

Supporting Information for

## Validation of the CoGEF Method as a Predictive Tool for Polymer Mechanochemistry

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## I. General Methods

CoGEF calculations were performed using Spartan '18 Parallel Suite according to previously reported methods.<sup>1</sup> Chemical structures were composed in ChemDraw, saved as .mol files, and then imported into Spartan. Structures were truncated to include tethers that accurately reflect the structure of the molecules used in the experimental studies. Ground state energies were calculated using DFT at the B3LYP/6-31G\* level of theory in vacuum, unless specified otherwise. For the three mechanophores in the heterolytic category, CoGEF calculations were also performed using a polarizable continuum model (dielectric constant of 37) to simulate a polar solvent. Starting from the equilibrium geometry of the unconstrained molecule (relative energy = 0 kJ/mol), the distance between the terminal anchor atoms of the truncated structure was increased in increments of 0.05 Å and the energy was minimized at each step. This operation was carried out automatically using the Energy Profile calculation in Spartan. Calculations were run until a chemical transformation was predicted to occur, as evidenced by the rupture and reorganization of one or more covalent bonds. In some cases, an initial equilibrium conformer calculation was performed using Molecular Mechanics (MMFF) before performing the steps outlined above. The maximum number of geometry optimization cycles was increased beyond the default value using the GEOMETRYCYCLE option to ensure convergence at each step in the CoGEF profile.

**Determination of  $F_{\max}$ .** The maximum force predicted for each mechanochemical transformation was calculated from the slope between contiguous points in the energy–displacement curve. In most cases,  $F_{\max}$  coincides with the displacement immediately prior to a discontinuity in the relative energy profile. The value of  $F_{\max}$  is thus calculated from the slope between the two data points preceding the abrupt attenuation in energy. More rarely, a continuous change in energy is observed that approaches an apparent plateau value at long displacements. In these cases,  $F_{\max}$  occurs at the inflection point in the CoGEF curve. The value of the slope is divided by the Avogadro constant and adjusted to provide force in units of nJ/m (nN).

**Determination of  $E_{\max}$ .** The maximum energy relative to the energy of the unconstrained molecule at equilibrium is reported as  $E_{\max}$ . The value of  $E_{\max}$  is determined from the CoGEF curve at the displacement corresponding to  $F_{\max}$ . Typically, this means that  $E_{\max}$  represents the highest relative energy on the CoGEF curve; however, for instances in which the CoGEF profile exhibits a sigmoidal shape and/or a discontinuity is absent,  $E_{\max}$  corresponds to the relative energy at the inflection point.

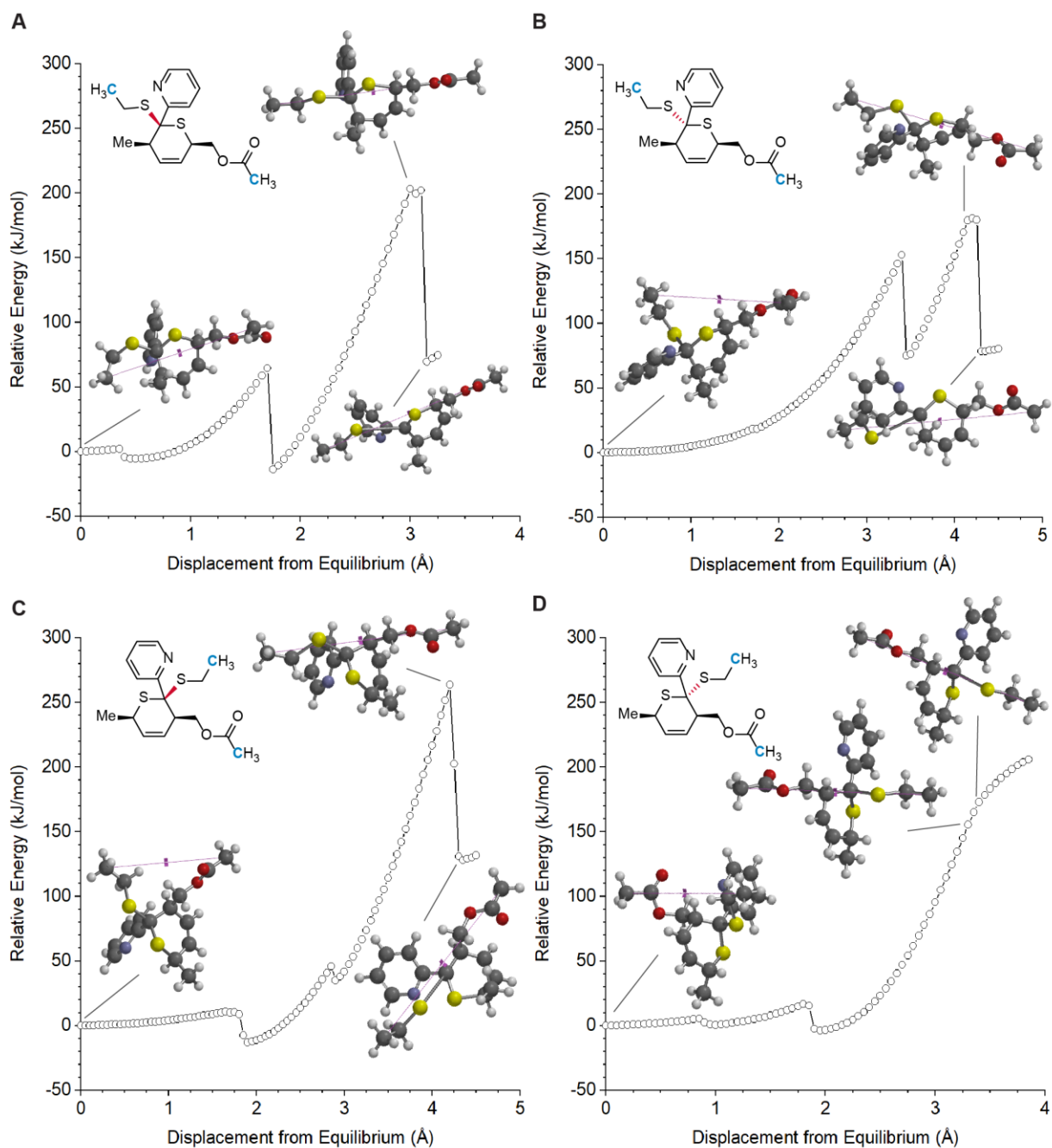
**Determination of Force–Bond Angle.** Force–bond angles were calculated according to the previously described method using structural models from CoGEF calculations at the displacement corresponding to  $F_{\max}$ .<sup>2</sup> The external force vector was approximated using the coordinates of the two terminal atoms that define the distance constraint in the CoGEF calculation.

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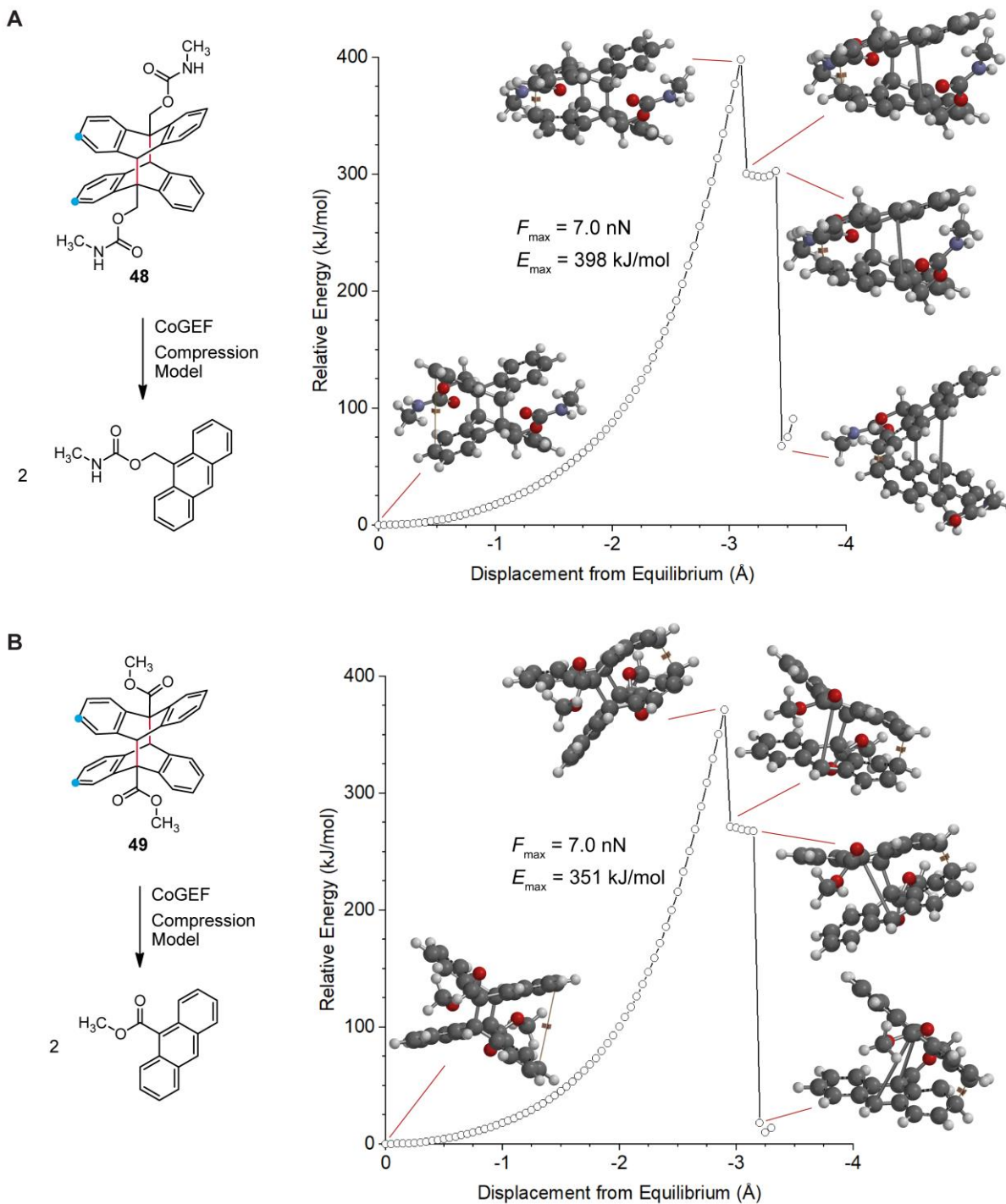
(1) (a) Beyer, M. K. The Mechanical Strength of a Covalent Bond Calculated by Density Functional Theory. *J. Chem. Phys.* **2000**, *112*, 7307–7312. (b) Kryger, M. J.; Munaretto, A. M.; Moore, J. S. Structure-Mechanochemical Activity Relationships for Cyclobutane Mechanophores. *J. Am. Chem. Soc.* **2011**, *133*, 18992–18998.

(2) Robb, M. J.; Kim, T. A.; Halmes, A. J.; White, S. R.; Sottos, N. R.; Moore, J. S. Regioisomer-Specific Mechanochromism of Naphthopyran in Polymeric Materials. *J. Am. Chem. Soc.* **2016**, *138*, 12328–12331.

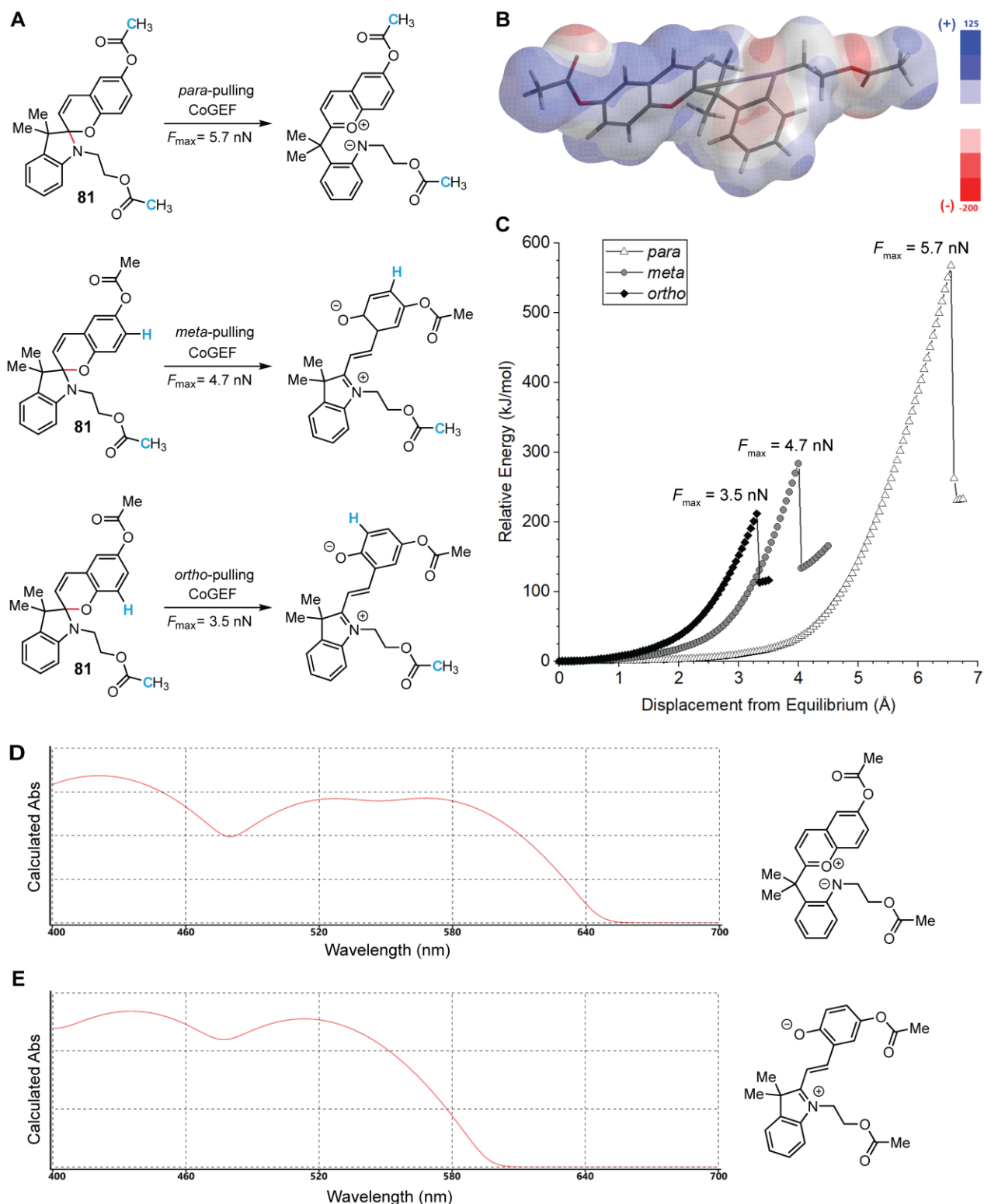
## II. Supplementary Figures



**Figure S1.** CoGEF results for four possible isomers of a hetero-Diels-Alder adduct corresponding to the reactive subunits of reported mechanophore **36**. All isomers are predicted to undergo C-S bond scission rather than the formal retro-[4+2] cycloaddition reaction.

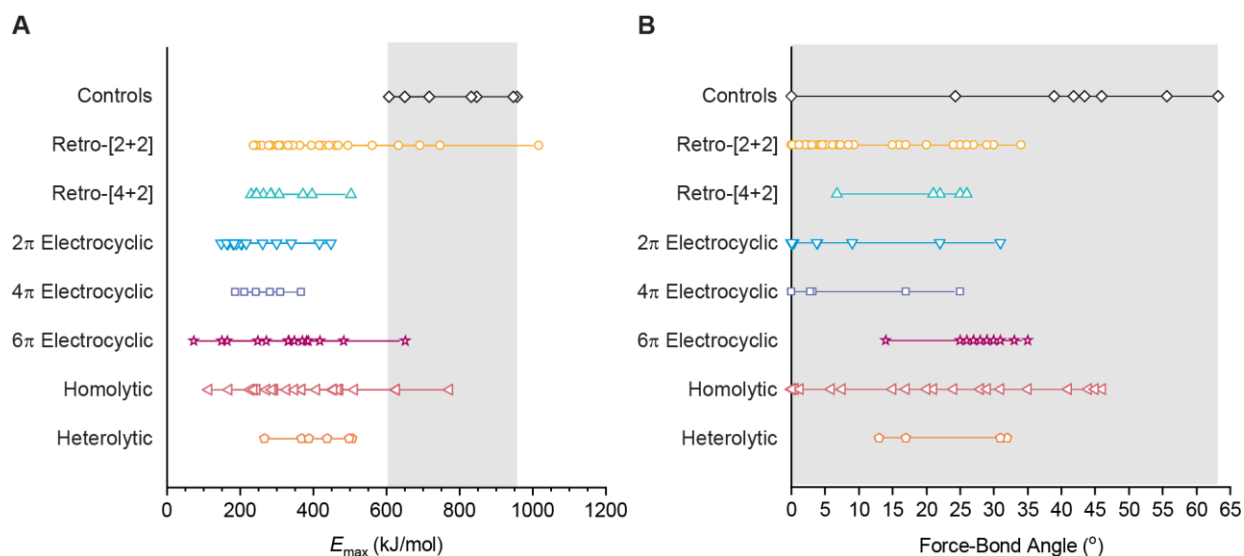


**Figure S2.** CoGEF calculations performed in an alternative compression mode for head-to-tail anthracene dimer mechanophores (A) **48** and (B) **49**. The distance between carbon atoms labeled with a blue dot was decreased incrementally starting from the force-free equilibrium geometry. At each step, the geometry was optimized at the B3LYP/6-31G\* level of DFT. Both molecules are predicted to undergo a formal retro-[4+4] cycloaddition reaction upon simulated compression. The transformation proceeds through an apparent stepwise pathway suggesting an intermediate with diradicaloid character.

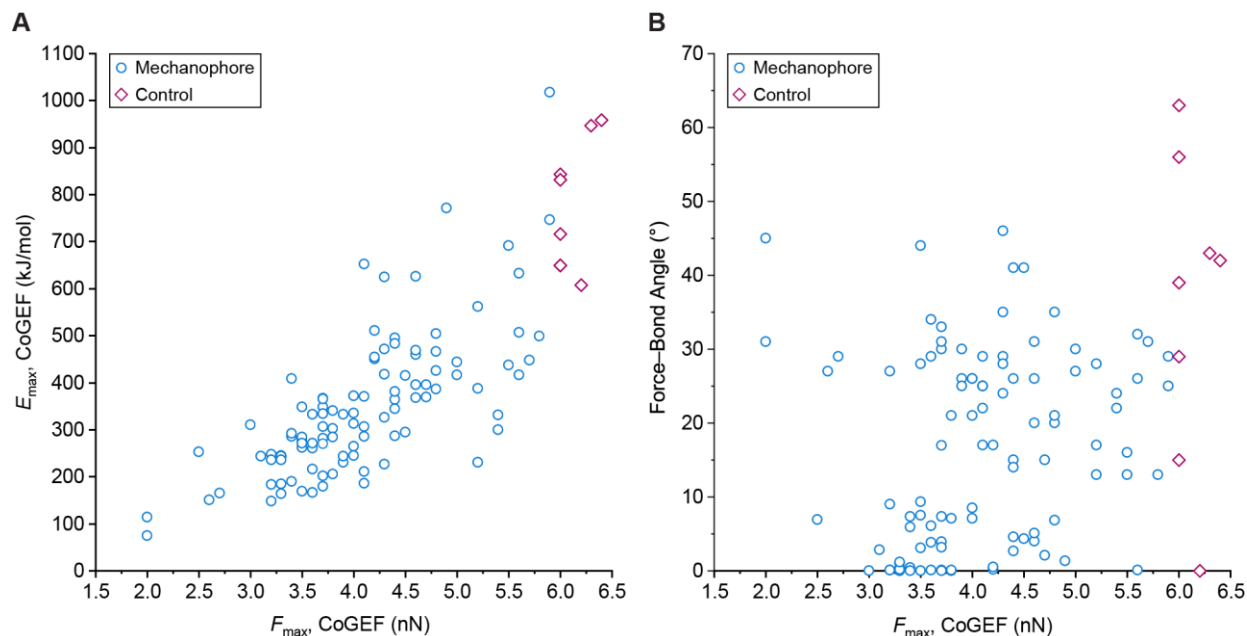


**Figure S3.** Investigation of regiochemical effects on the predicted mechanochemical reactivity of spiropyran **81**. (A) Changing the pulling position results in the anticipated scission of the C–O pyran bond leading to formation of the merocyanine. (B) Electrostatic potential map of the product predicted by CoGEF (*para*-pulling) indicating heterolytic fragmentation of the C–N bond. (C) CoGEF profiles associated with the schemes in panel A. (D, E) Visible absorption spectra calculated at the B3LYP/6-31G\* level of TD-DFT for the product resulting from C–N bond scission, and the expected merocyanine species.

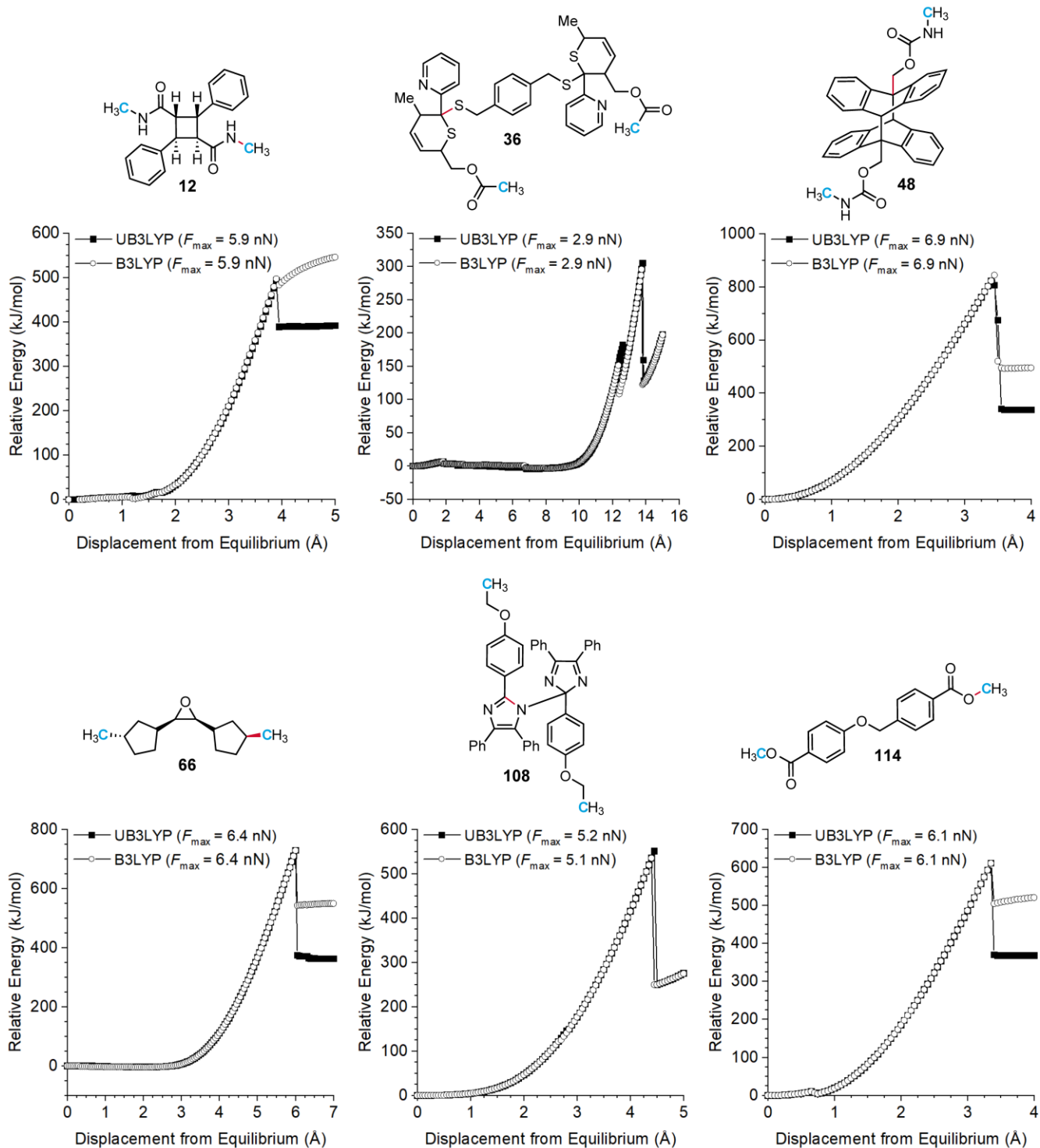




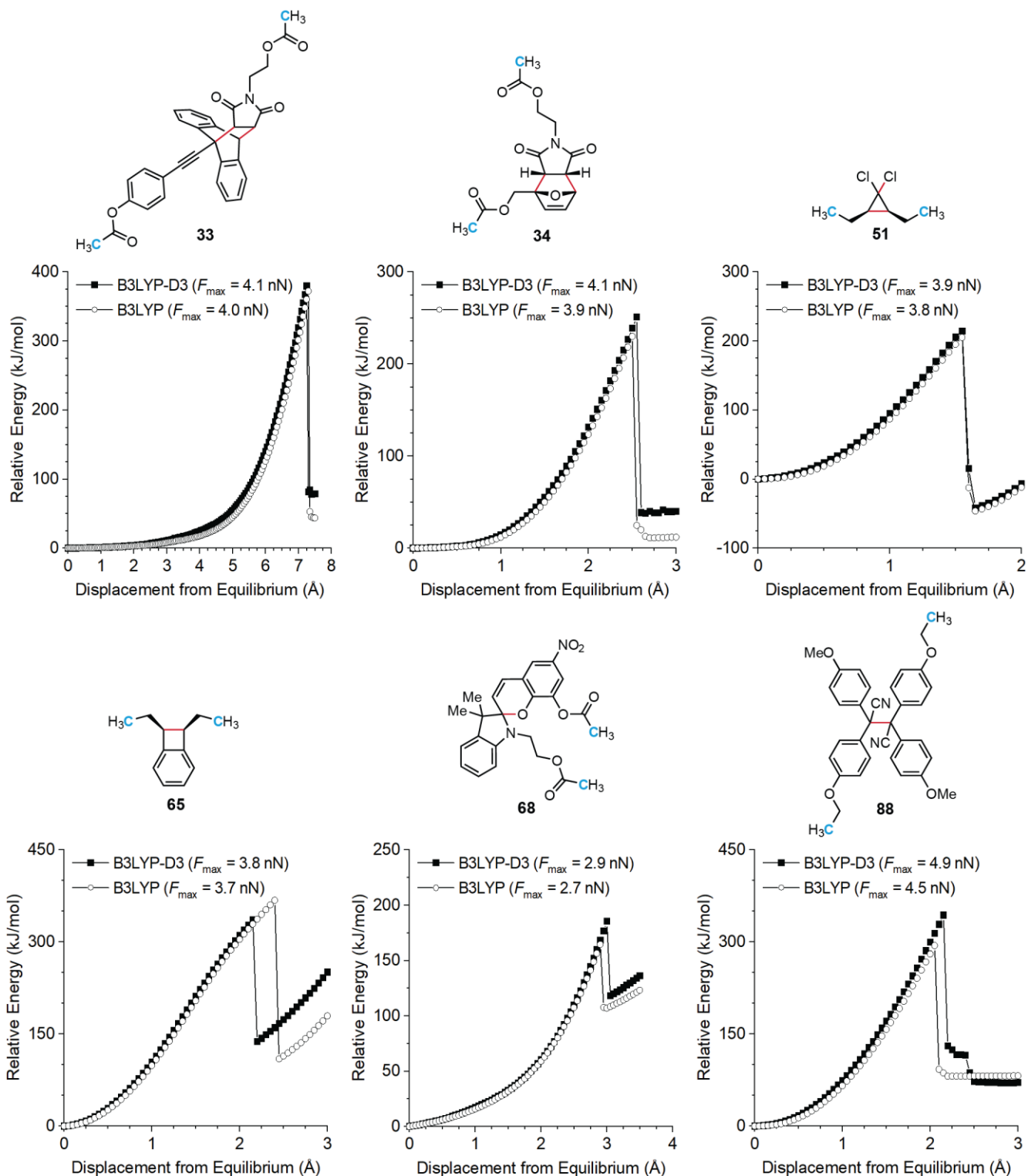
**Figure S4.** Summary of (A)  $E_{\max}$  values and (B) force–bond angles determined using the CoGEF method for each mechanochemical reaction class. The CoGEF results for control structures are universally indistinguishable from the mechanophores when alternative quantitative metrics  $E_{\max}$  and force–bond angle are compared, indicating that these metrics are poor predictors of mechanochemical activity. Data from calculations that are inconsistent with reported experimentally determined reactivity are excluded.



**Figure S5.** Relationship between calculated values of (A)  $E_{\max}$  and (B) force–bond angle with the calculated values of  $F_{\max}$  determined with the CoGEF method at the B3LYP/6-31G\* level of density functional theory. There is a positive correlation between values of  $E_{\max}$  and  $F_{\max}$ , while there is no apparent correlation between force–bond angle and values of  $F_{\max}$ .



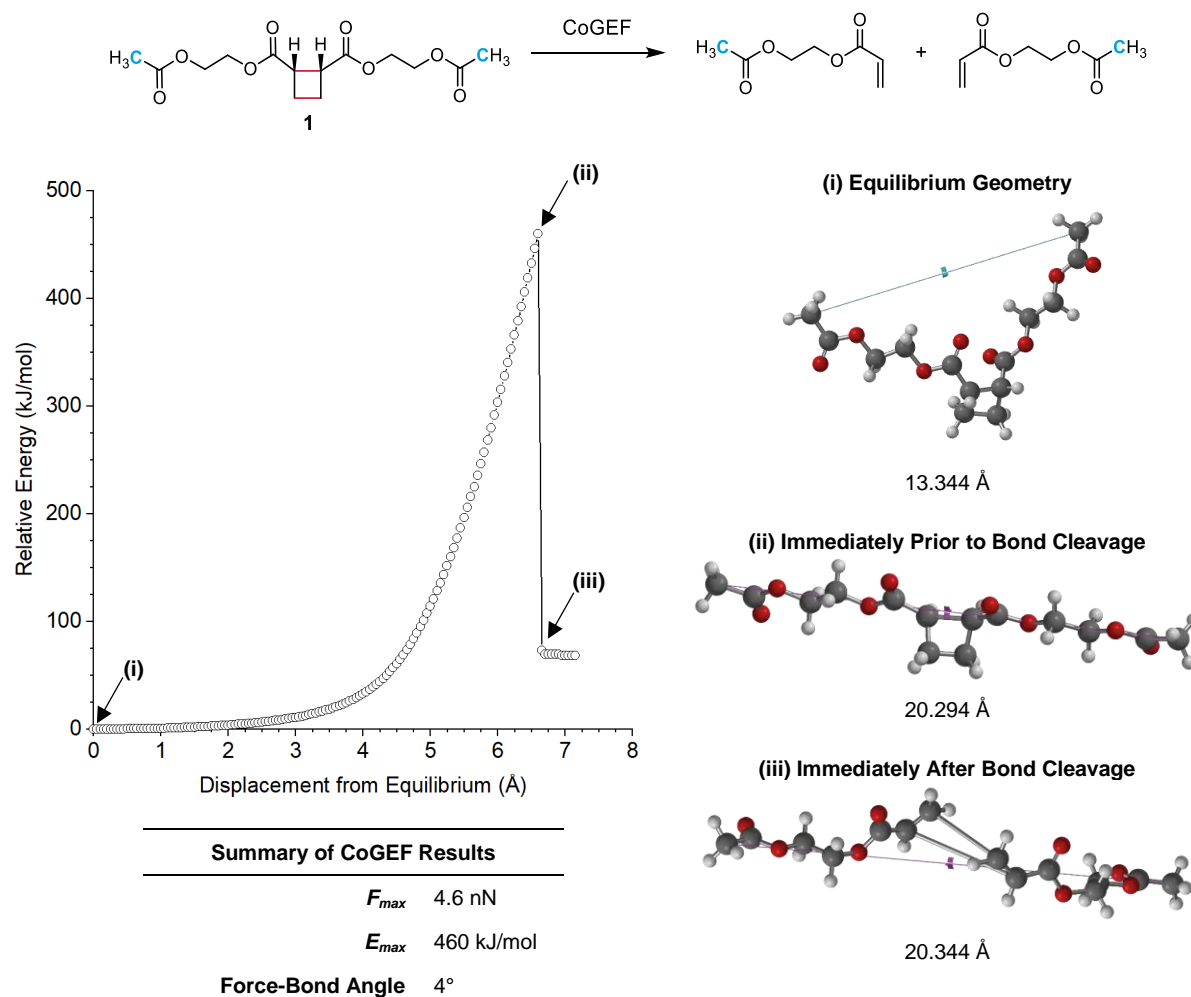
**Figure S6.** CoGEF calculations performed using unrestricted DFT (UB3LYP/6-31G\*) on representative mechanophores for which CoGEF calculations at the B3LYP/6-31G\* level of DFT predict reactions that are inconsistent with the reported experimental behavior. Use of the UB3LYP functional has minimal influence on the results of the CoGEF simulations. The same chemical transformations are predicted in each case.

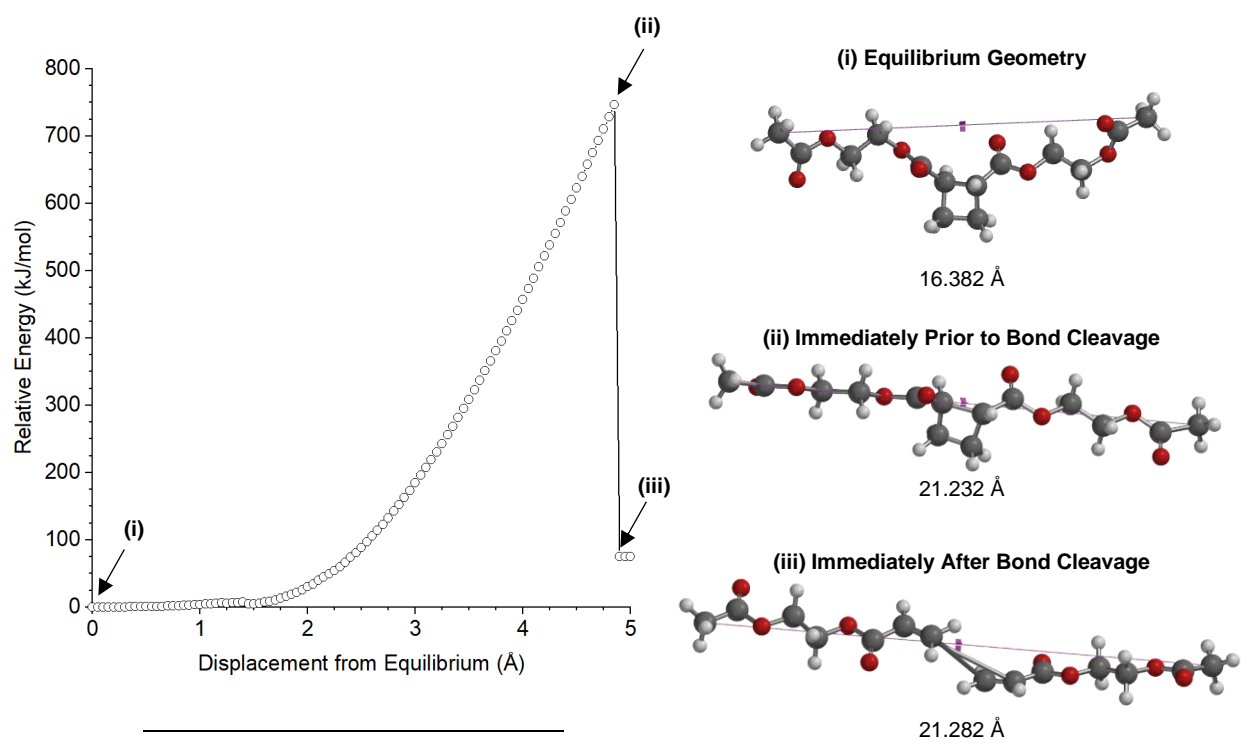


**Figure S7.** Comparison of CoGEF calculations performed on representative mechanophores at the B3LYP/6-31G\* level of DFT and using a dispersion-corrected functional (B3LYP-D3/6-31G\*). Use of the dispersion-corrected B3LYP-D3 functional has minimal influence on the results of the CoGEF simulations. The same chemical transformations are predicted in each case.

### III. Summaries of Individual CoGEF Calculations

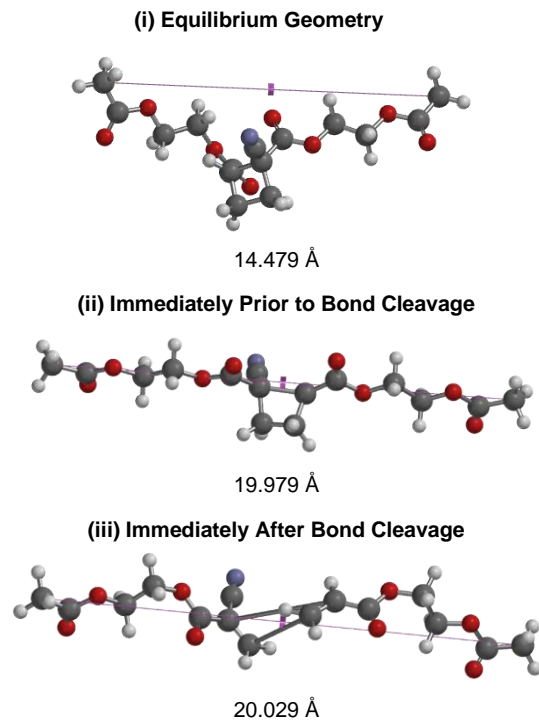
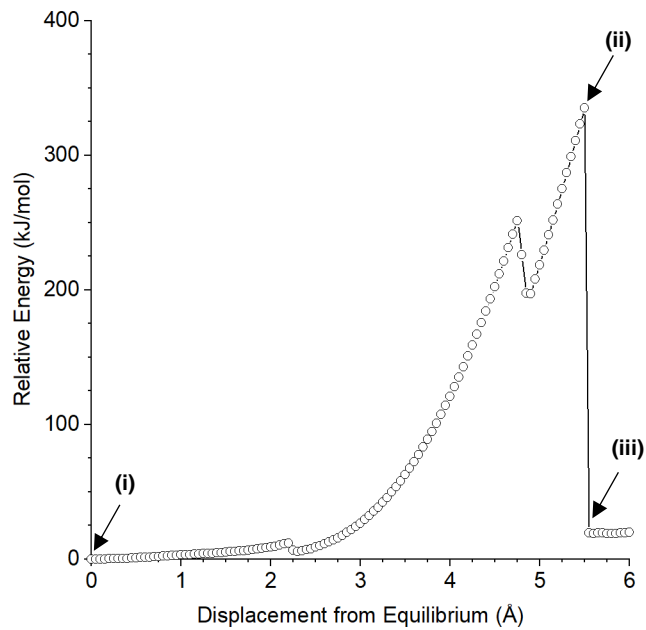
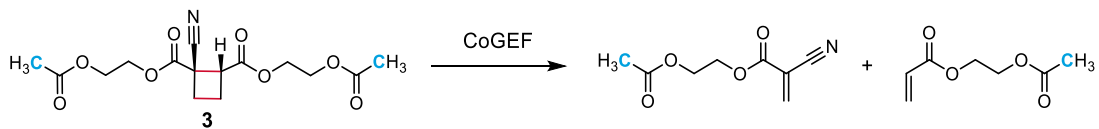
A summary of the results of each individual CoGEF calculation are presented on the pages below. All calculations were performed using DFT at the B3LYP/6-31G\* level of theory in vacuum, unless specified otherwise. A reaction scheme depicts the structure of the truncated molecule and the product(s) predicted from the CoGEF calculation. The atoms colored blue indicate the anchor positions (i.e., pulling points) for defining the distance constraint and the bonds that are predicted to cleave are colored red. Representative images of computed structures at critical points in the CoGEF profile are included that depict the force-free equilibrium geometry as well as the structure(s) immediately before and after bond cleavage events. The length of the distance constraint is included below each computed structure and the corresponding positions on the CoGEF curve are denoted. Electrostatic potential maps are included for the products predicted by CoGEF calculations in the heterolytic category. The calculated values of  $F_{max}$ ,  $E_{max}$ , and force-bond angle are tabulated for each calculation. Note that the former bonds persist as artifacts in Spartan after a reaction is predicted to occur. For references to the primary literature describing the experimental reactivity of each compound, refer to the tables in the main text.





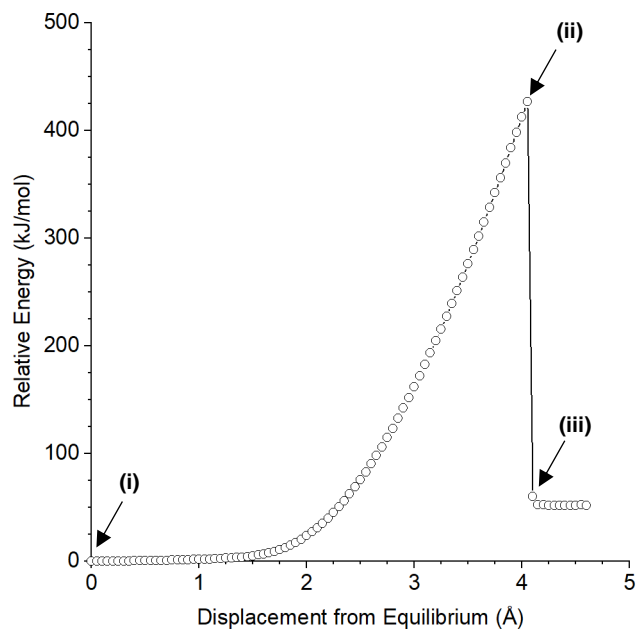
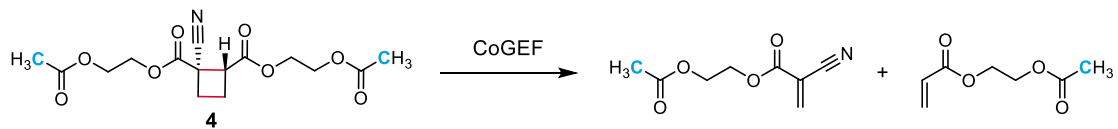
**Summary of CoGEF Results**

$F_{max}$	5.9 nN
$E_{max}$	746 kJ/mol
<b>Force-Bond Angle</b>	25°

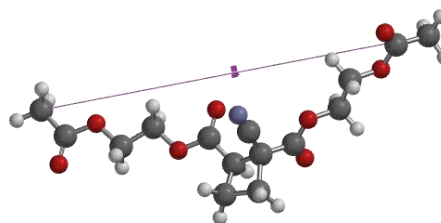


**Summary of CoGEF Results**

$F_{max}$	4.0 nN
$E_{max}$	335 kJ/mol
<b>Force-Bond Angle</b>	7.1°

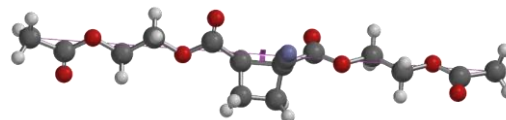


(i) Equilibrium Geometry



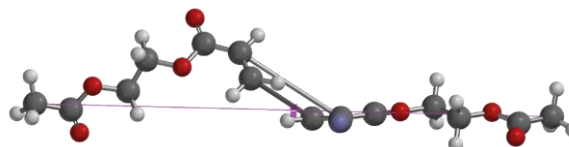
16.271 Å

(ii) Immediately Prior to Bond Cleavage



20.321 Å

(iii) Immediately After Bond Cleavage

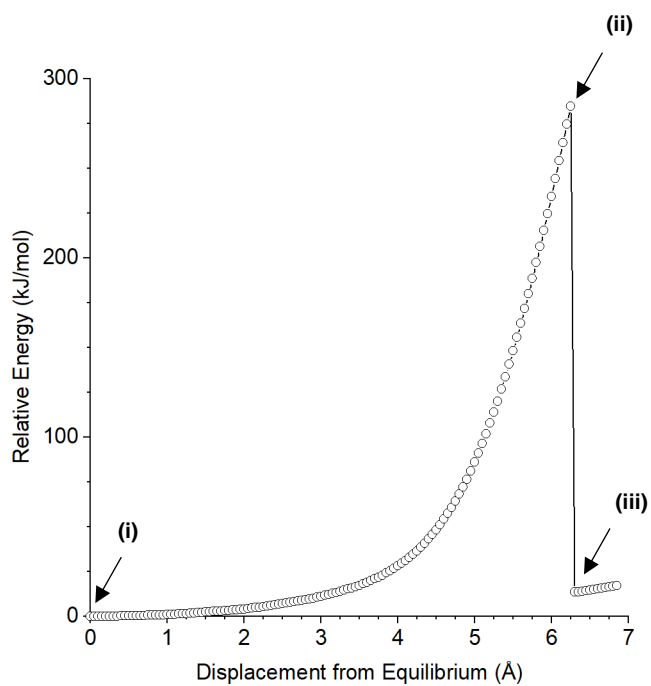
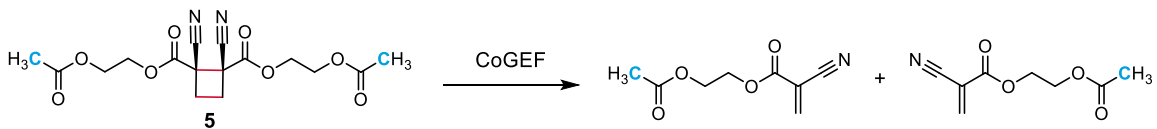


20.371 Å

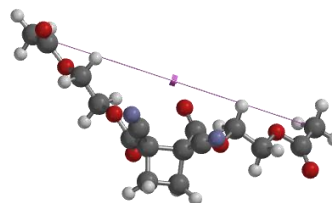
**Summary of CoGEF Results**

$F_{max}$  4.8 nN  
 $E_{max}$  426 kJ/mol

Force-Bond Angle 20°

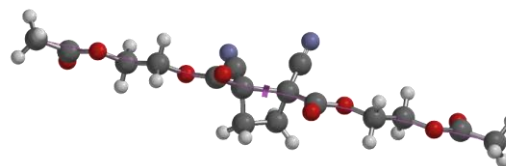


(i) Equilibrium Geometry



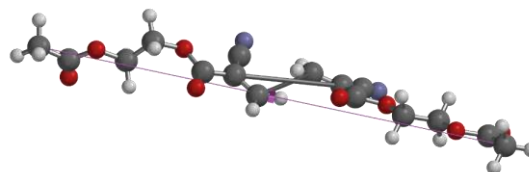
13.303 Å

(ii) Immediately Prior to Bond Cleavage



19.553 Å

(iii) Immediately After Bond Cleavage

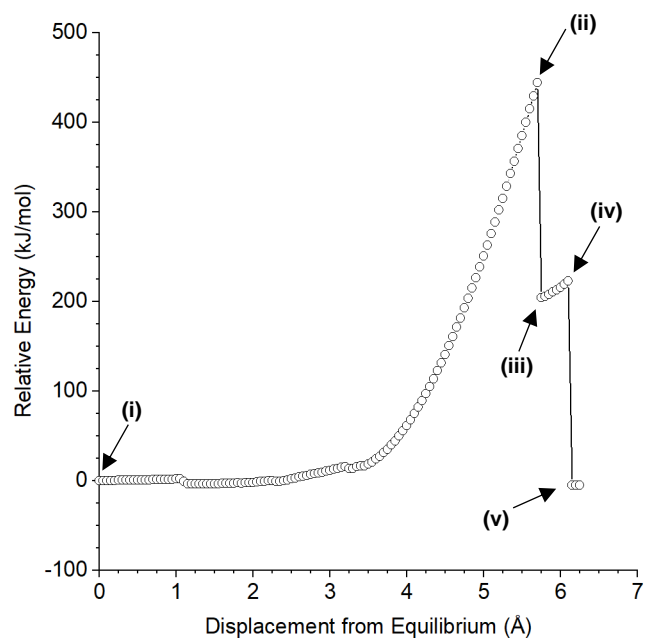
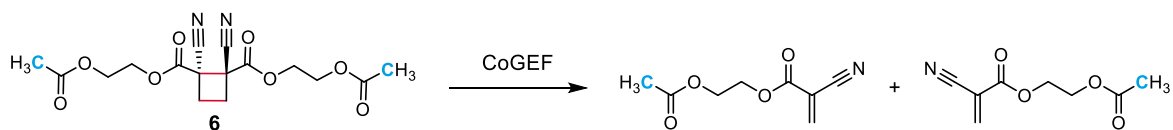


19.603 Å

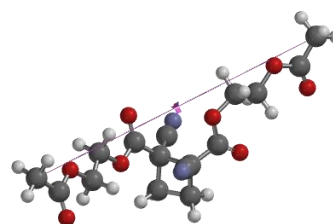
**Summary of CoGEF Results**

$F_{max}$	3.4 nN
$E_{max}$	285 kJ/mol
Force-Bond angle	7.3°





(i) Equilibrium Geometry



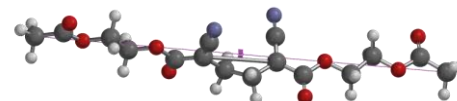
14.667 Å

(ii) Immediately Prior to First Bond Cleavage



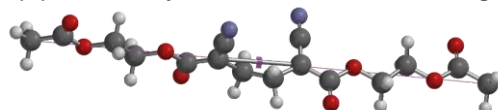
20.417 Å

(iii) Immediately After First Bond Cleavage



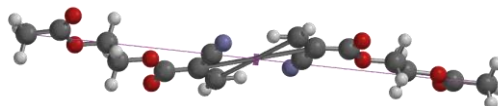
20.467 Å

(iv) Immediately Prior to Second Bond Cleavage



20.817 Å

(iv) Immediately After Second Bond Cleavage



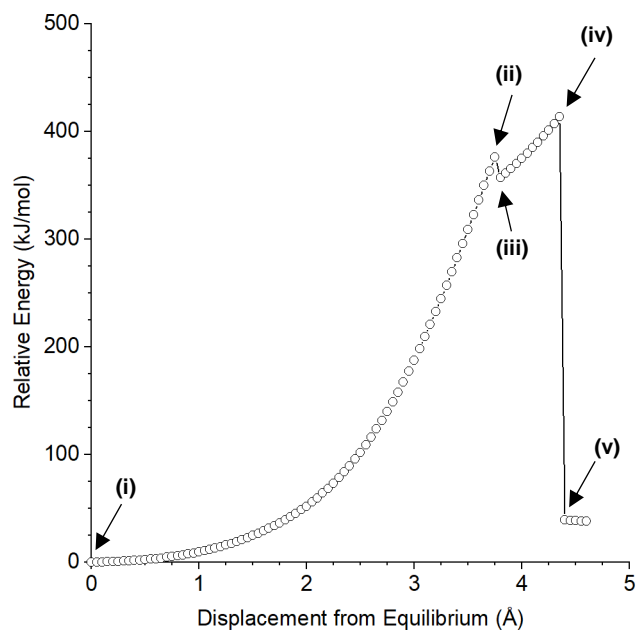
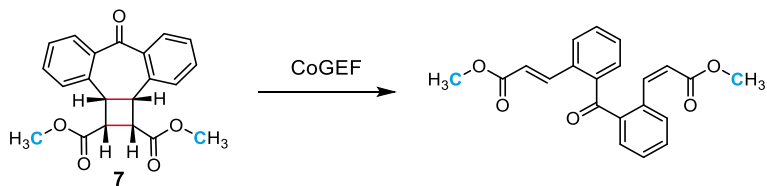
20.867 Å

**Summary of CoGEF Results**

$F_{max}$  5.0 nN

$E_{max}$  444 kJ/mol

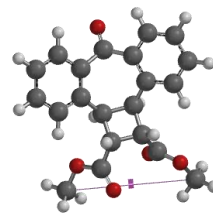
Force-Bond Angle 27°



**Summary of CoGEF Results**

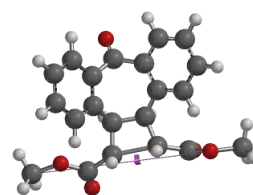
$F_{max}$	4.5 nN
$E_{max}$	413 kJ/mol
Force-Bond Angle	4.3°

**(i) Equilibrium Geometry**



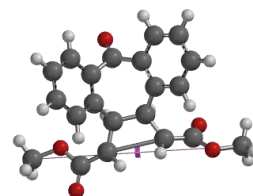
6.295 Å

**(ii) Immediately Prior to First Bond Cleavage**



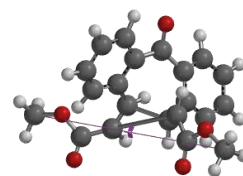
10.045 Å

**(iii) Immediately After First Bond Cleavage**



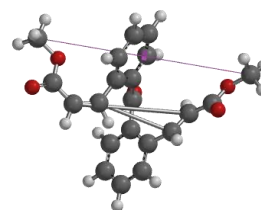
10.095 Å

**(iv) Immediately Before Second Bond Cleavage**

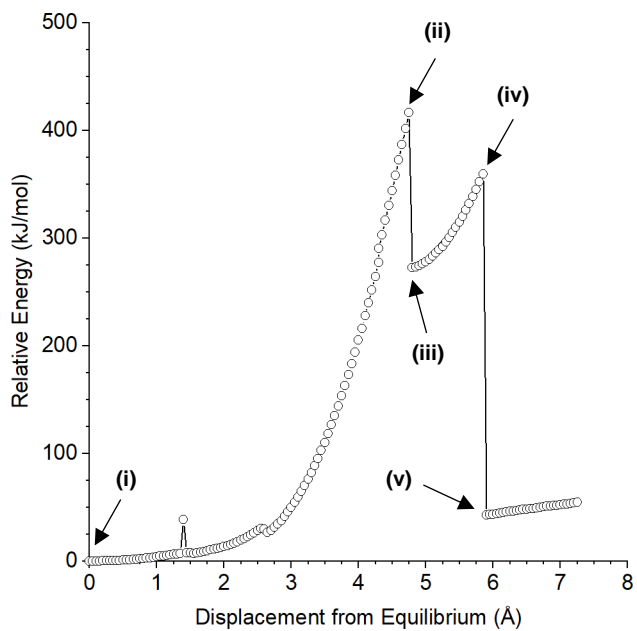
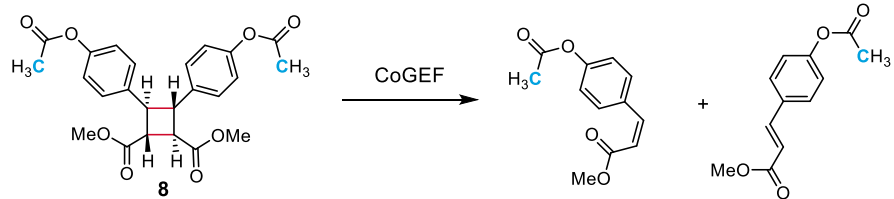


10.645 Å

**(v) Immediately After Second Bond Cleavage**



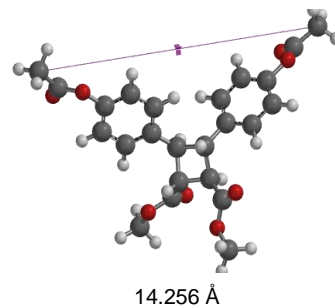
10.695 Å



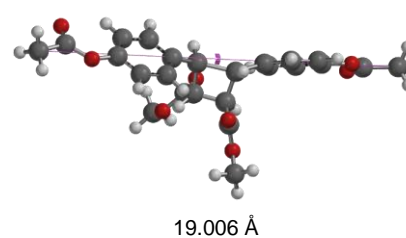
**Summary of CoGEF Results**

$F_{max}$	5.0 nN
$E_{max}$	417 kJ/mol
Force-Bond Angle	30°

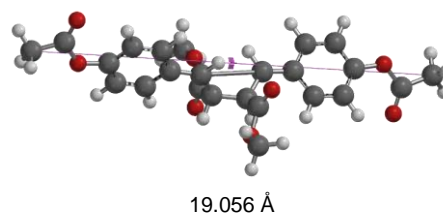
**(i) Equilibrium Geometry**



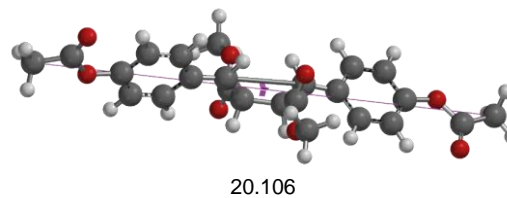
**(ii) Immediately Prior to First Bond Cleavage**



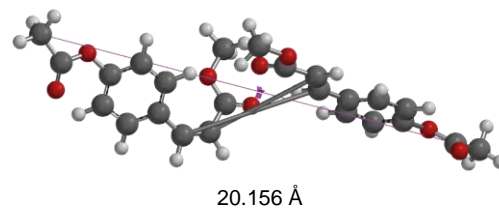
**(iii) Immediately After First Bond Cleavage**

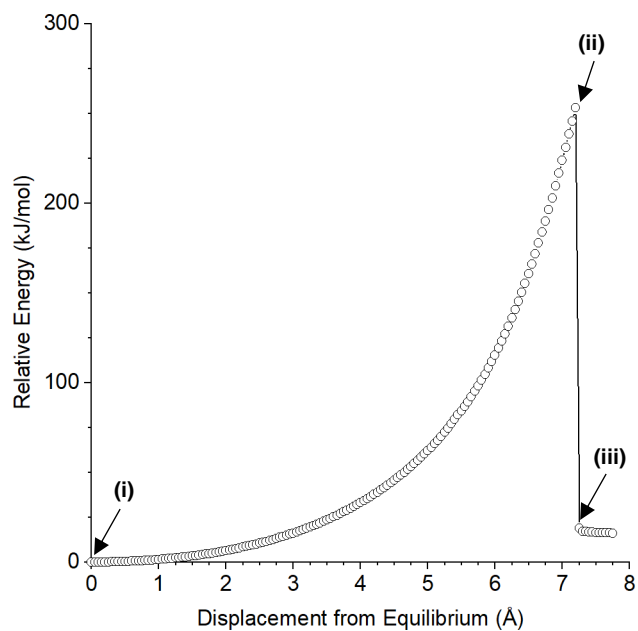
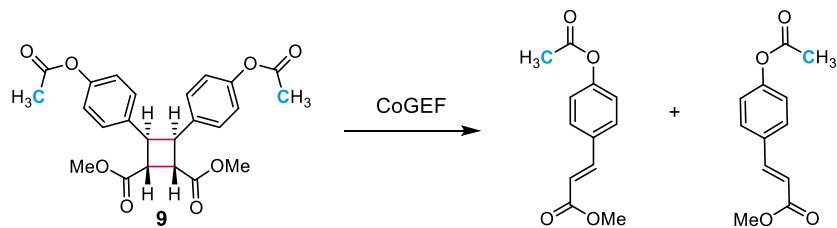


**(iv) Immediately Prior to Second Bond Cleavage**

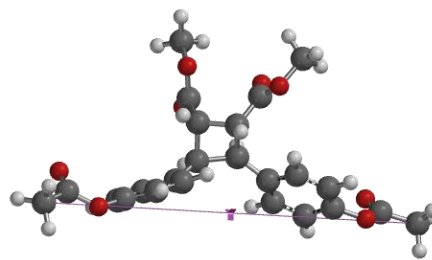


**(v) Immediately After Second Bond Cleavage**



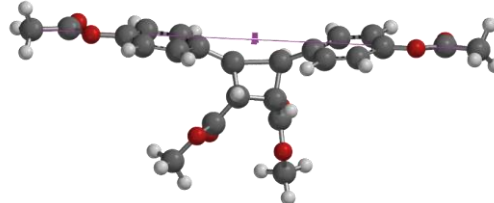


(i) Equilibrium Geometry



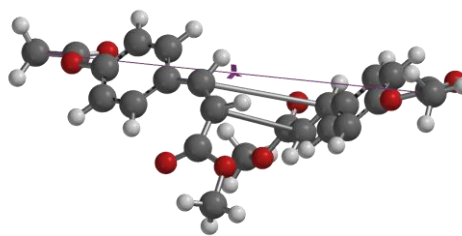
10.962 Å

(ii) Immediately Prior to First Bond Cleavage



18.162 Å

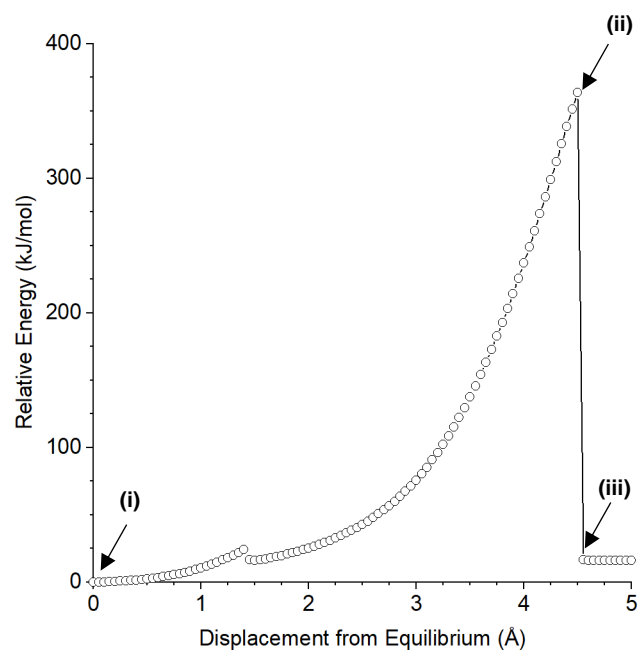
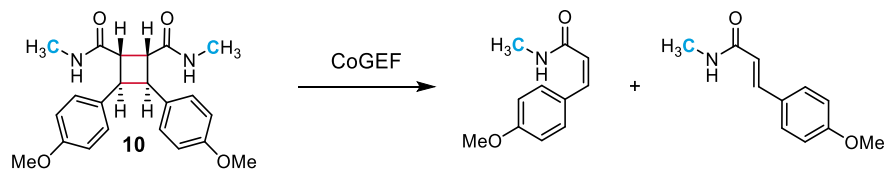
(iii) Immediately After First Bond Cleavage



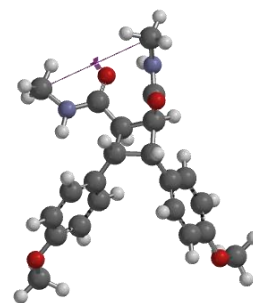
18.212 Å

**Summary of CoGEF Results**

$F_{max}$	2.5 nN
$E_{max}$	253 kJ/mol
<b>Force-Bond Angle</b>	6.9°

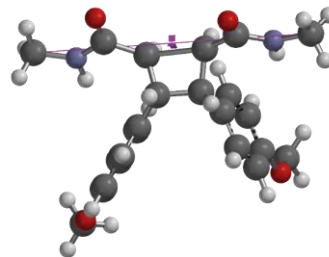


(i) Equilibrium Geometry



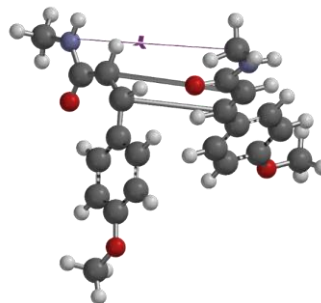
5.759 Å

(ii) Immediately Prior to First Bond Cleavage



10.259 Å

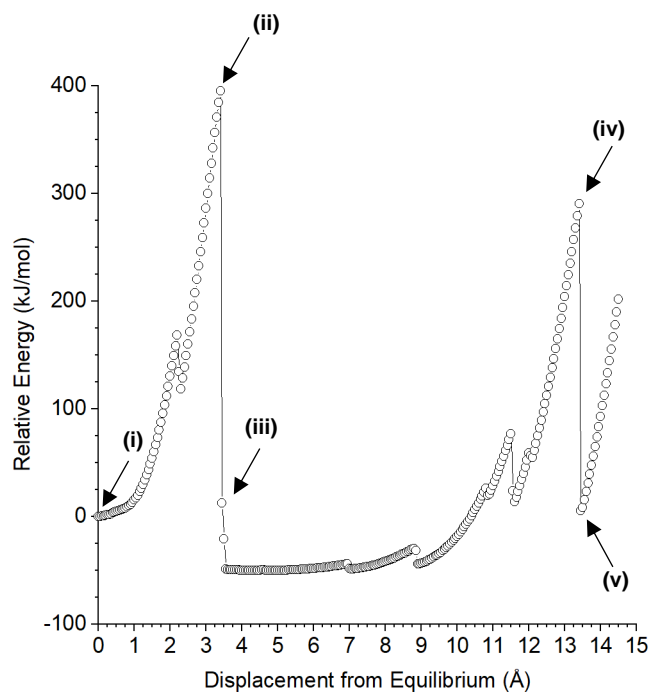
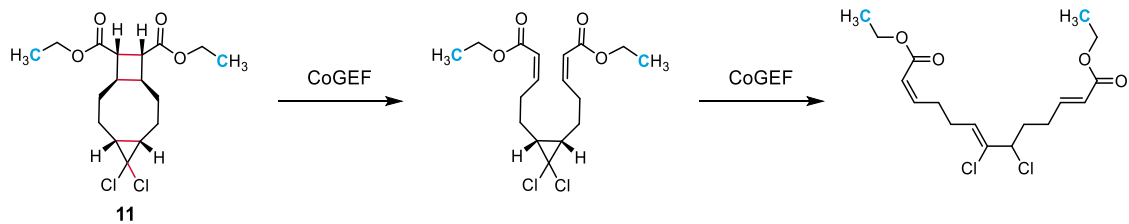
(iii) Immediately After First Bond Cleavage



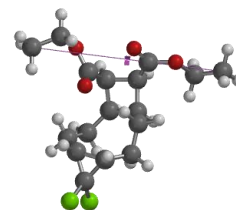
10.309 Å

**Summary of CoGEF Results**

$F_{max}$	4.4 nN
$E_{max}$	364 kJ/mol
<b>Force-Bond Angle</b>	2.7°

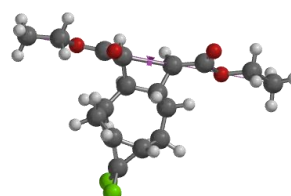


(i) Equilibrium Geometry



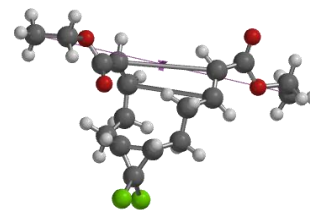
9.485 Å

(ii) Immediately Prior to First Bond Cleavage



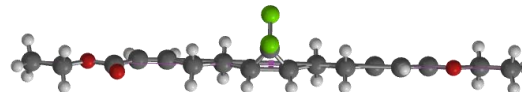
12.885 Å

(iii) Immediately After First Bond Cleavage



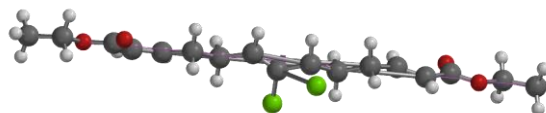
12.935 Å

(iv) Immediately Before Second Bond Cleavage



22.885 Å

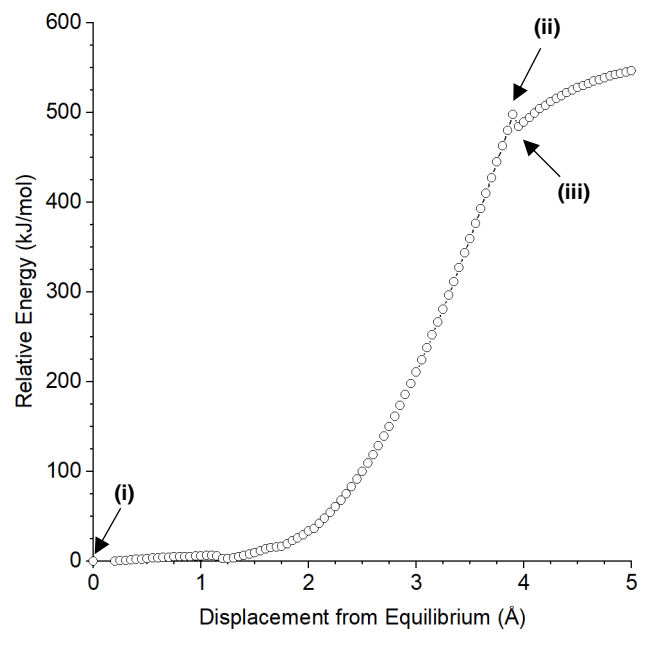
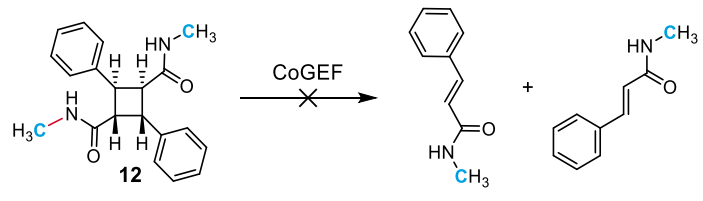
(v) Immediately After Second Bond Cleavage



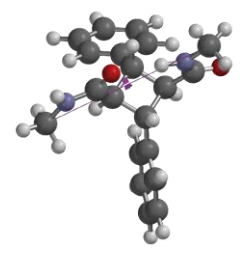
22.935 Å

Summary of CoGEF Results

	cyclobutane	gDCC
$F_{max}$	4.7 nN	3.8 nN
$E_{max}$	395 kJ/mol	291 kJ/mol
Force-Bond Angle	2.1°	0.4°

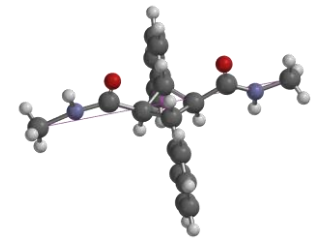


(i) Equilibrium Geometry



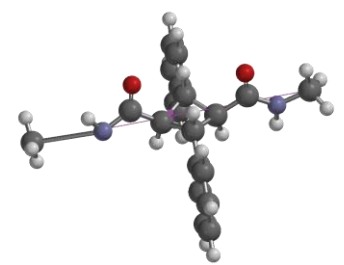
7.497 Å

(ii) Immediately Prior to Bond Cleavage



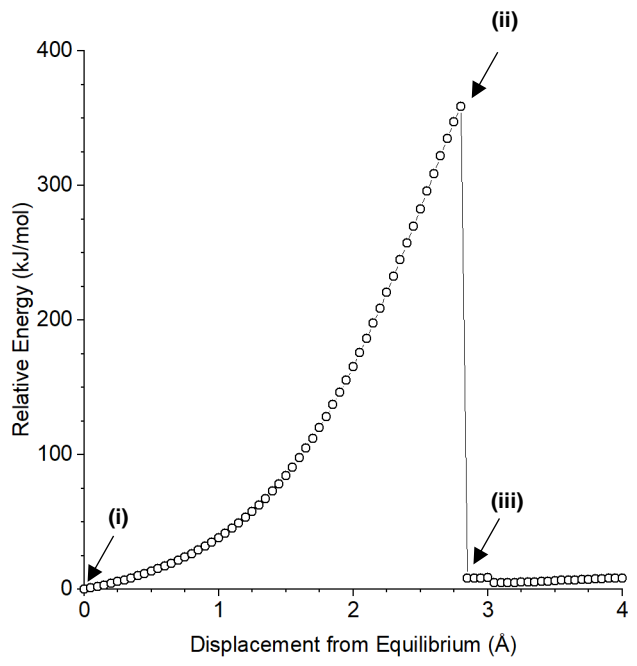
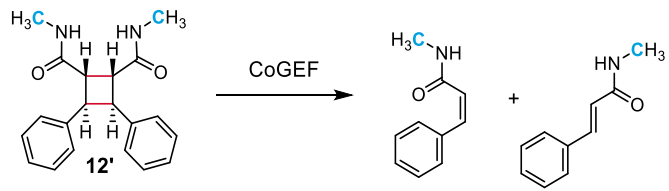
11.397 Å

(iii) Immediately After Bond Cleavage

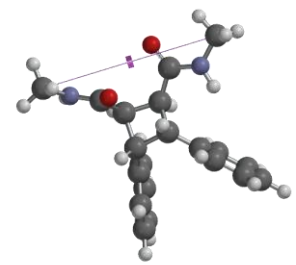


11.5447 Å

Summary of CoGEF Results	
$F_{max}$	5.9 nN
$E_{max}$	498 kJ/mol
Force-Bond Angle	44°

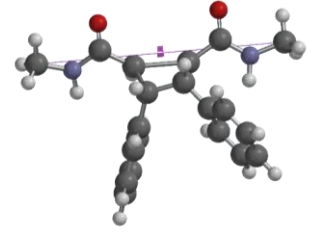


(i) Equilibrium Geometry



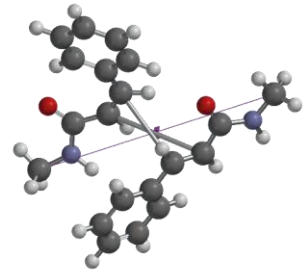
7.519 Å

(ii) Immediately Prior to Bond Cleavage



10.319 Å

(iii) Immediately After Bond Cleavage

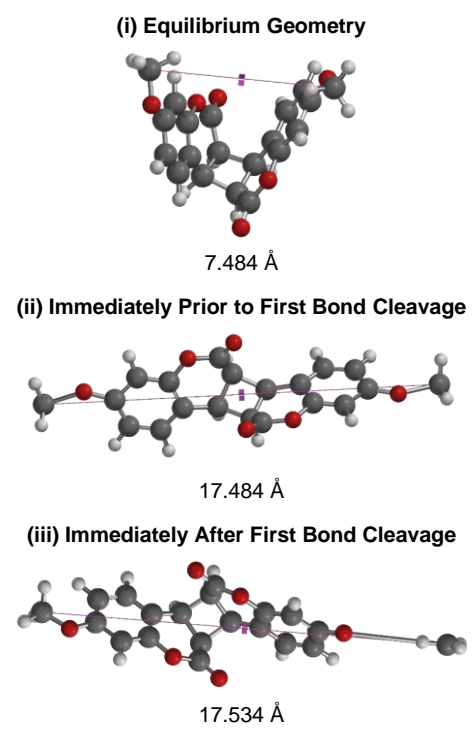
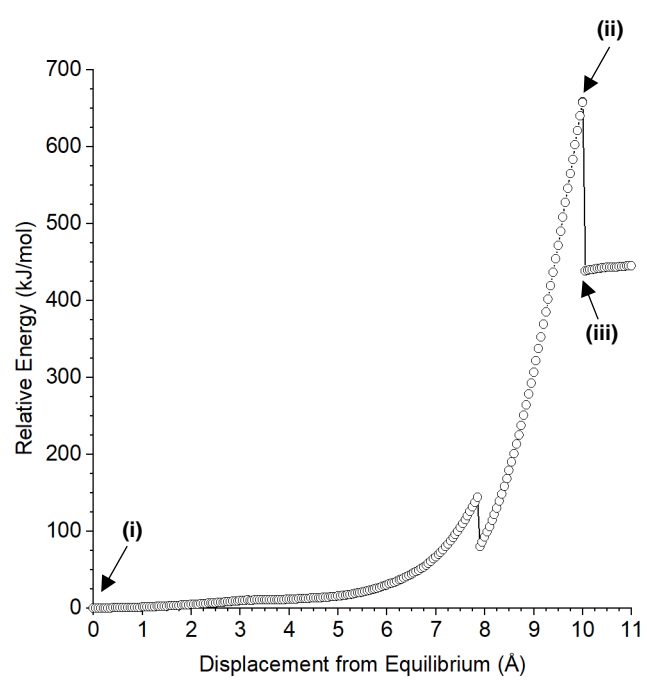
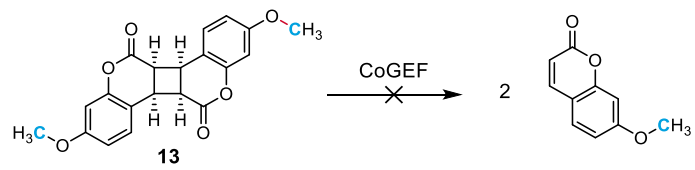


10.369 Å

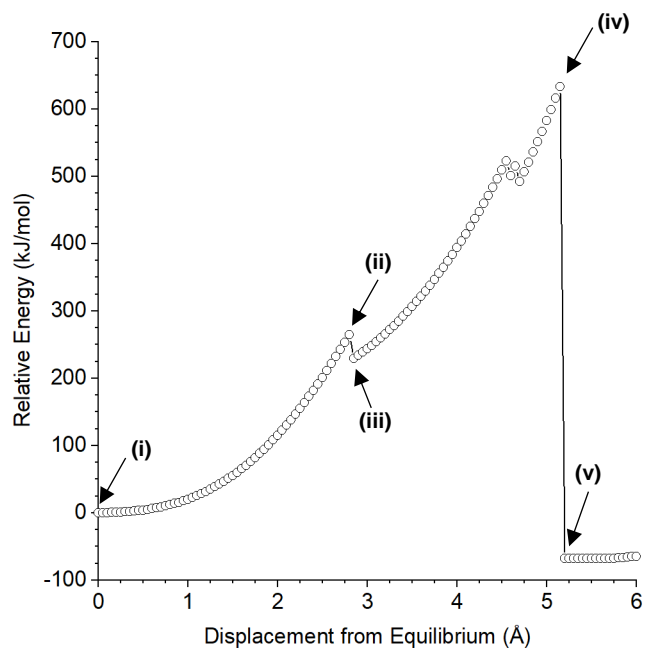
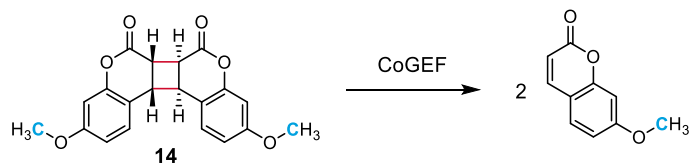
**Summary of CoGEF Results**

$F_{max}$	4.4 nN
$E_{max}$	359 kJ/mol
<b>Force-Bond Angle</b>	2.2°





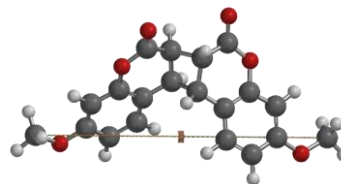
Summary of CoGEF Results	
$F_{max}$	6.3 nN
$E_{max}$	658 kJ/mol
Force-Bond Angle	28°



**Summary of CoGEF Results**

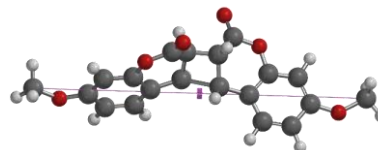
$F_{max}$	5.6 nN
$E_{max}$	633 kJ/mol
<b>Force-Bond Angle</b>	26°

**(i) Equilibrium Geometry**



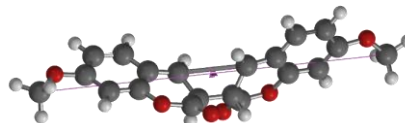
13.066 Å

**(ii) Immediately Prior to First Bond Cleavage**



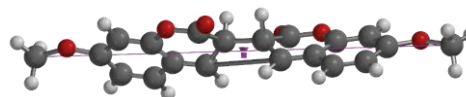
15.866 Å

**(iii) Immediately After First Bond Cleavage**



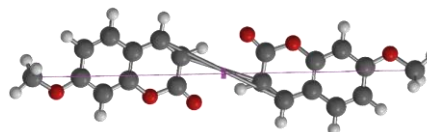
15.916 Å

**(iv) Immediately Before Second Bond Cleavage**

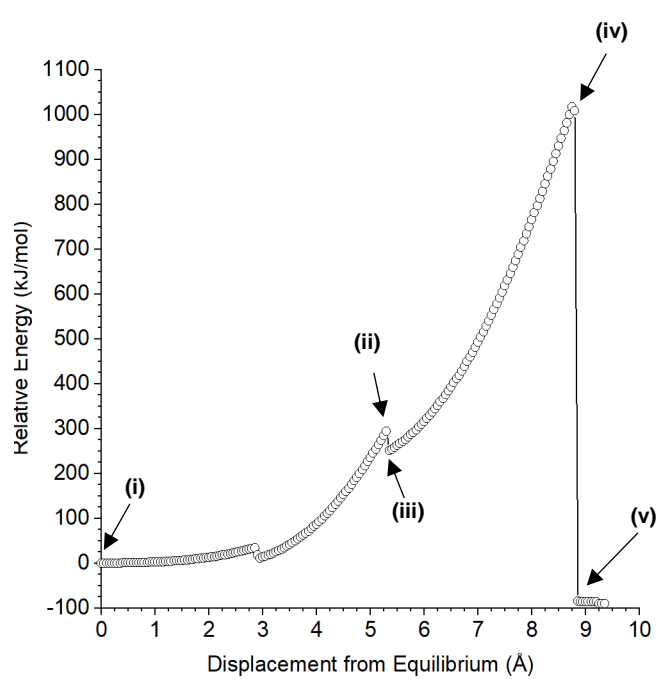
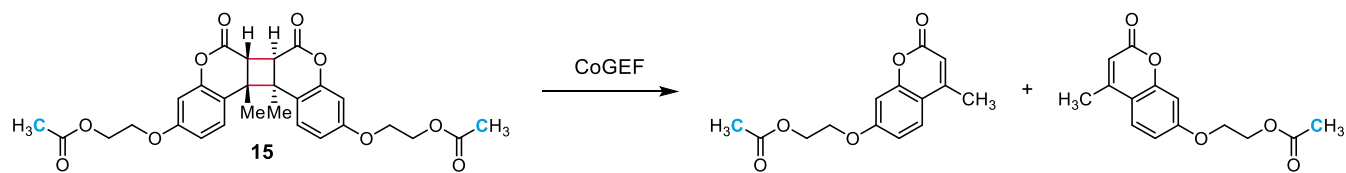


18.216 Å

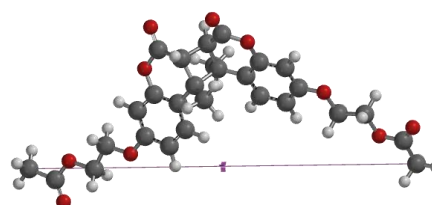
**(v) Immediately After Second Bond Cleavage**



18.266 Å

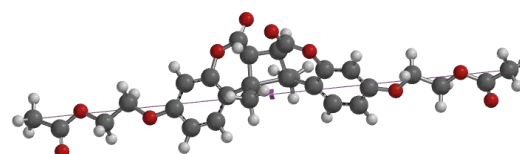


(i) Equilibrium Geometry



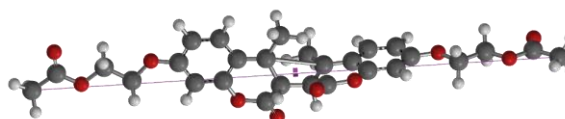
20.607 Å

(ii) Immediately Prior to First Bond Cleavage



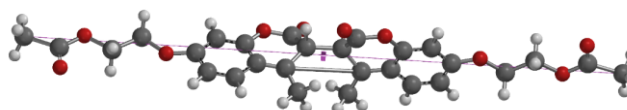
25.907 Å

(iii) Immediately After First Bond Cleavage



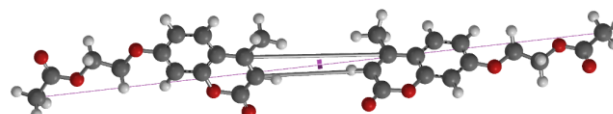
25.957 Å

(iv) Immediately Before Second Bond Cleavage



29.407 Å

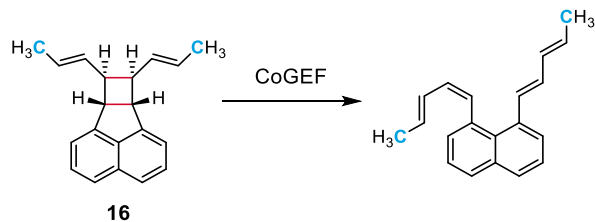
(v) Immediately After Second Bond Cleavage



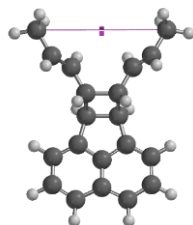
29.457 Å

**Summary of CoGEF Results**

$F_{max}$	5.9 nN
$E_{max}$	1017 kJ/mol
Force-Bond Angle	29°

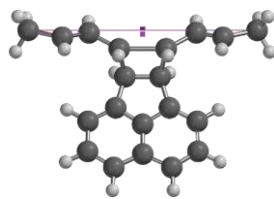


**(i) Equilibrium Geometry**



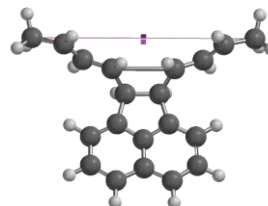
6.366 Å

**(ii) Immediately Prior to First Bond Cleavage**



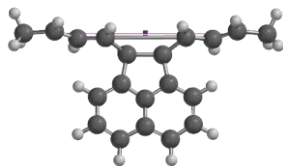
10.066 Å

**(iii) Immediately After First Bond Cleavage**



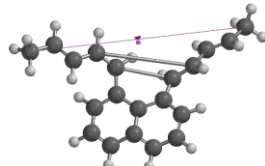
10.116 Å

**(v) Immediately Prior to Second Bond Cleavage**

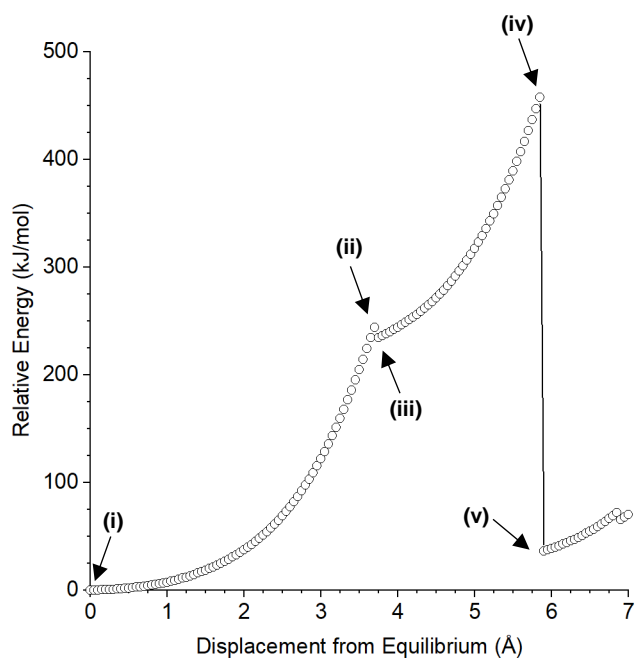


12.216 Å

**(vi) Immediately After Second Bond Cleavage**

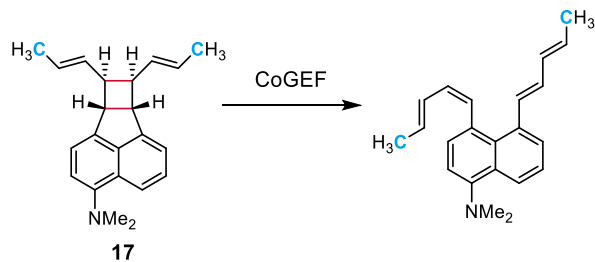


12.266 Å

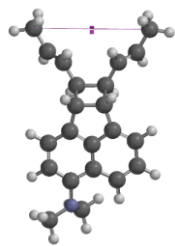


**Summary of CoGEF Results**

$F_{max}$	3.3 nN
$E_{max}$	244 kJ/mol
<b>Force-Bond Angle</b>	0.0°

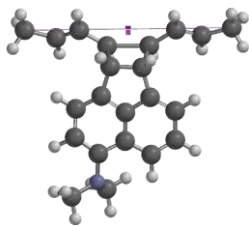


(i) Equilibrium Geometry



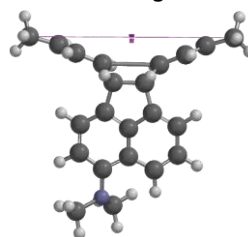
6.351 Å

(ii) Immediately Prior to First Bond Cleavage



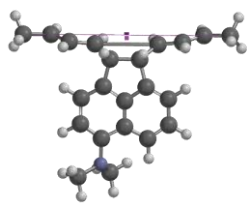
10.051 Å

(iii) Immediately After First Bond Cleavage



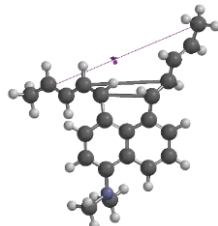
10.101 Å

(v) Immediately Prior to Second Bond Cleavage

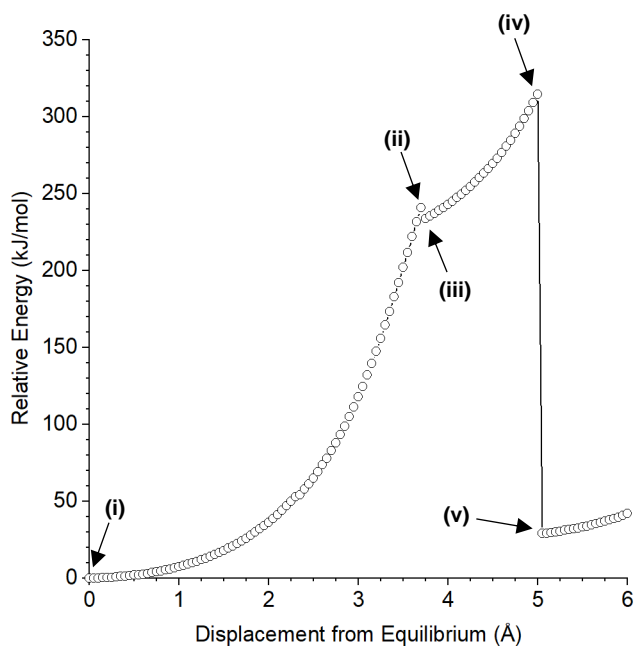


11.351 Å

(vi) Immediately After Second Bond Cleavage

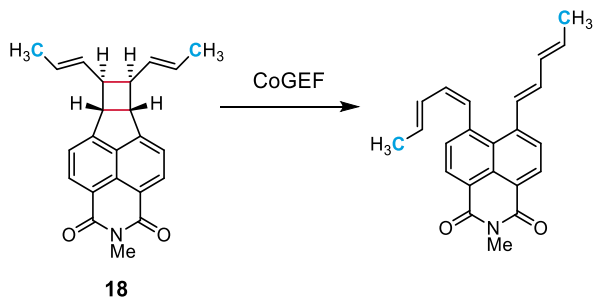


11.401 Å

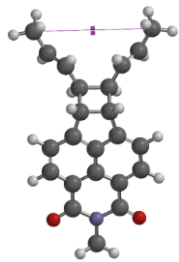


**Summary of CoGEF Results**

$F_{max}$	3.3 nN
$E_{max}$	241 kJ/mol
Force-Bond Angle	1.0°

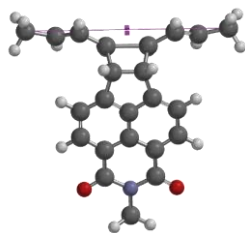


**(i) Equilibrium Geometry**



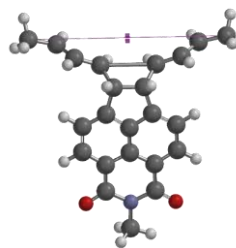
6.319 Å

**(ii) Immediately Prior to First Bond Cleavage**



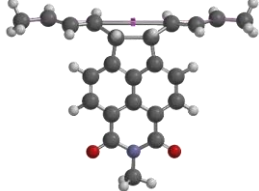
10.069 Å

**(iii) Immediately After First Bond Cleavage**



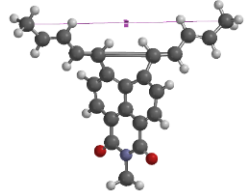
10.119 Å

**(v) Immediately Prior to Second Bond Cleavage**

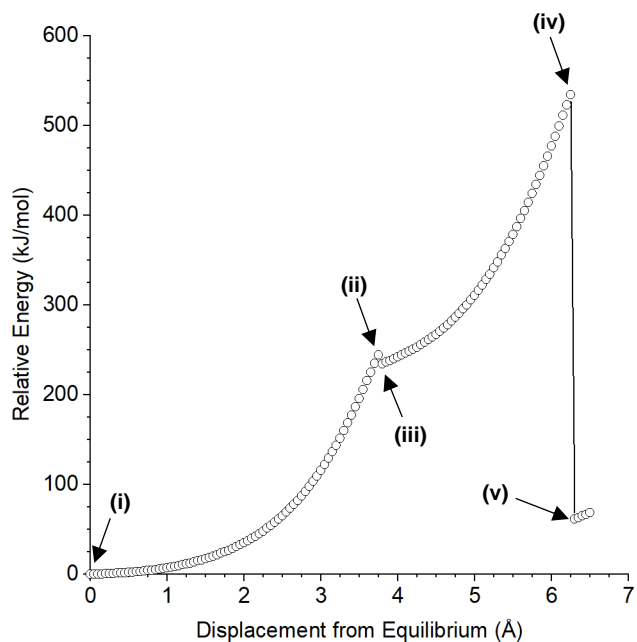


12.569 Å

**(vi) Immediately After Second Bond Cleavage**

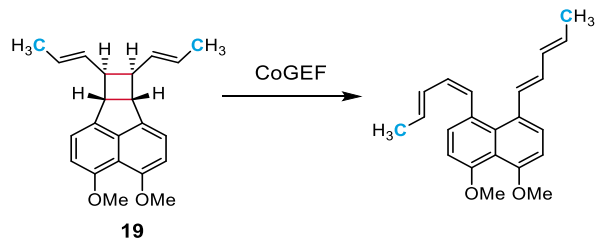


12.619 Å

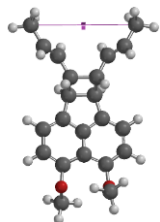


**Summary of CoGEF Results**

$F_{max}$	3.3 nN
$E_{max}$	244 kJ/mol
<b>Force-Bond Angle</b>	0.2°

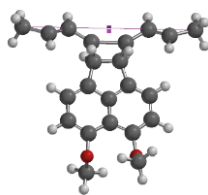


**(i) Equilibrium Geometry**



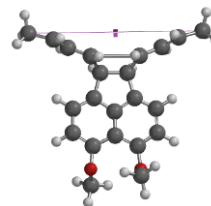
6.325 Å

**(ii) Immediately Prior to First Bond Cleavage**



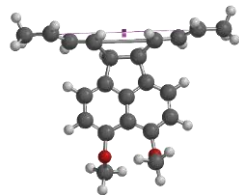
10.025 Å

**(iii) Immediately After First Bond Cleavage**



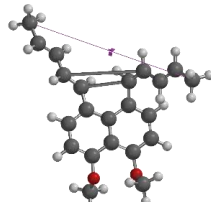
10.075 Å

**(v) Immediately Prior to Second Bond Cleavage**

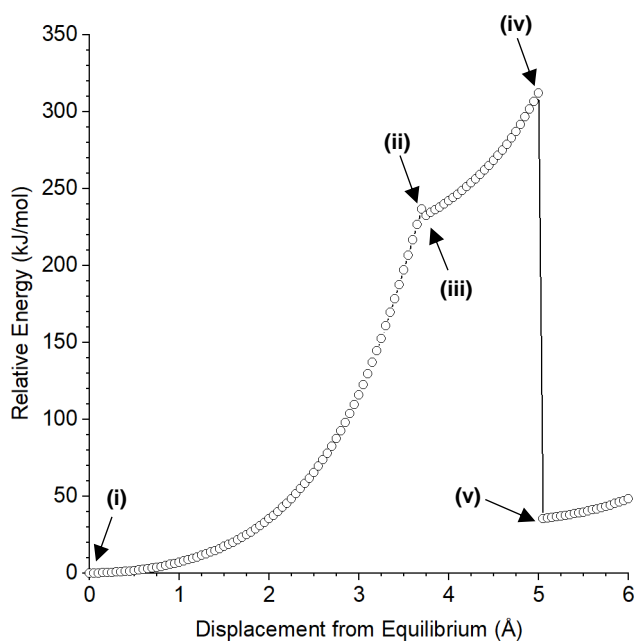


11.325 Å

**(vi) Immediately After Second Bond Cleavage**

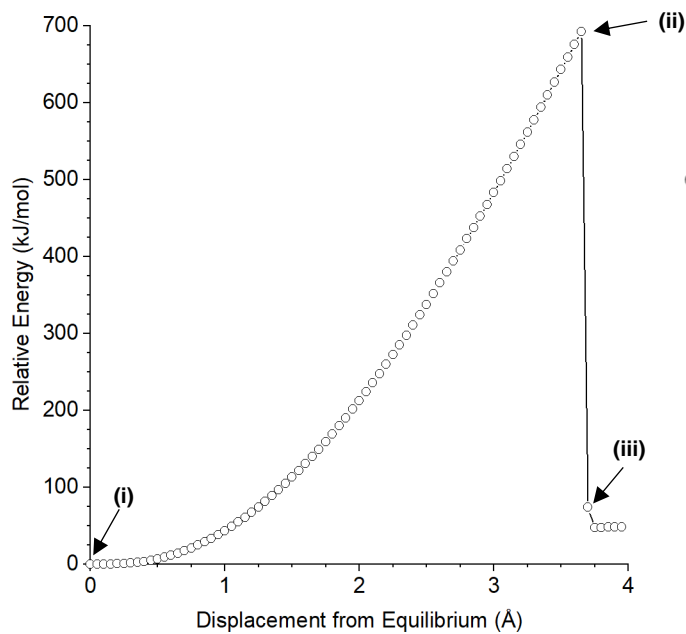
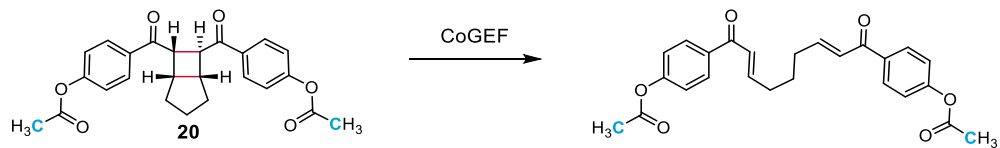


11.375 Å

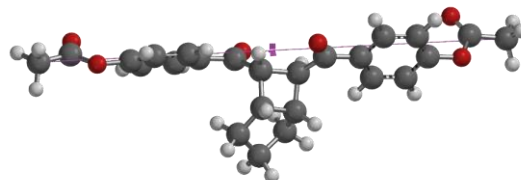


**Summary of CoGEF Results**

$F_{max}$	3.3 nN
$E_{max}$	236 kJ/mol
<b>Force-Bond Angle</b>	1.2°

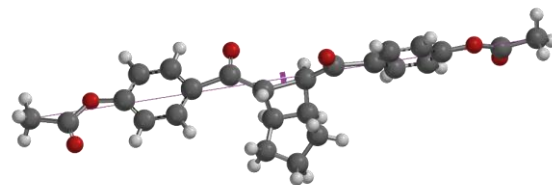


(i) Equilibrium Geometry



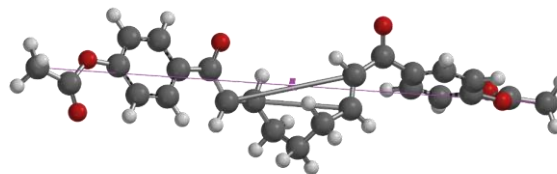
18.900 Å

(i) Immediately Prior to Bond Cleavage



22.550 Å

(iii) Immediately After Bond Cleavage



22.600 Å

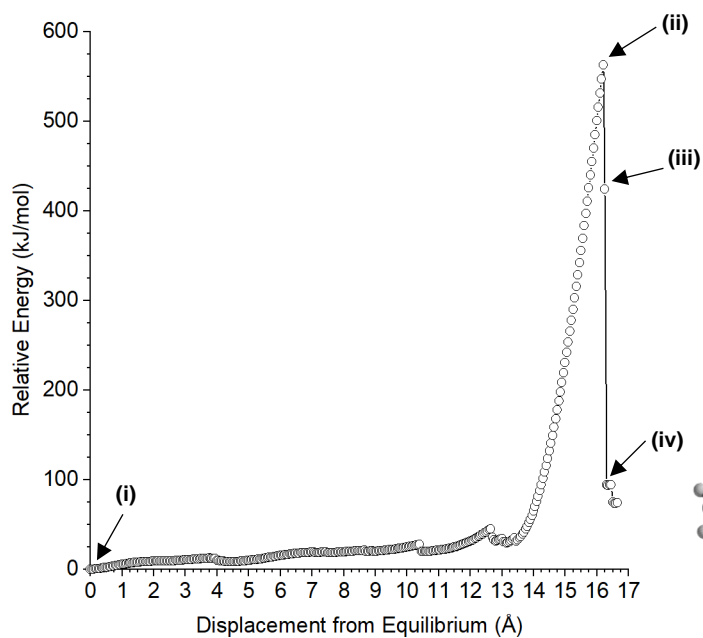
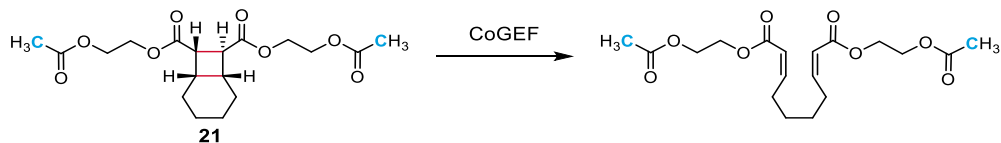
**Summary of CoGEF Results**

$F_{max}$  5.5 nN

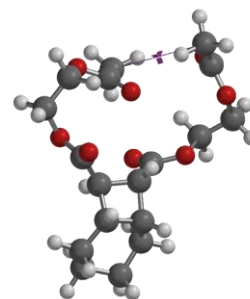
$E_{max}$  692 kJ/mol

Force-Bond Angle 16°



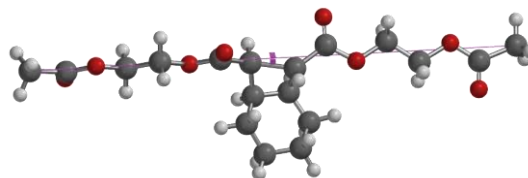


(i) Equilibrium Geometry



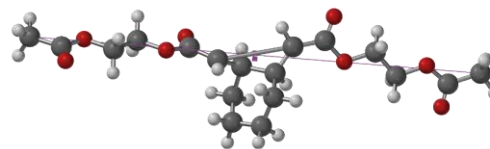
4.462 Å

(ii) Immediately Prior to First Bond Cleavage



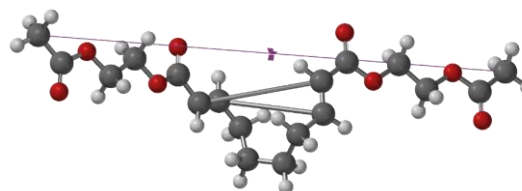
20.662 Å

(iii) Immediately After First Bond Cleavage



20.712 Å

(iv) Immediately After Second Bond Cleavage



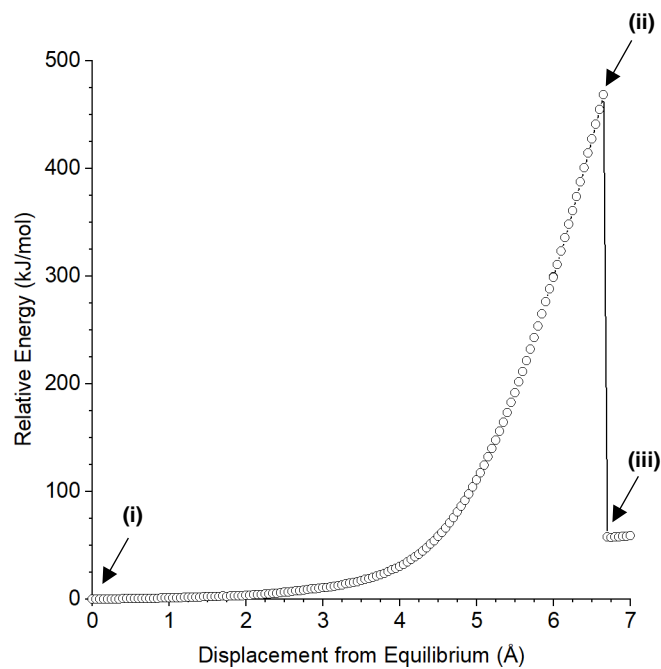
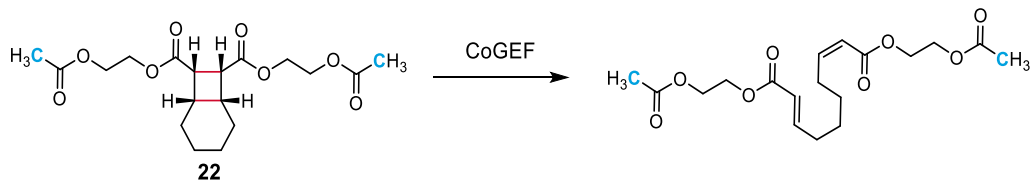
20.762 Å

**Summary of CoGEF Results**

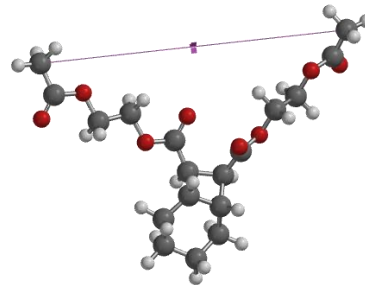
$F_{max}$  5.2 nN

$E_{max}$  562 kJ/mol

Force-Bond Angle 17°

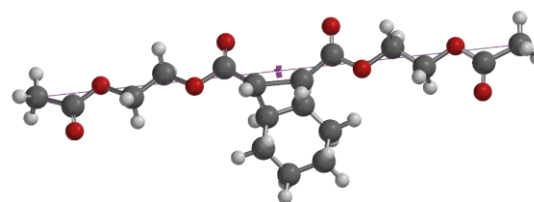


(i) Equilibrium Geometry



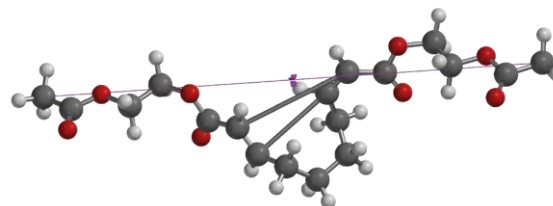
13.678 Å

(ii) Immediately Prior to Bond Cleavage



20.328 Å

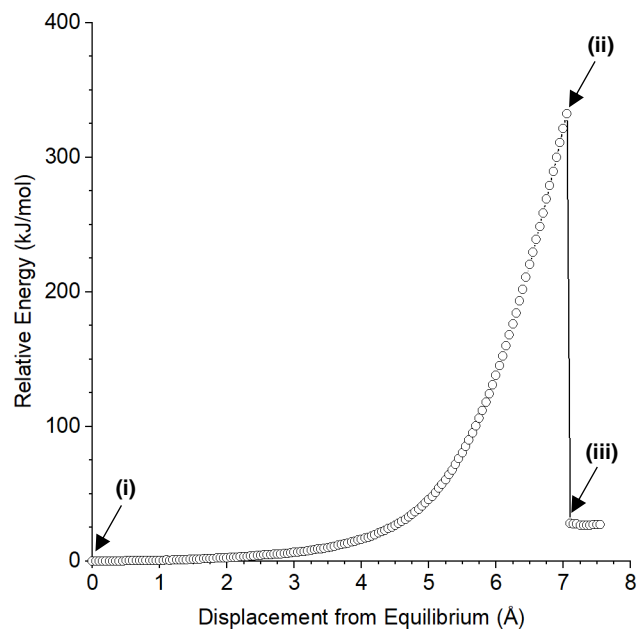
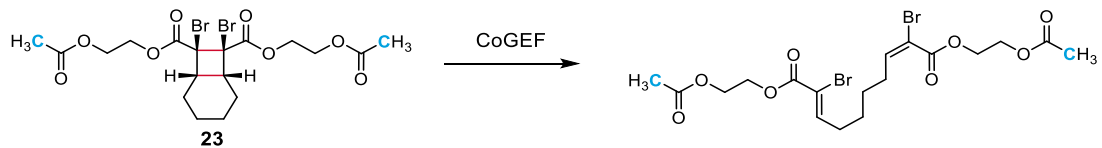
(iii) Immediately After Bond Cleavage



20.378 Å

**Summary of CoGEF Results**

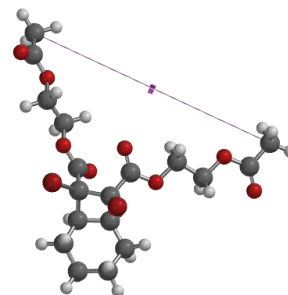
$F_{max}$	4.6 nN
$E_{max}$	469 kJ/mol
Force-Bond Angle	4.9°



**Summary of CoGEF Results**

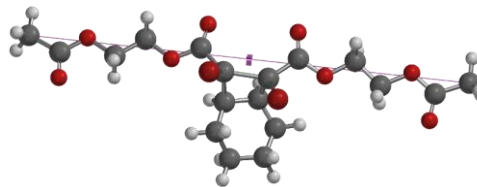
$F_{max}$	3.6 nN
$E_{max}$	332 kJ/mol
<b>Force-Bond Angle</b>	6.2°

**(i) Equilibrium Geometry**



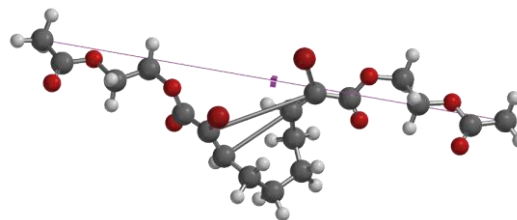
12.604 Å

**(ii) Immediately Prior to First Bond Cleavage**

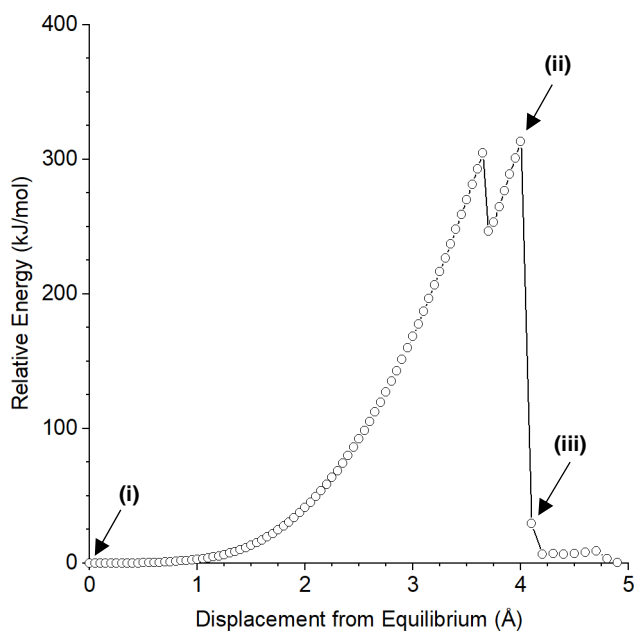
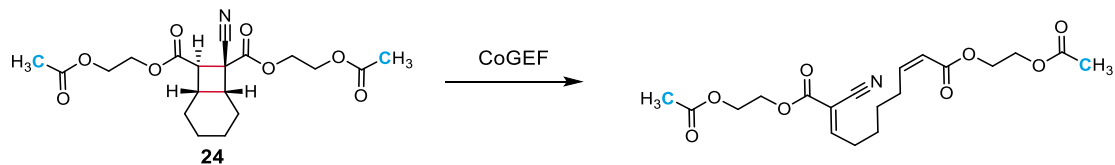


19.654 Å

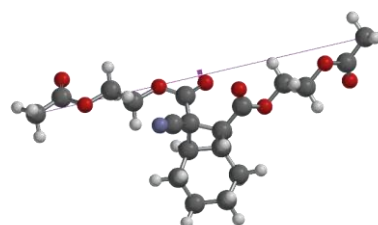
**(iii) Immediately After First Bond Cleavage**



19.704 Å

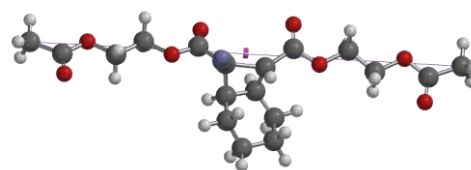


(i) Equilibrium Geometry



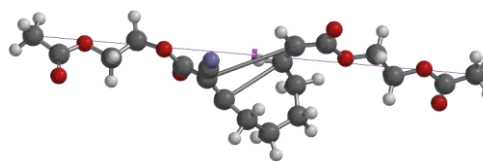
15.909 Å

(ii) Immediately Prior to Bond Cleavage



19.909 Å

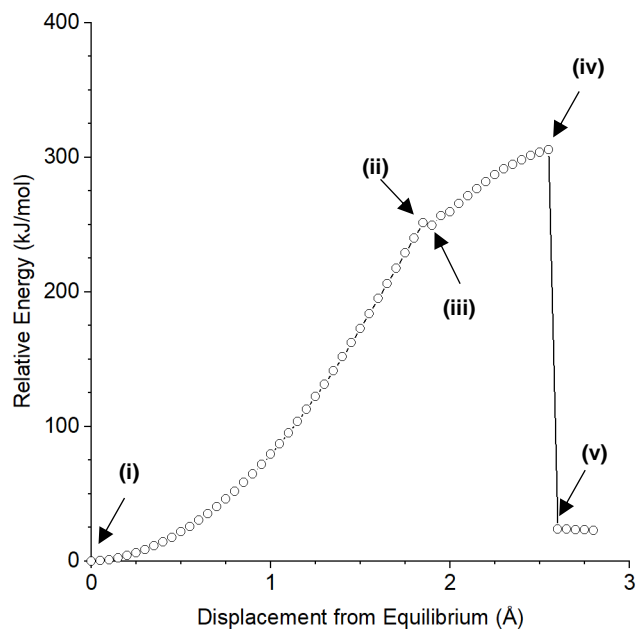
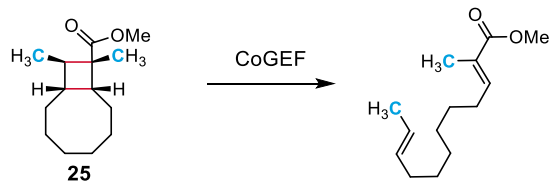
(iii) Immediately After Bond Cleavage



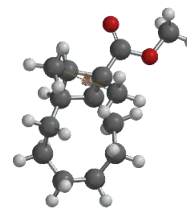
20.009 Å

**Summary of CoGEF Results**

$F_{max}$	4.0 nN
$E_{max}$	313 kJ/mol
Force-Bond Angle	8.5°

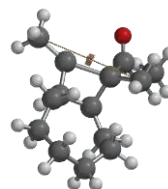


**(i) Equilibrium Geometry**



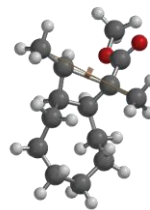
3.052 Å

**(ii) Immediately Prior to First Bond Cleavage**



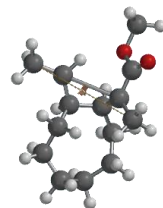
4.902 Å

**(iii) Immediately After First Bond Cleavage**



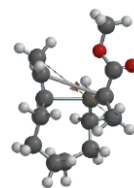
4.952 Å

**(iv) Immediately Prior to Second Bond Cleavage**



5.552 Å

**(v) Immediately After Second Bond Cleavage**



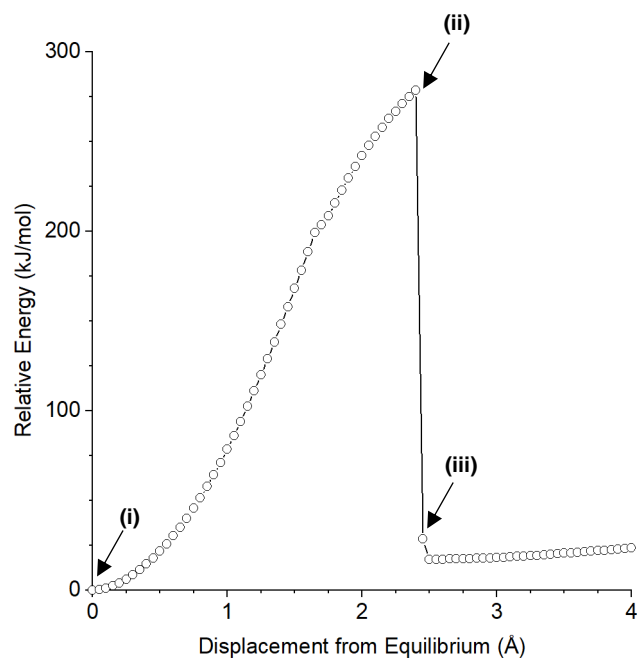
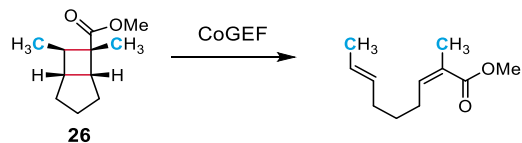
5.602 Å

**Summary of CoGEF Results**

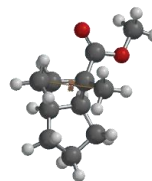
$F_{max}$  3.8 nN

$E_{max}$  302 kJ/mol

**Force-Bond Angle** 7.1°

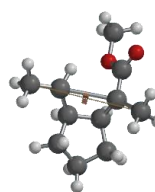


**(i) Equilibrium Geometry**



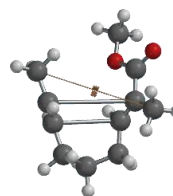
3.057 Å

**(ii) Immediately Prior to Bond Cleavage**



5.457 Å

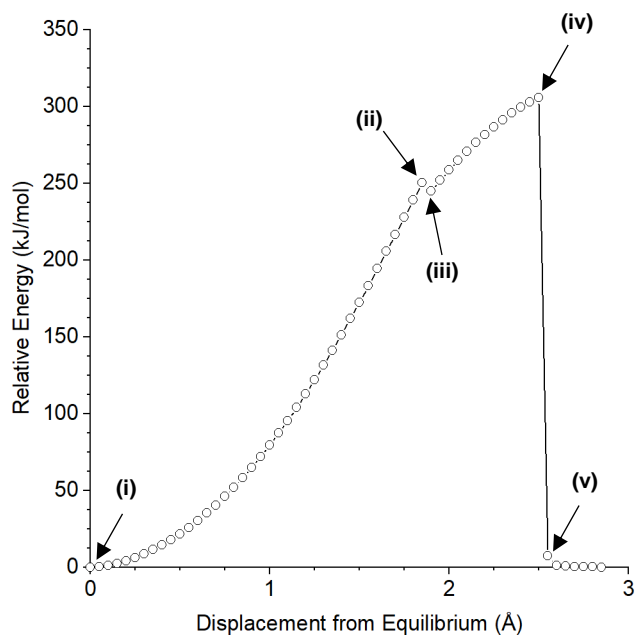
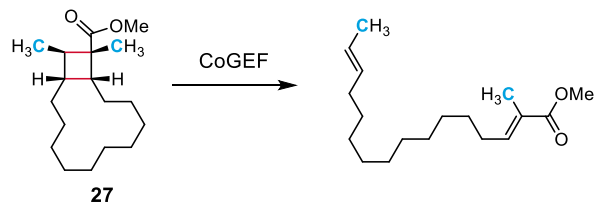
**(iii) Immediately After Bond Cleavage**



5.507 Å

**Summary of CoGEF Results**

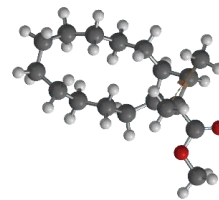
$F_{max}$	3.5 nN
$E_{max}$	278 kJ/mol
<b>Force-Bond Angle</b>	3.1°



**Summary of CoGEF Results**

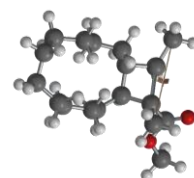
$F_{max}$	3.7 nN
$E_{max}$	306 kJ/mol
Force-Bond Angle	7.3°

**(i) Equilibrium Geometry**



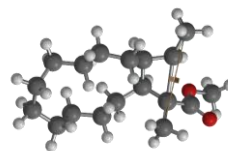
3.051 Å

**(ii) Immediately Prior to First Bond Cleavage**



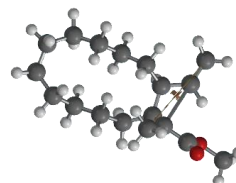
4.901 Å

**(iii) Immediately After First Bond Cleavage**



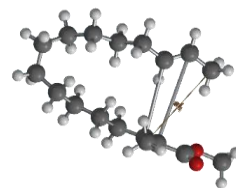
4.951 Å

**(iv) Immediately Prior to Second Bond Cleavage**

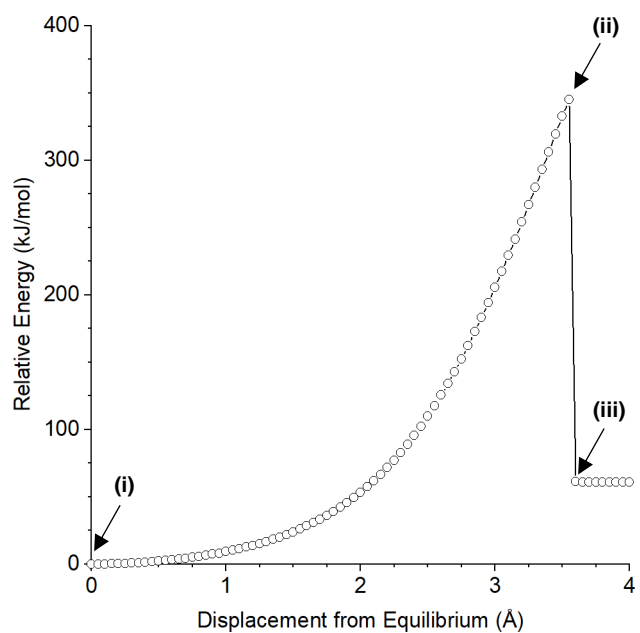
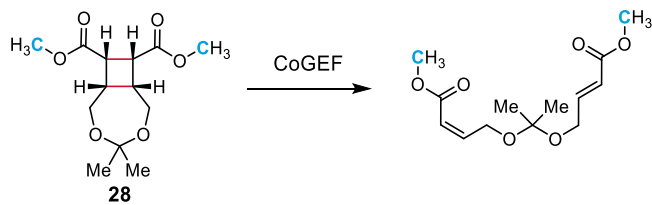


5.551 Å

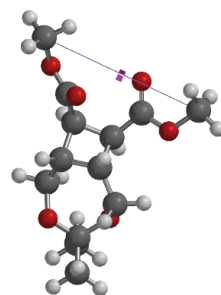
**(v) Immediately After Second Bond Cleavage**



5.601 Å

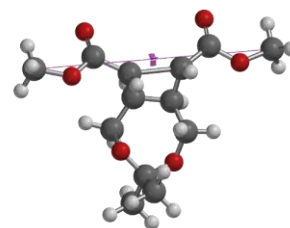


(i) Equilibrium Geometry



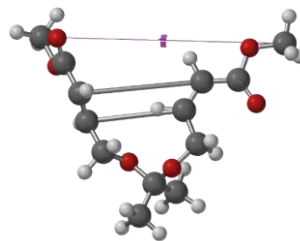
6.476 Å

(ii) Immediately Prior to Bond Cleavage



10.026 Å

(iii) Immediately After Bond Cleavage

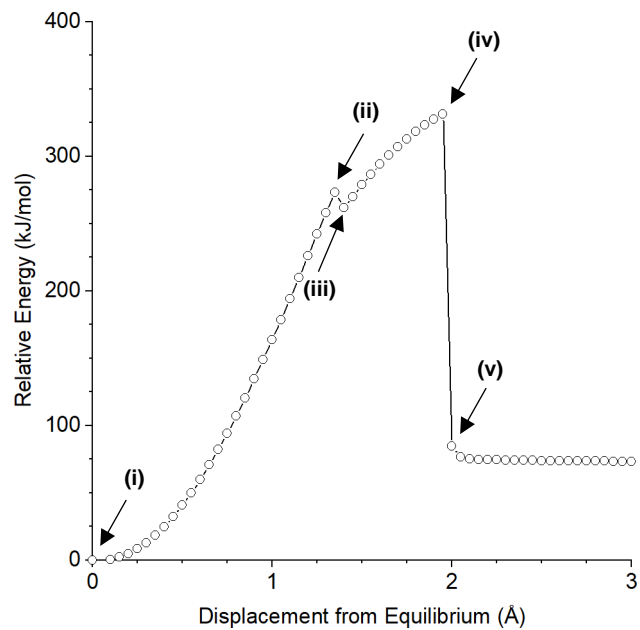
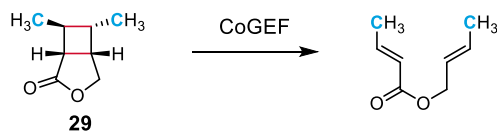


10.076 Å

**Summary of CoGEF Results**

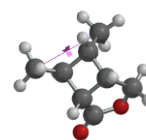
$F_{max}$	4.4 nN
$E_{max}$	345 kJ/mol
Force-Bond Angle	4.6 °





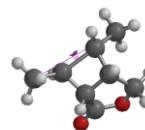
Summary of CoGEF Results	
$F_{max}$	5.4 nN
$E_{max}$	331 kJ/mol
Force-Bond Angle	24°

(i) Equilibrium Geometry



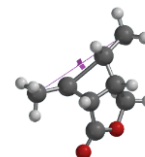
3.769 Å

(ii) Immediately Prior to First Bond Cleavage



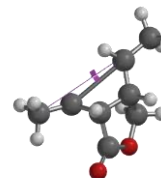
5.119 Å

(iii) Immediately After First Bond Cleavage



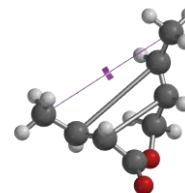
5.169 Å

(iv) Immediately Prior to Second Bond Cleavage

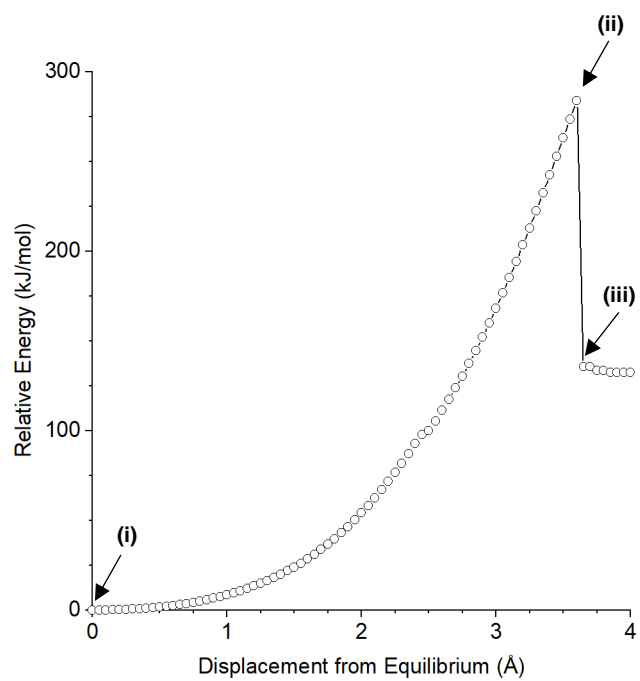
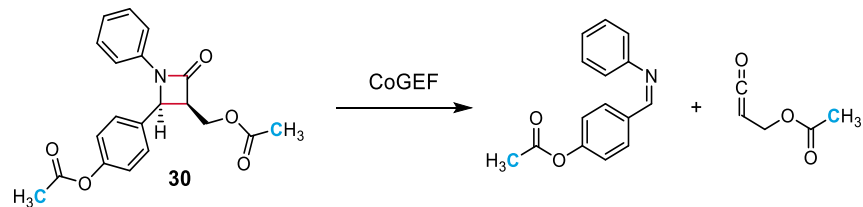


5.719 Å

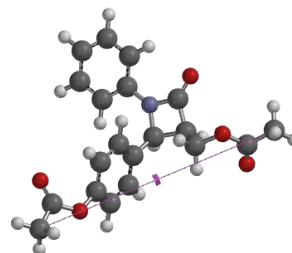
(v) Immediately After Second Bond Cleavage



5.769 Å

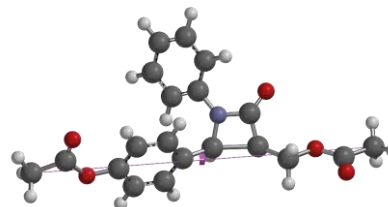


(i) Equilibrium Geometry



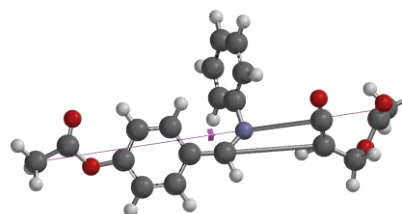
11.759 Å

(ii) Immediately Prior to Bond Cleavage



15.359 Å

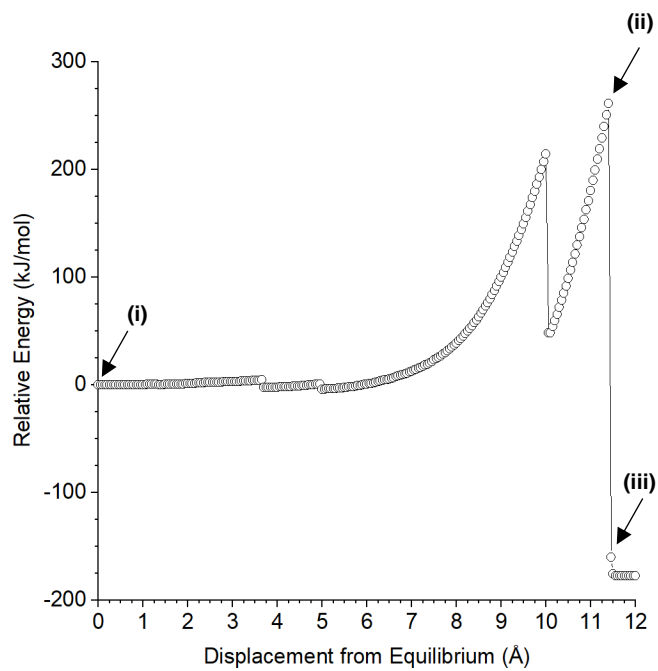
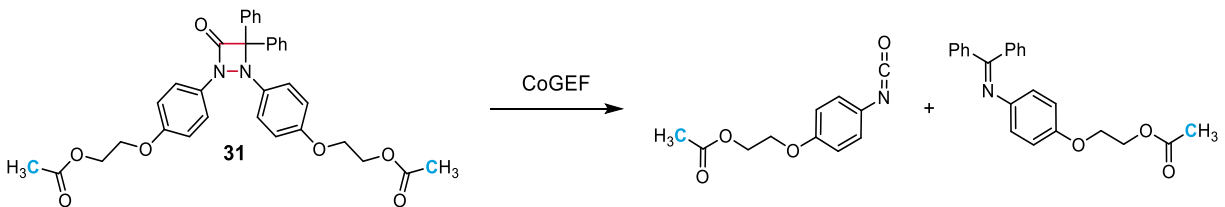
(iii) Immediately After Bond Cleavage



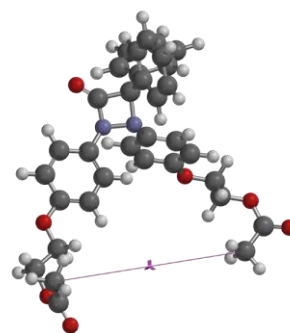
15.409 Å

**Summary of CoGEF Results**

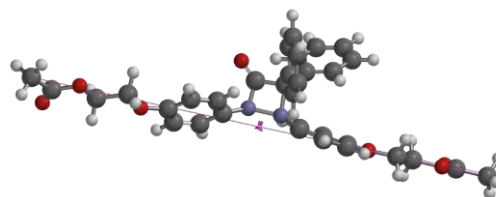
$F_{max}$	3.5 nN
$E_{max}$	284 kJ/mol
<b>Force-Bond Angle</b>	9.3°



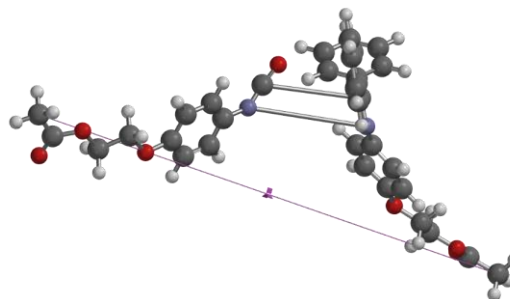
(i) Equilibrium Geometry



(ii) Immediately Prior to Bond Cleavage



(iii) Immediately After Bond Cleavage

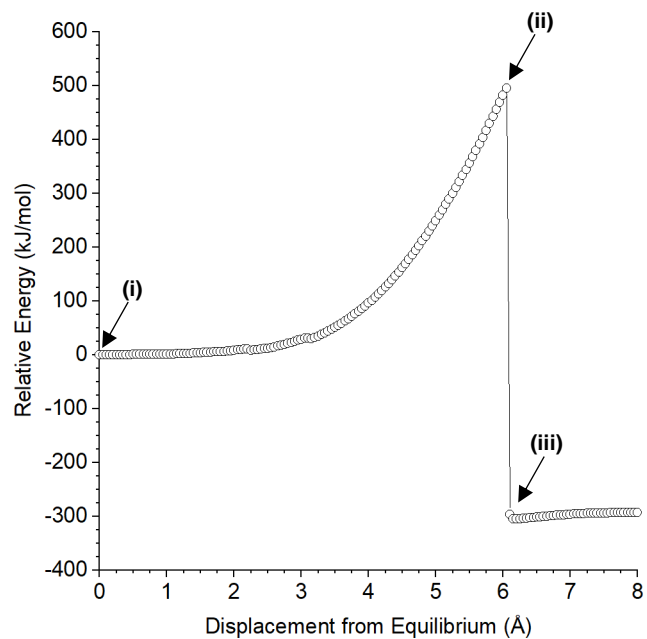
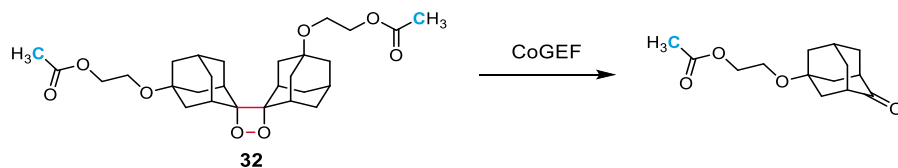


**Summary of CoGEF Results**

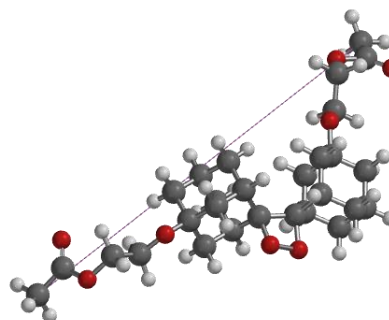
$F_{max}$  3.6 nN

$E_{max}$  260 kJ/mol

Force-Bond Angle 34°

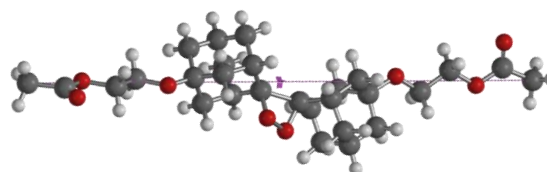


(i) Equilibrium Geometry



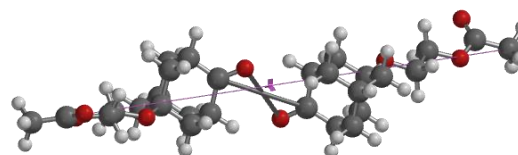
18.153 Å

(ii) Immediately Prior to Bond Cleavage



24.203 Å

(iii) Immediately After Bond Cleavage



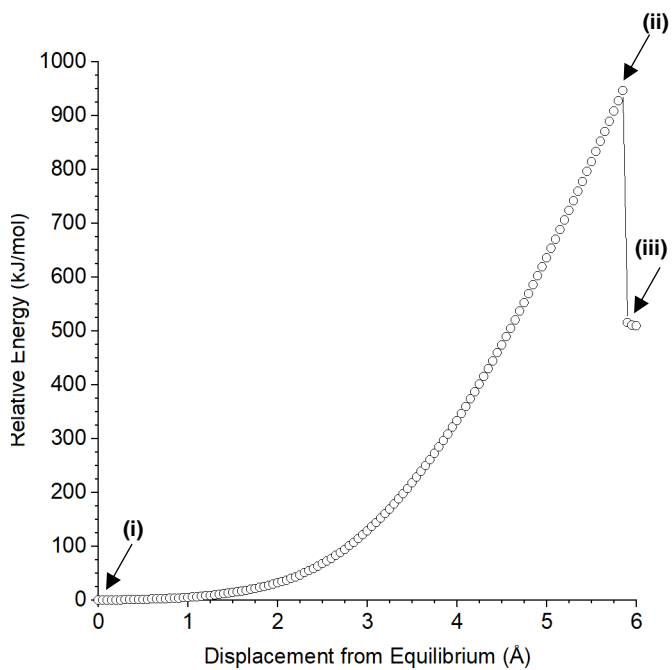
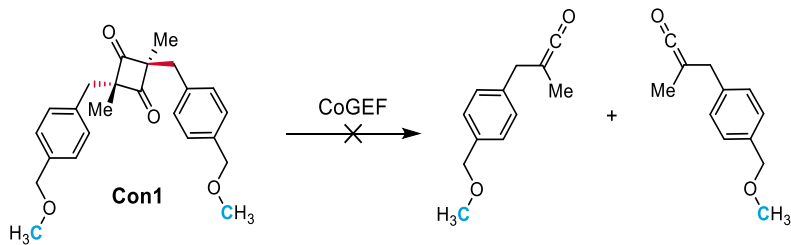
24.253 Å

**Summary of CoGEF Results**

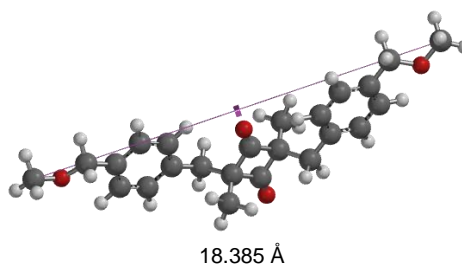
$F_{max}$  4.4 nN

$E_{max}$  495 kJ/mol

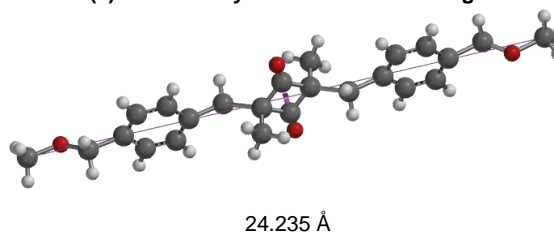
Force-Bond Angle 15°



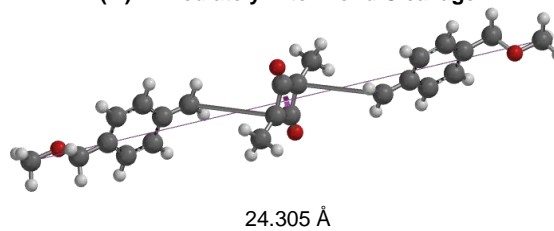
**(i) Equilibrium Geometry**



**(ii) Immediately Prior to Bond Cleavage**



**(iii) Immediately After Bond Cleavage**

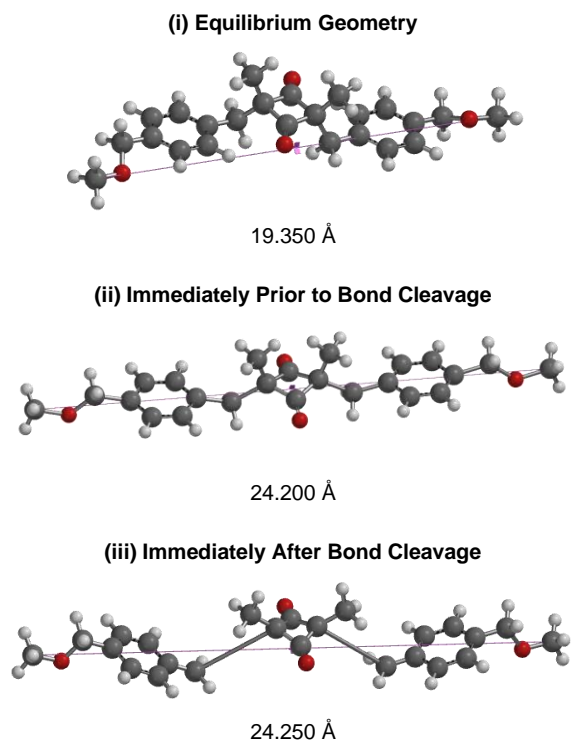
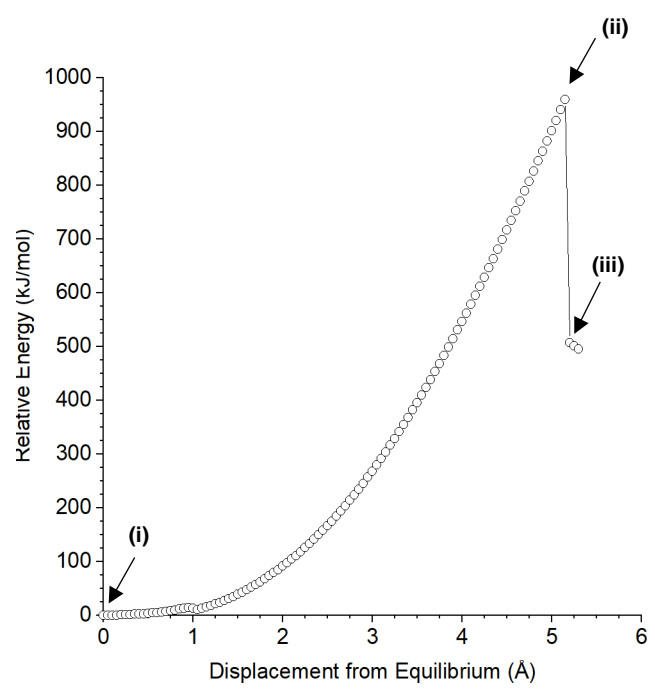
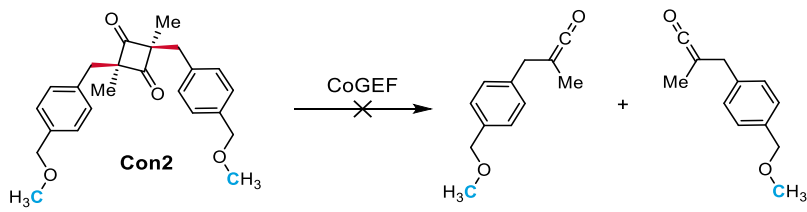


**Summary of CoGEF Results**

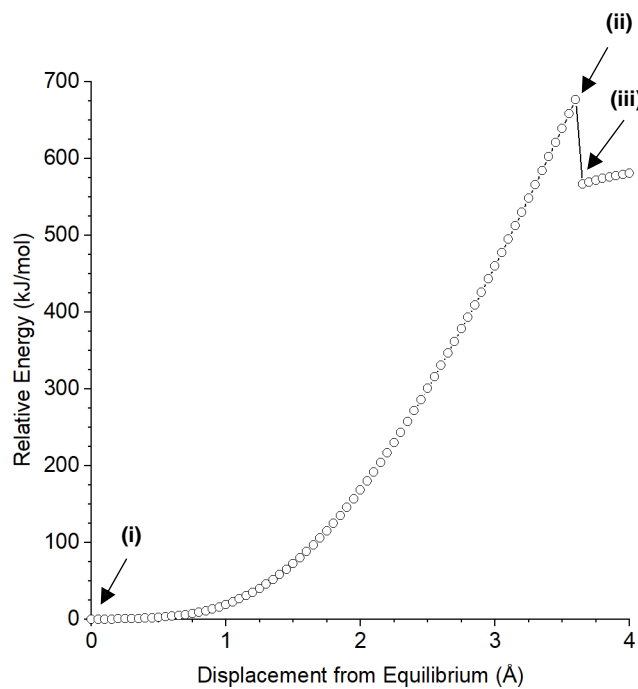
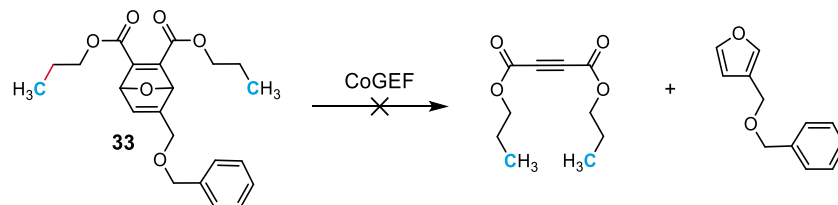
$F_{max}$  6.3 nN

$E_{max}$  947 kJ/mol

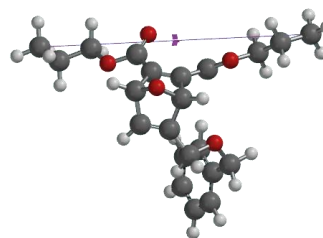
**Force-Bond Angle** 43°



Summary of CoGEF Results	
$F_{max}$	6.4 nN
$E_{max}$	959 kJ/mol
Force-Bond Angle	42°

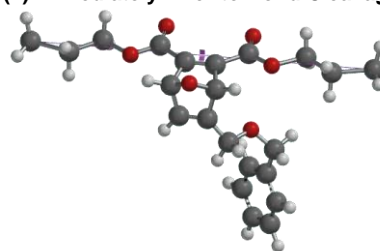


**(i) Equilibrium Geometry**



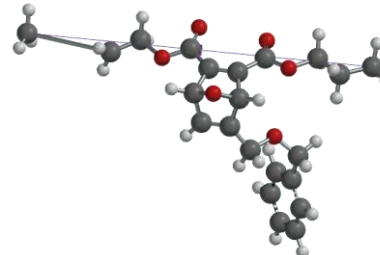
12.509 Å

**(ii) Immediately Prior to Bond Cleavage**



16.109 Å

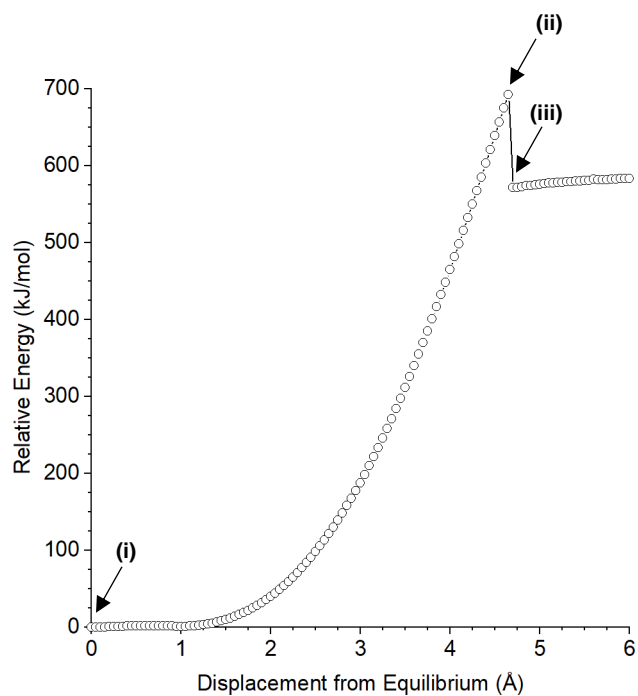
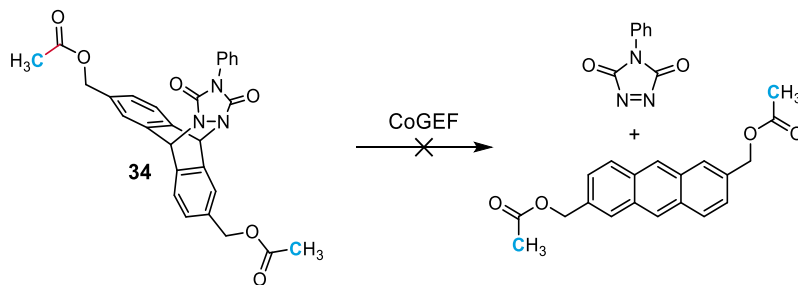
**(iii) Immediately After Bond Cleavage**



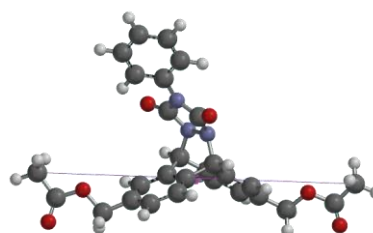
16.159 Å

**Summary of CoGEF Results**

$F_{max}$	6.2 nN
$E_{max}$	676 kJ/mol
<b>Force-Bond Angle</b>	78°

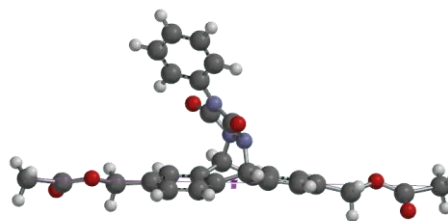


(i) Equilibrium Geometry



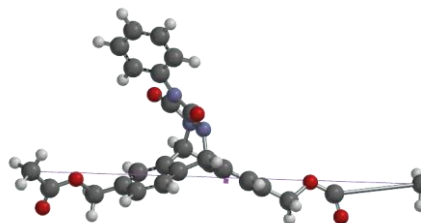
15.358 Å

(ii) Immediately Prior to Bond Cleavage



20.008 Å

(iii) Immediately After Bond Cleavage

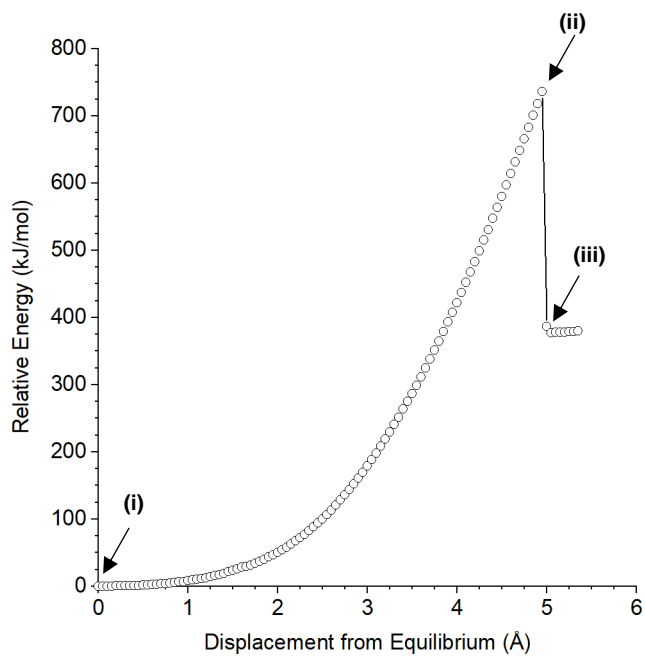
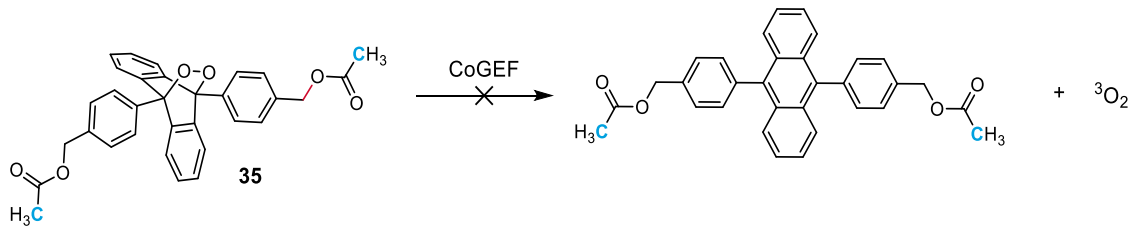


20.058 Å

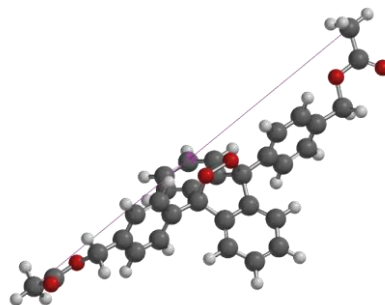
**Summary of CoGEF Results**

$F_{max}$	6.0 nN
$E_{max}$	693 kJ/mol
<b>Force-Bond Angle</b>	85°



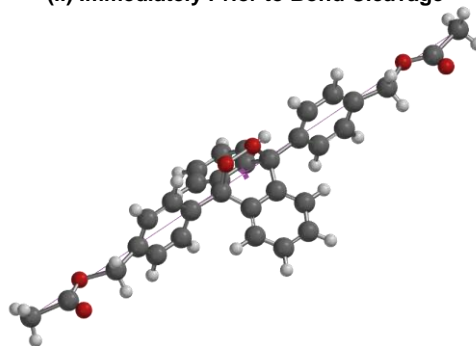


(i) Equilibrium Geometry



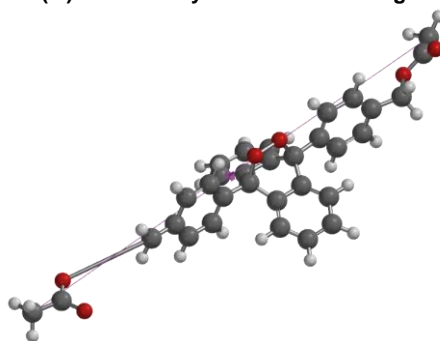
19.243 Å

(ii) Immediately Prior to Bond Cleavage



24.193 Å

(iii) Immediately After Bond Cleavage



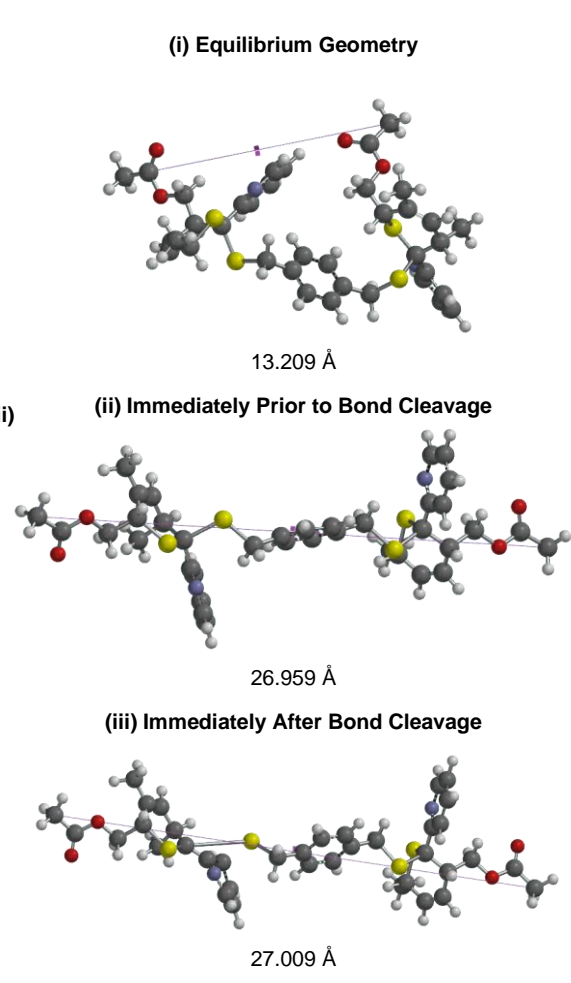
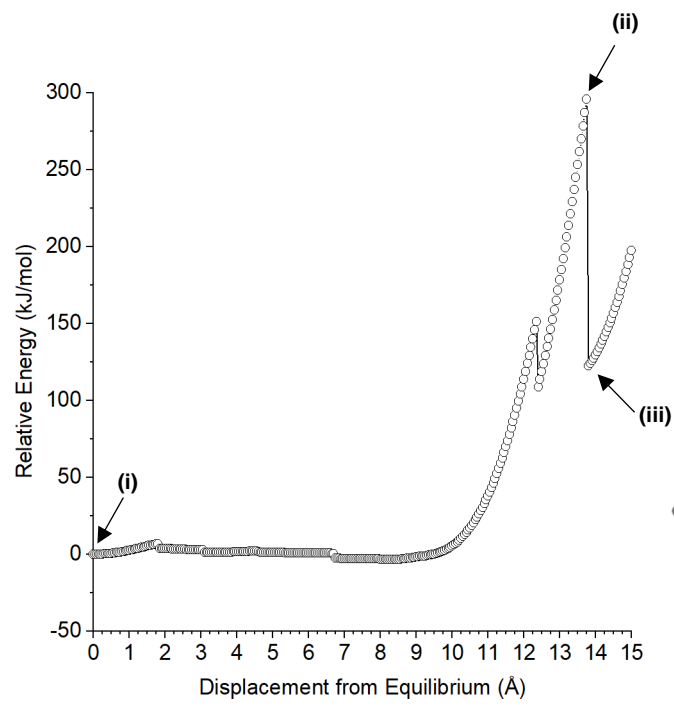
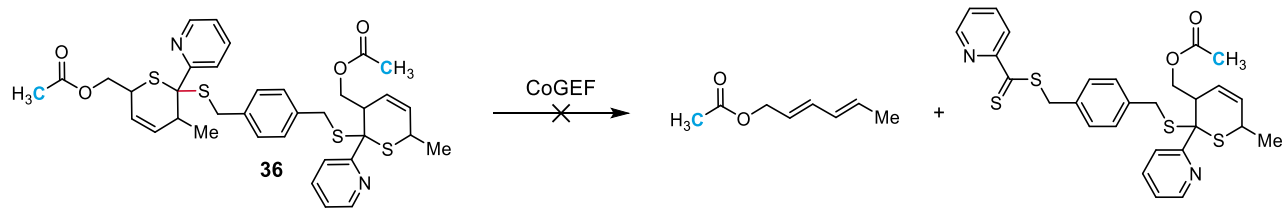
24.243 Å

**Summary of CoGEF Results**

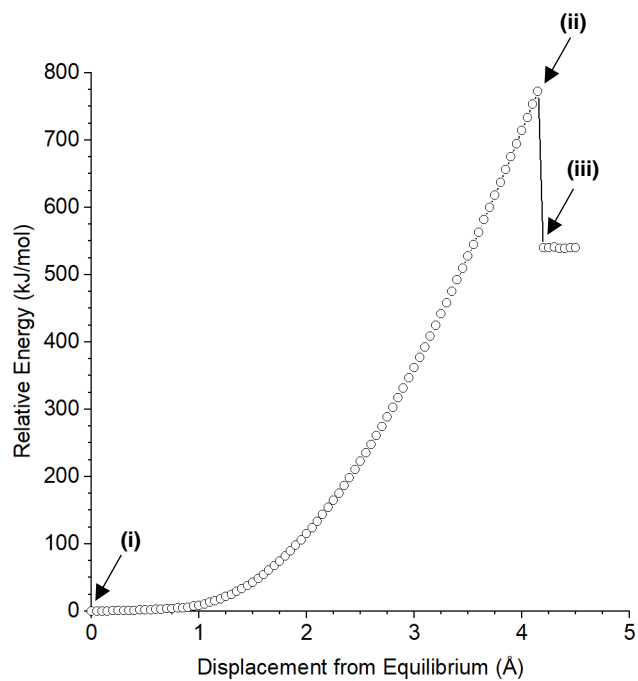
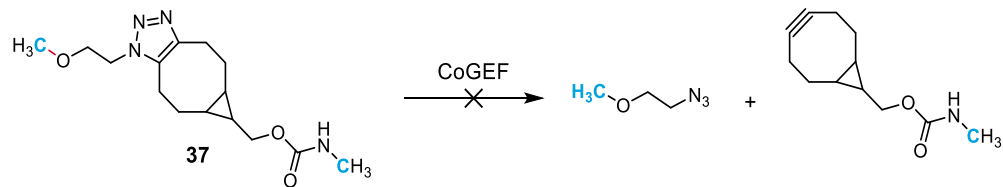
$F_{max}$  5.8 nN

$E_{max}$  736 kJ/mol

Force-Bond Angle 66°



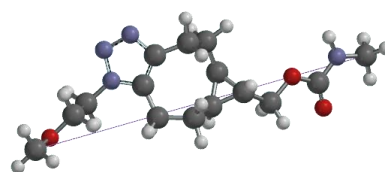
Summary of CoGEF Results	
$F_{max}$	2.9 nN
$E_{max}$	295 kJ/mol
Force-Bond Angle	32°



**Summary of CoGEF Results**

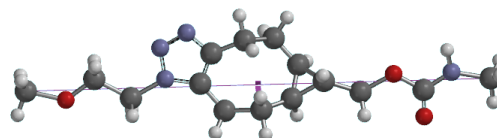
$F_{max}$	6.5 nN
$E_{max}$	772 kJ/mol
Force/Bond angle	8.9°

**(i) Equilibrium Geometry**



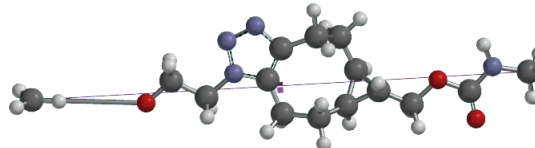
15.627 Å

**(ii) Immediately Prior to Bond Cleavage**

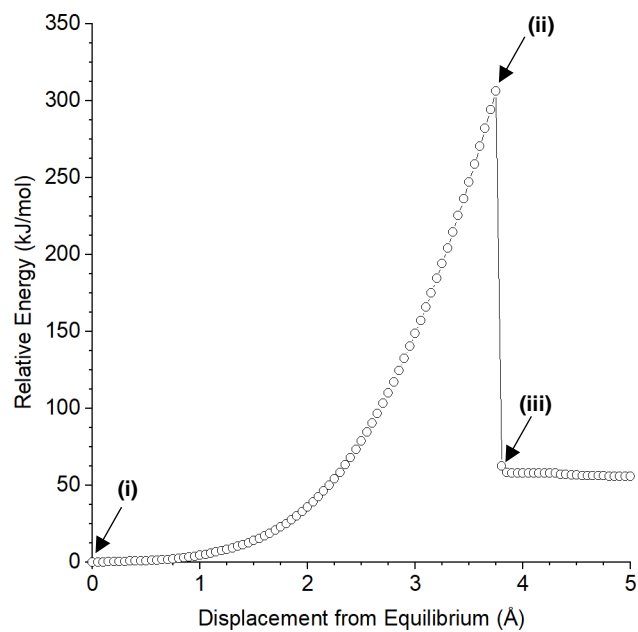
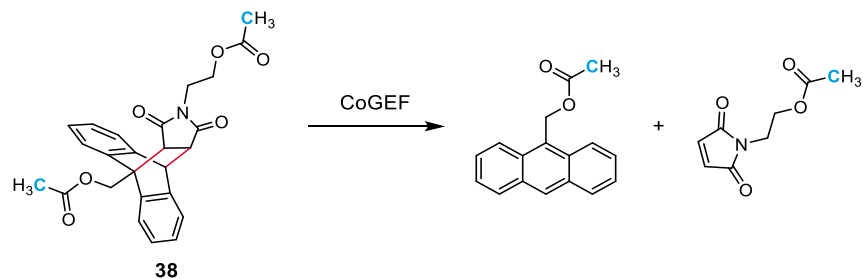


19.777 Å

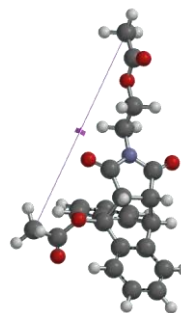
**(iii) Immediately After Bond Cleavage**



19.827 Å

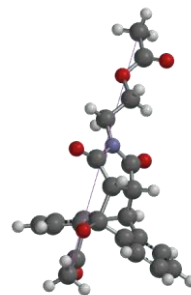


**(i) Equilibrium Geometry**



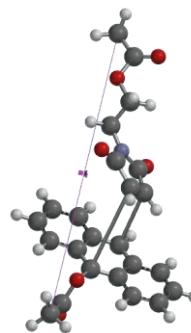
10.918 Å

**(ii) Immediately Prior to Bond Cleavage**



14.668 Å

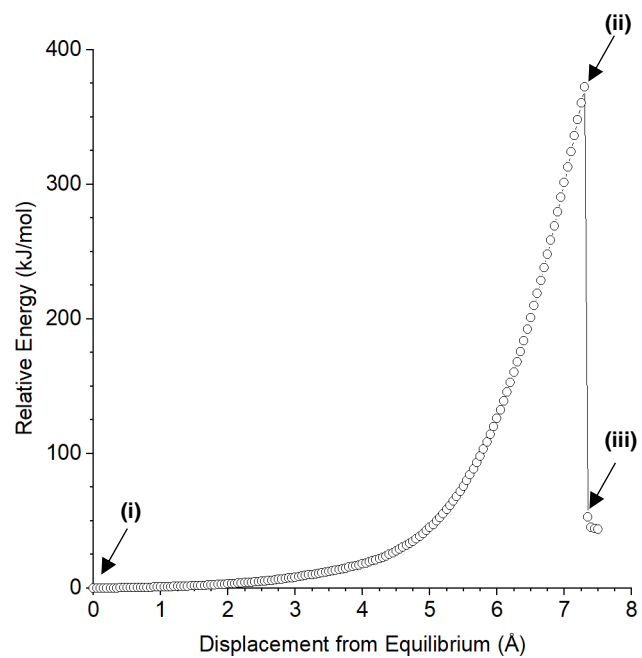
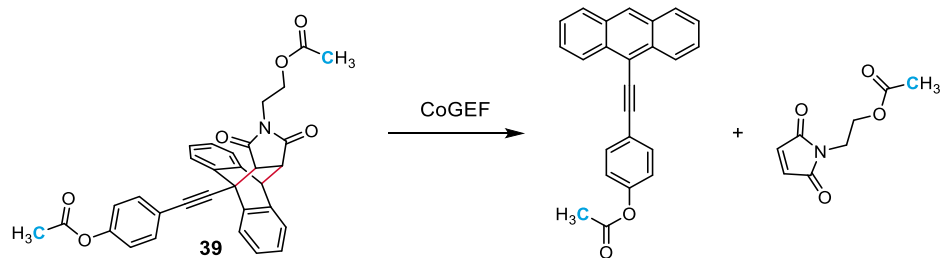
**(iii) Immediately After Bond Cleavage**



14.718 Å

**Summary of CoGEF Results**

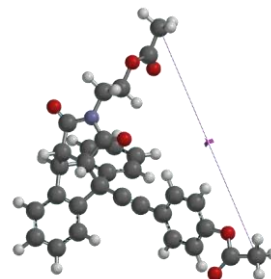
$F_{max}$	4.1 nN
$E_{max}$	306 kJ/mol
Force/Bond angle	25°



**Summary of CoGEF Results**

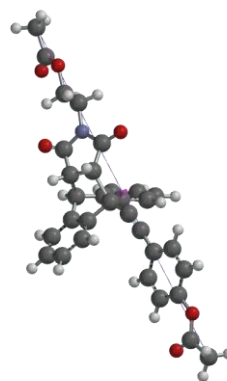
$F_{max}$	4.0 nN
$E_{max}$	372 kJ/mol
<b>Force-Bond Angle</b>	26°

**(i) Equilibrium Geometry**



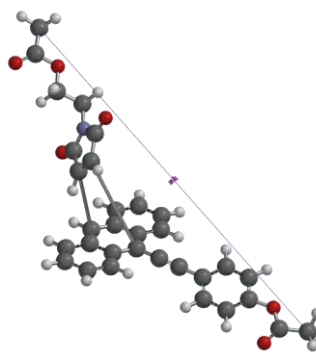
14.542 Å

**(ii) Immediately Prior to Bond Cleavage**

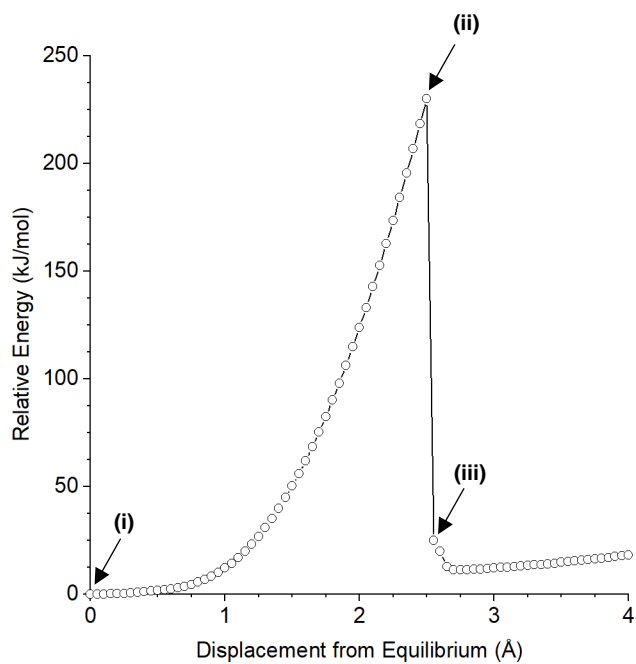
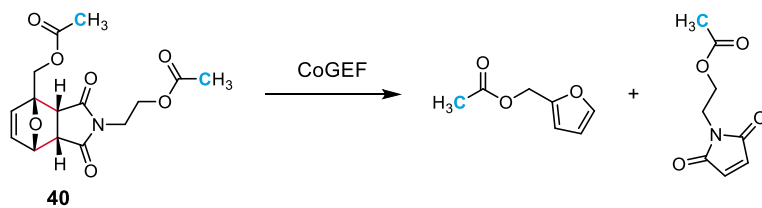


21.842 Å

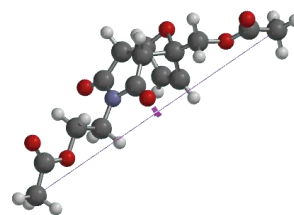
**(iii) Immediately After Bond Cleavage**



21.892 Å

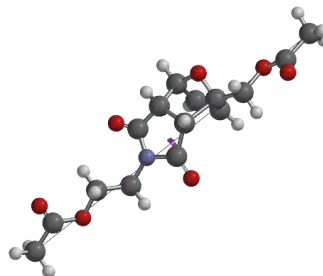


(i) Equilibrium Geometry



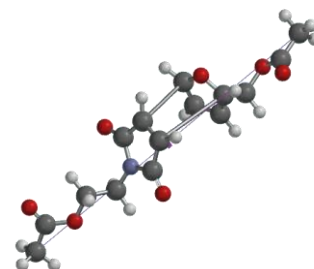
13.422 Å

(ii) Immediately Prior to Bond Cleavage



15.922 Å

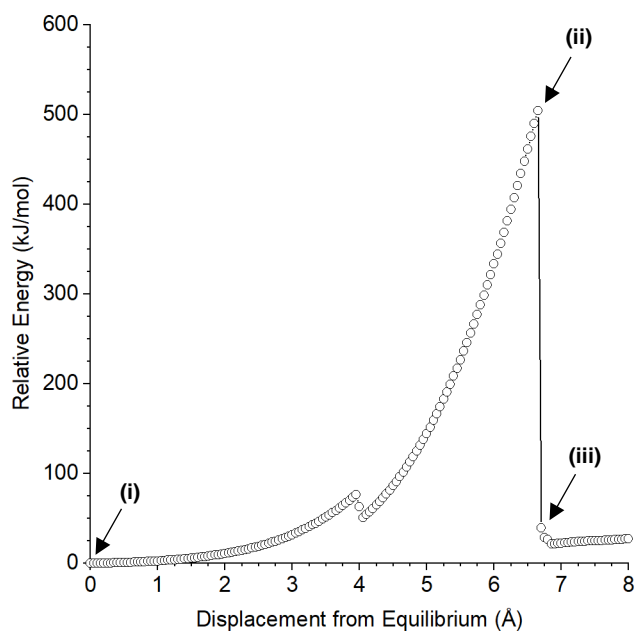
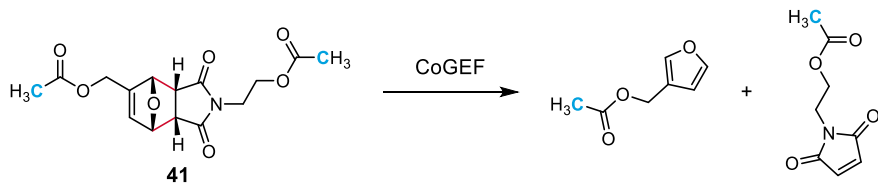
(iii) Immediately After Bond Cleavage



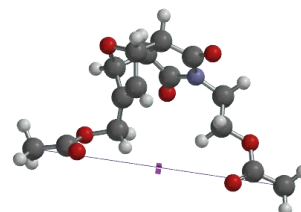
15.972 Å

**Summary of CoGEF Results**

$F_{max}$	3.9 nN
$E_{max}$	230 kJ/mol
<b>Force-Bond Angle</b>	26°

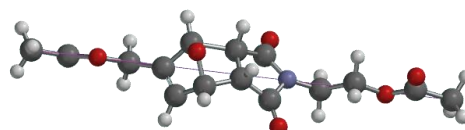


(i) Equilibrium Geometry



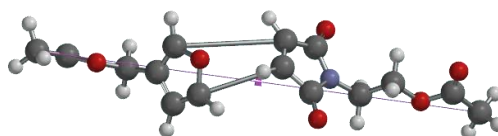
10.731 Å

(ii) Immediately Prior to Bond Cleavage



17.381 Å

(iii) Immediately After Bond Cleavage



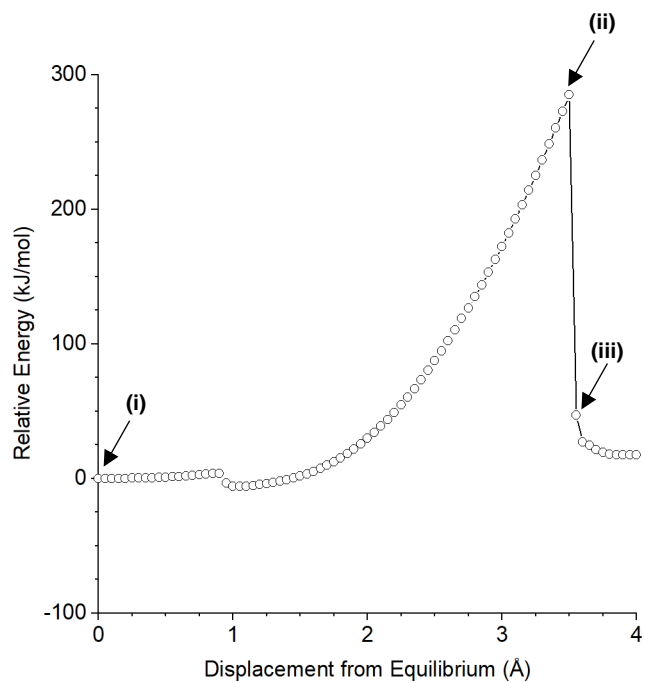
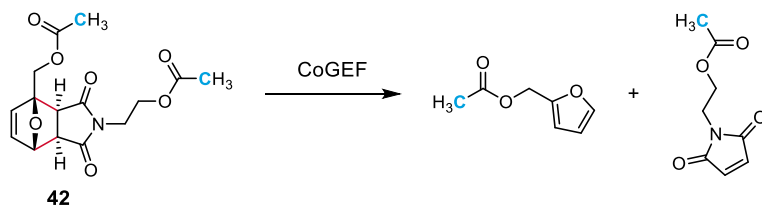
17.431 Å

**Summary of CoGEF Results**

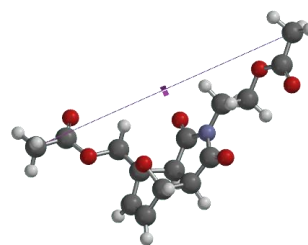
$F_{max}$  4.8 nN

$E_{max}$  504 kJ/mol

Force-Bond Angle 6.8°

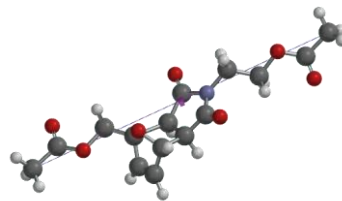


(i) Equilibrium Geometry



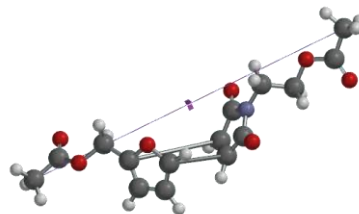
12.433 Å

(ii) Immediately Prior to Bond Cleavage



15.933 Å

(iii) Immediately After Bond Cleavage

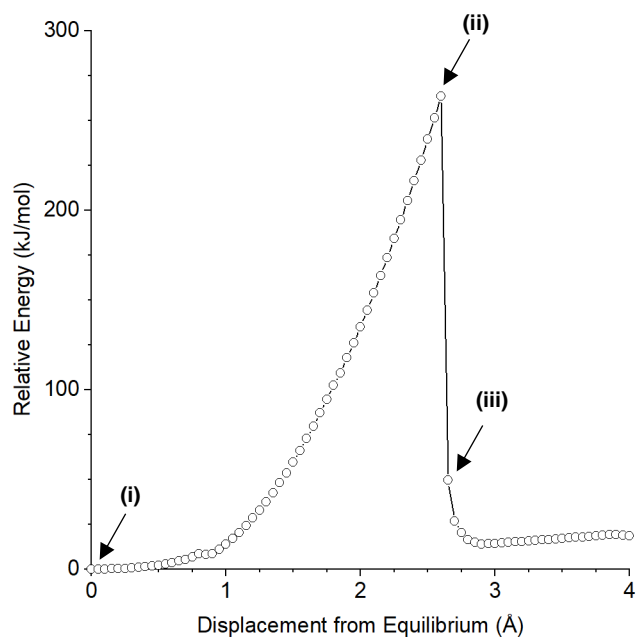
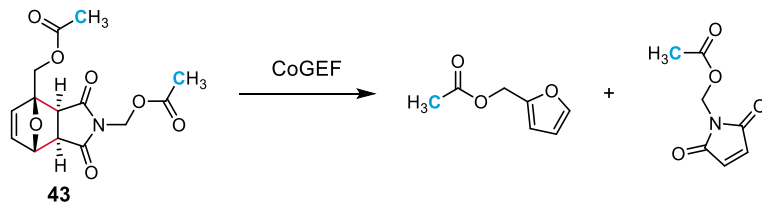


15.983 Å

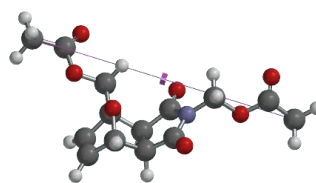
**Summary of CoGEF Results**

$F_{max}$	4.1 nN
$E_{max}$	285 kJ/mol
Force-Bond Angle	22°



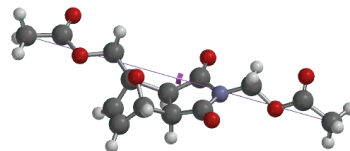


(i) Equilibrium Geometry



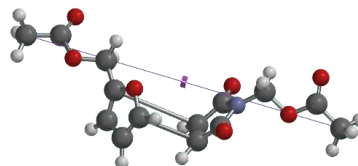
11.874 Å

(ii) Immediately Prior to Bond Cleavage



14.474 Å

(iii) Immediately After Bond Cleavage



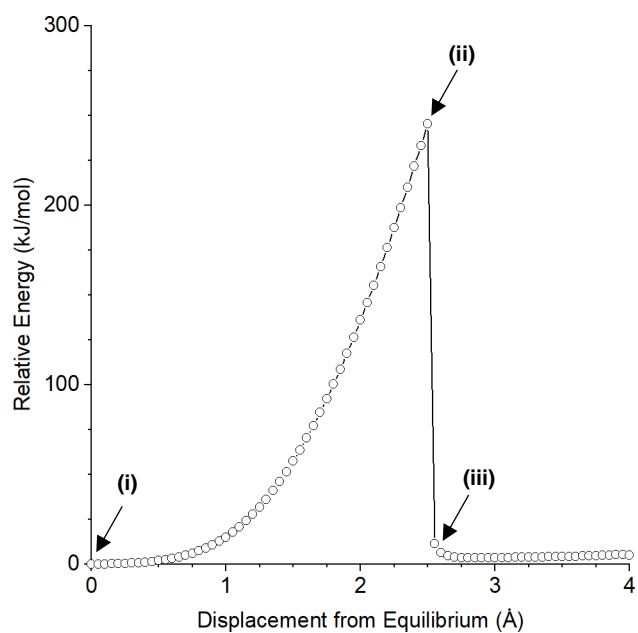
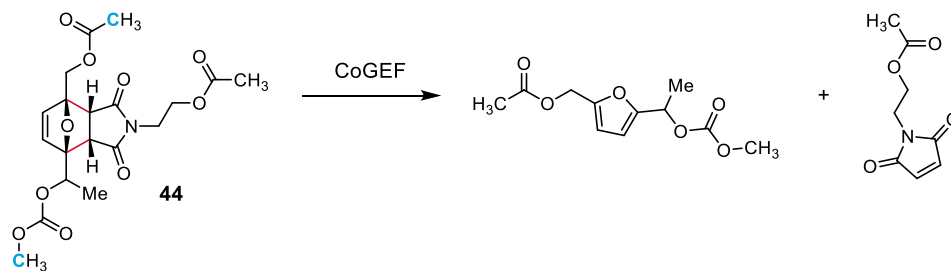
14.524 Å

**Summary of CoGEF Results**

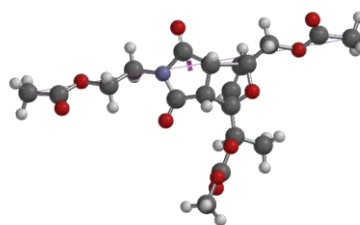
$F_{max}$  4.0 nN

$E_{max}$  264 kJ/mol

Force-Bond Angle 21°

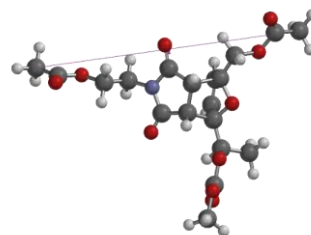


(i) Equilibrium Geometry



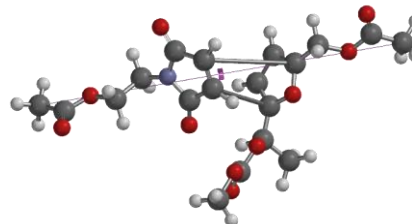
13.491 Å

(ii) Immediately Prior to Bond Cleavage



15.991 Å

(iii) Immediately After Bond Cleavage



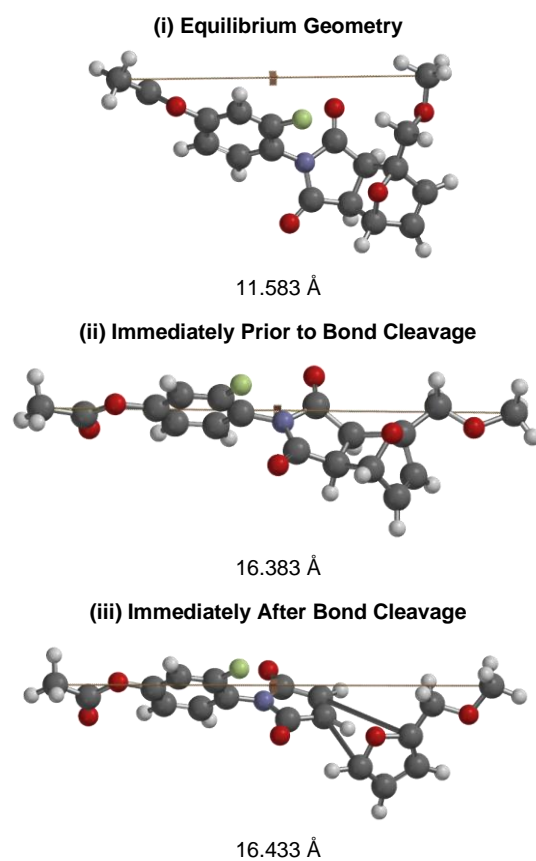
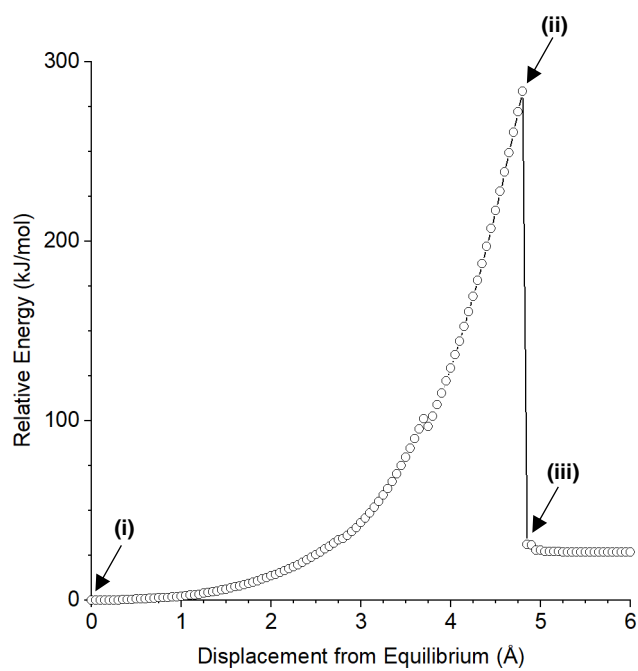
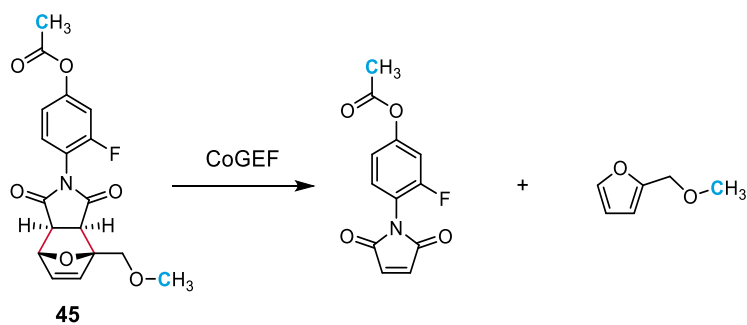
16.041 Å

**Summary of CoGEF Results**

$F_{max}$  4.0 nN

$E_{max}$  245 kJ/mol

Force-Bond Angle 26°

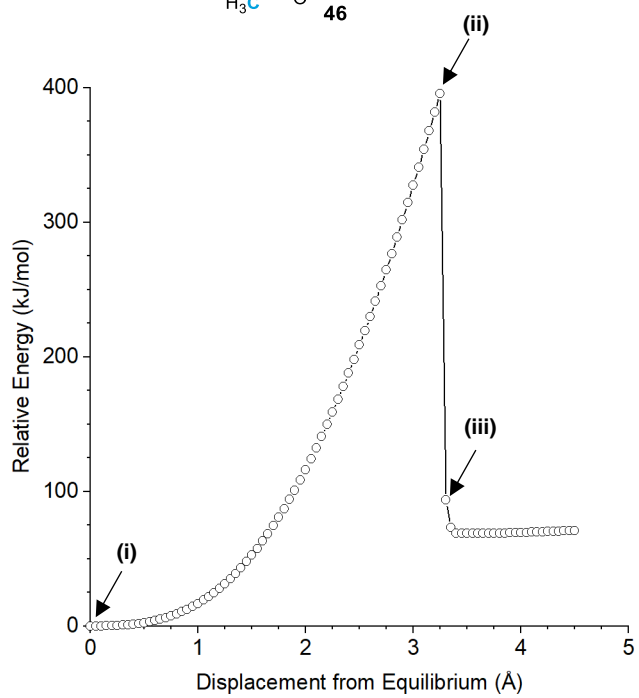
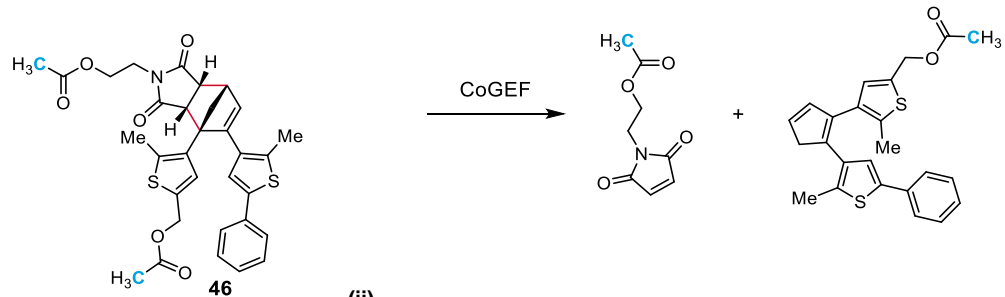


**Summary of CoGEF Results**

$F_{max}$  3.8 nN

$E_{max}$  284 kJ/mol

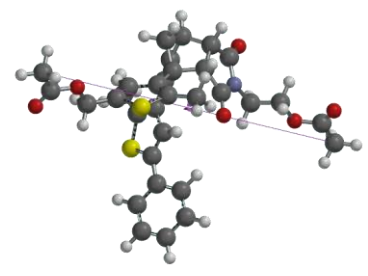
**Force-Bond Angle** 21°



**Summary of CoGEF Results**

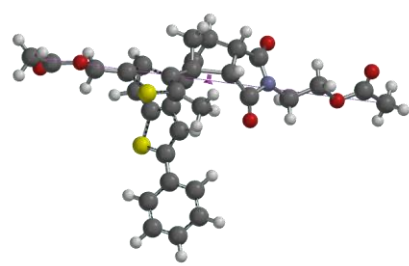
$F_{max}$	4.6 nN
$E_{max}$	396 kJ/mol
Force-Bond Angle	26°

**(i) Equilibrium Geometry**



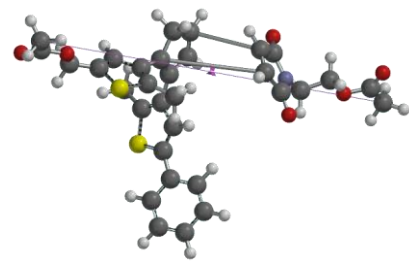
17.075 Å

**(ii) Immediately Prior to Bond Cleavage**

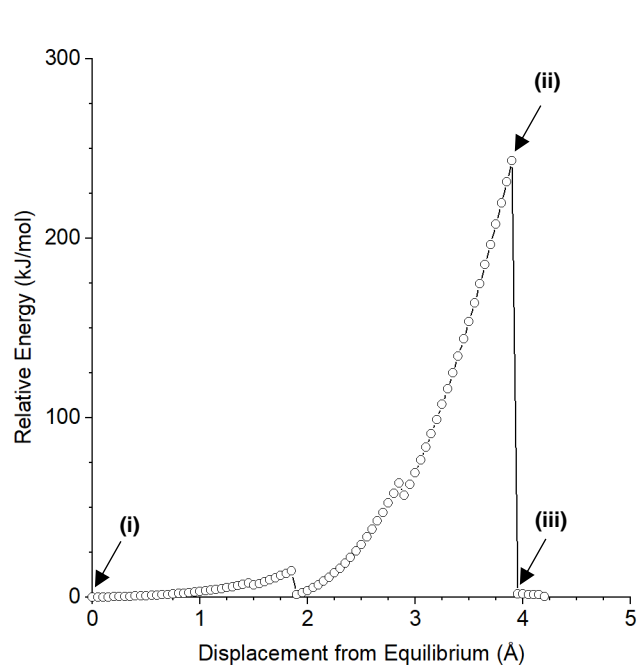
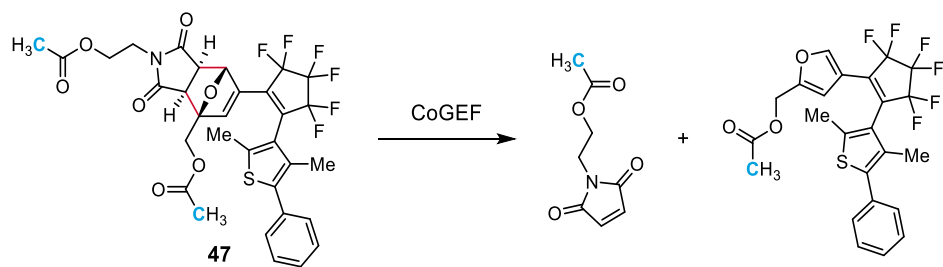


20.325 Å

**(iii) Immediately After Bond Cleavage**



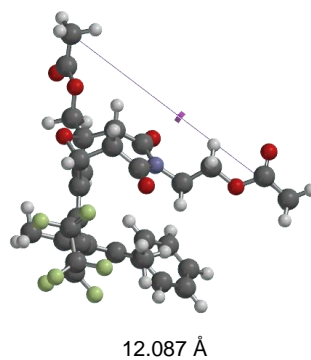
20.375 Å



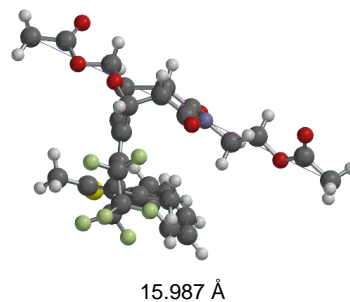
#### Summary of CoGEF Results

$F_{max}$	3.9 nN
$E_{max}$	243 kJ/mol
Force-Bond Angle	25°

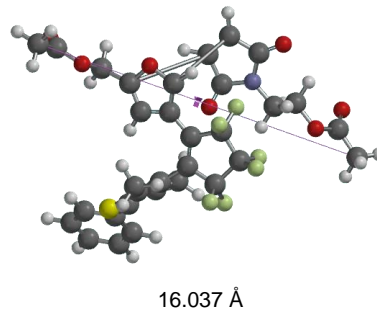
#### (i) Equilibrium Geometry

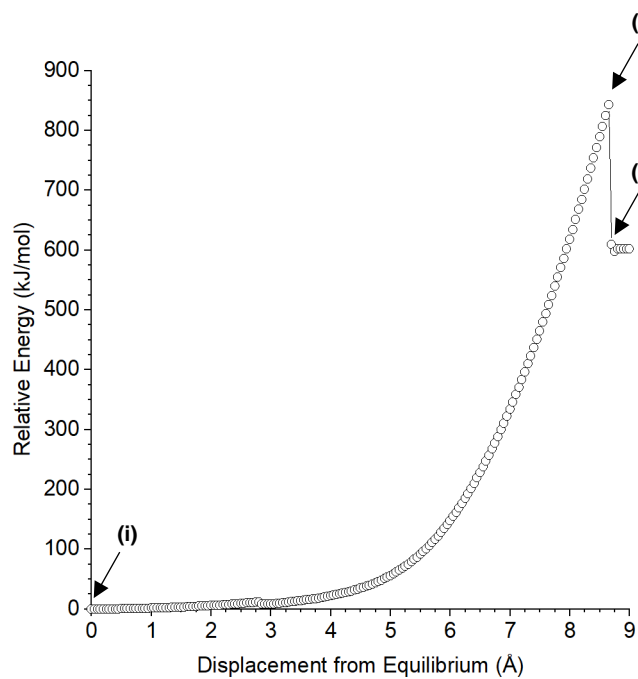
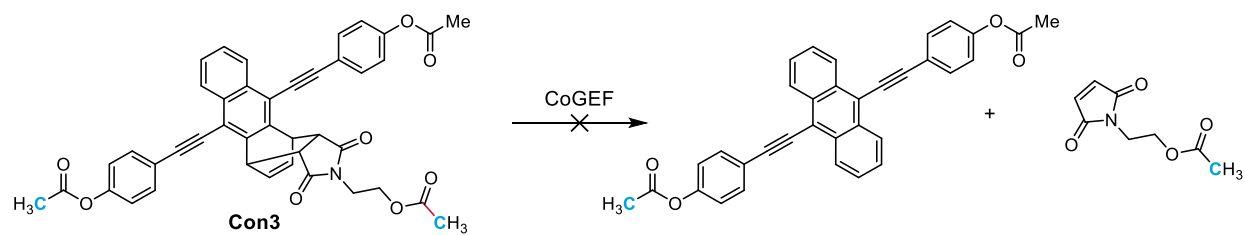


#### (ii) Immediately Prior to Bond Cleavage



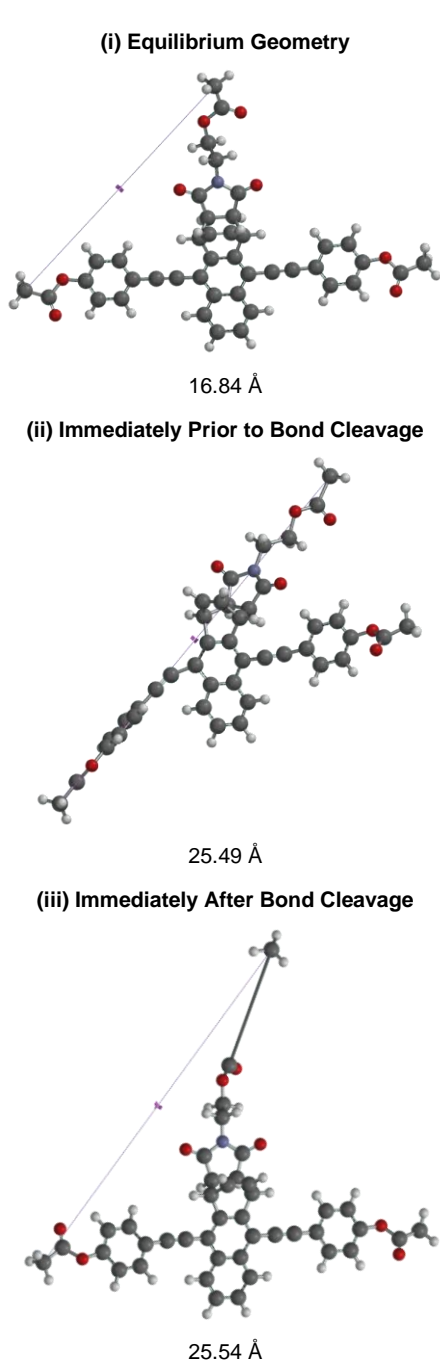
#### (iii) Immediately After Bond Cleavage

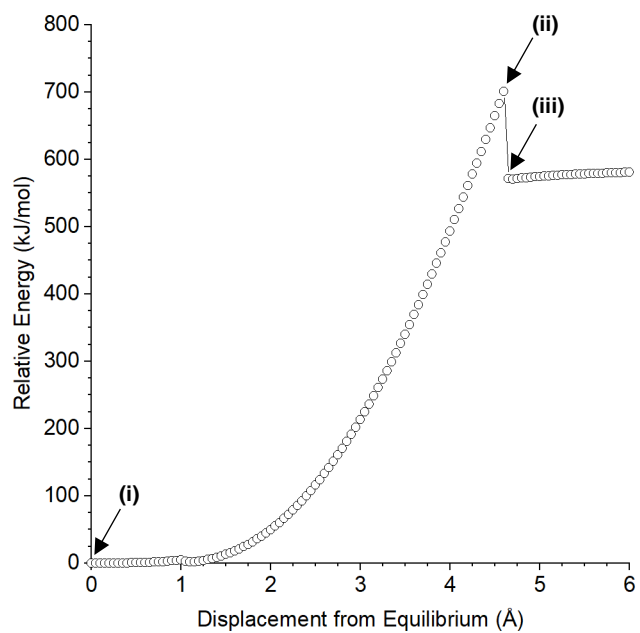
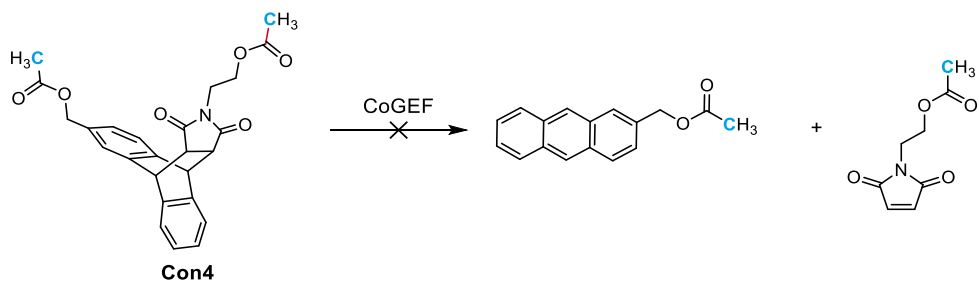




**Summary of CoGEF Results**

$F_{max}$	6.0 nN
$E_{max}$	843 kJ/mol
Force-Bond Angle	29°

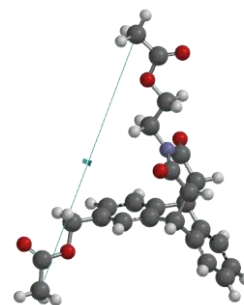




**Summary of CoGEF Results**

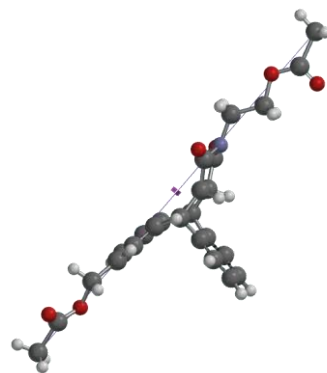
$F_{max}$	6.0 nN
$E_{max}$	832 kJ/mol
<b>Force-Bond Angle</b>	15°

**(i) Equilibrium Geometry**



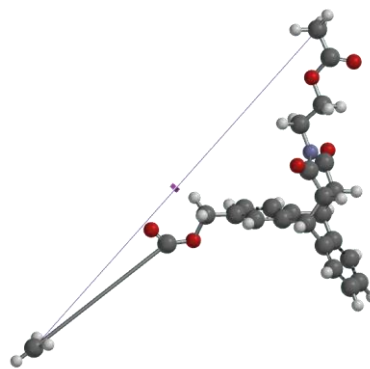
16.321 Å

**(ii) Immediately Prior to Bond Cleavage**

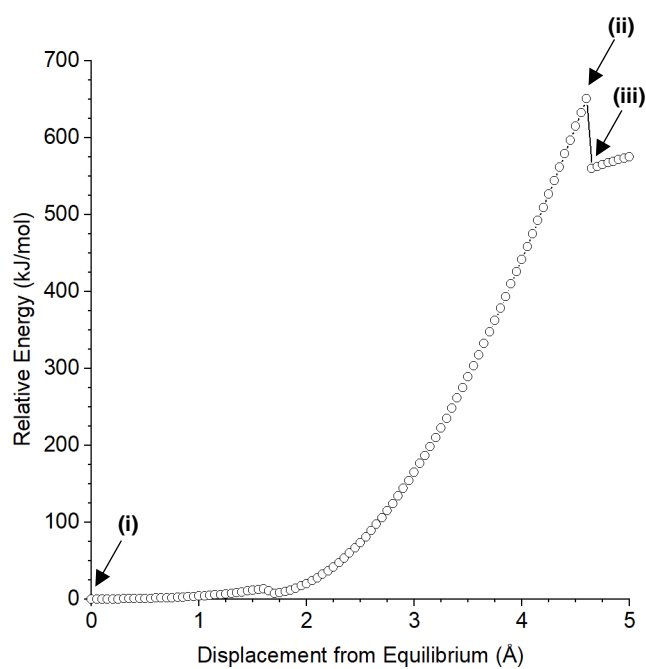
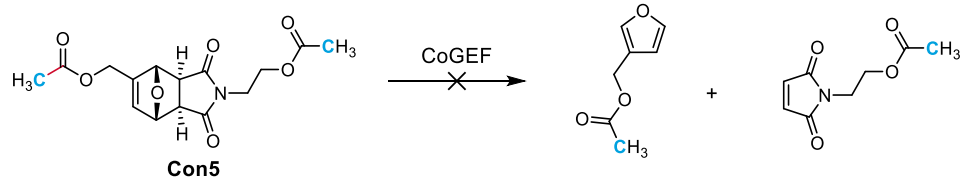


20.821 Å

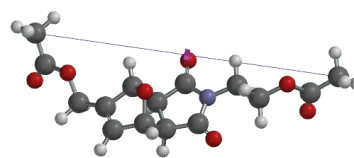
**(iii) Immediately After Bond Cleavage**



20.871 Å

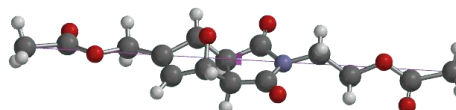


**(i) Equilibrium Geometry**



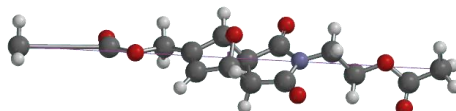
13.761 Å

**(ii) Immediately Prior to Bond Cleavage**



18.361 Å

**(iii) Immediately After Bond Cleavage**

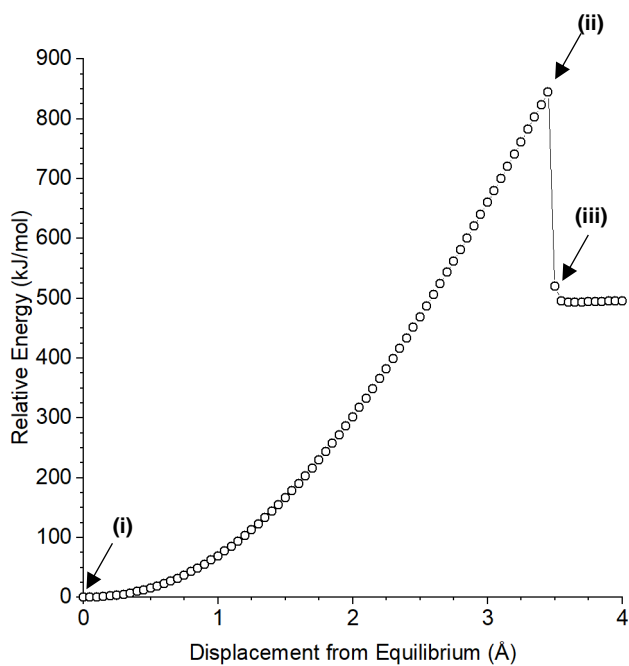
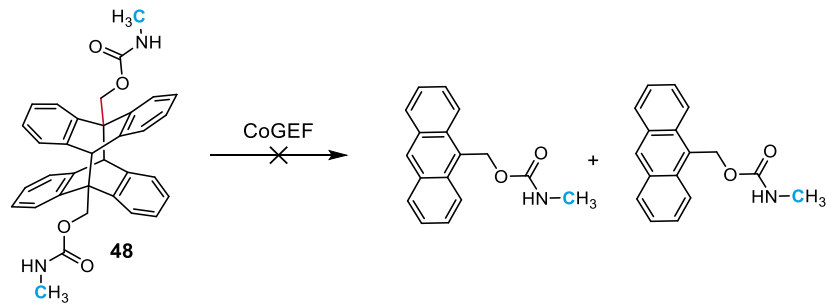


18.411 Å

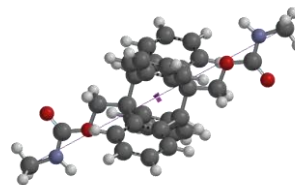
**Summary of CoGEF Results**

$F_{max}$	6.0 nN
$E_{max}$	650 kJ/mol
<b>Force-Bond Angle</b>	39°



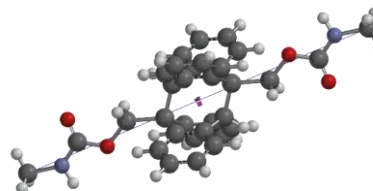


(i) Equilibrium Geometry



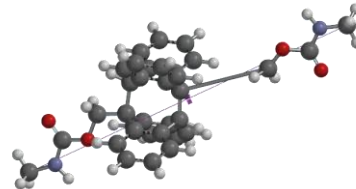
15.288 Å

(ii) Immediately Prior to Bond Cleavage



18.738 Å

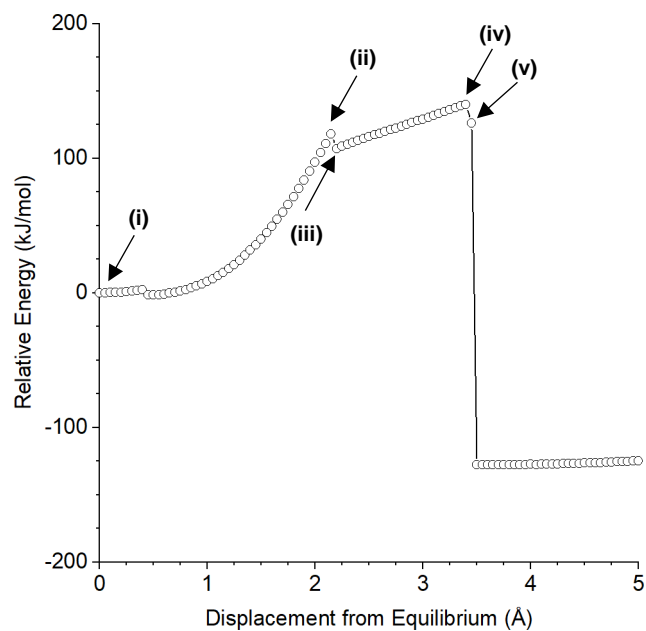
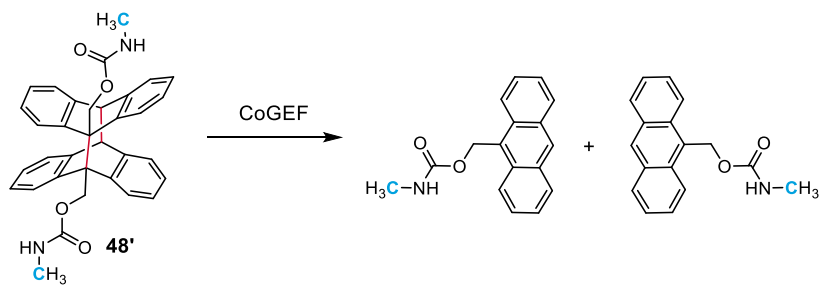
(iii) Immediately After Bond Cleavage



18.788 Å

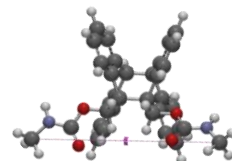
**Summary of CoGEF Results**

$F_{max}$	6.9 nN
$E_{max}$	844 kJ/mol
<b>Force-Bond Angle</b>	53°



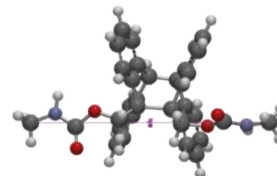
Summary of CoGEF Results	
$F_{max}$	2.3 nN
$E_{max}$	140 kJ/mol
Force-Bond Angle	5.7°

(i) Equilibrium Geometry



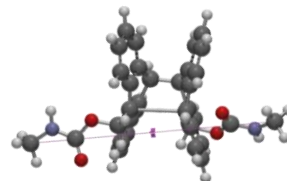
11.492 Å

(ii) Immediately Prior to First Bond Cleavage



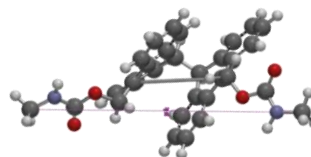
13.642 Å

(iii) Immediately After First Bond Cleavage



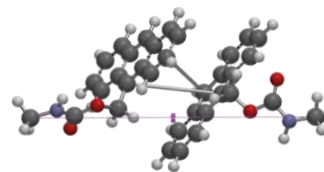
13.692 Å

(iv) Immediately Prior to Second Bond Cleavage

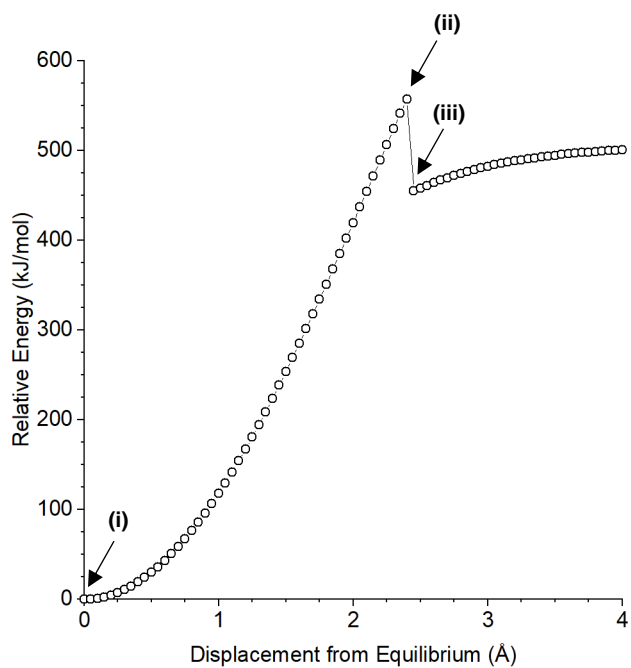
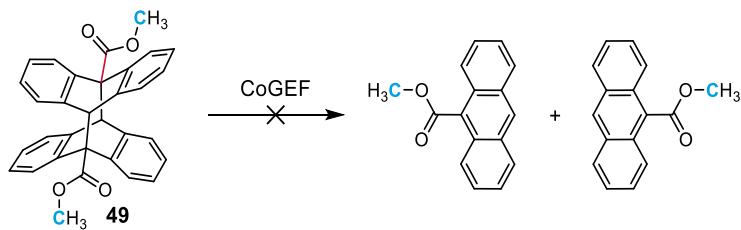


14.892 Å

(v) Immediately After Second Bond Cleavage



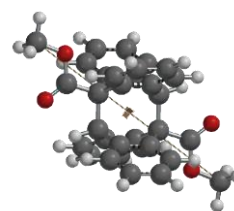
14.942 Å



**Summary of CoGEF Results**

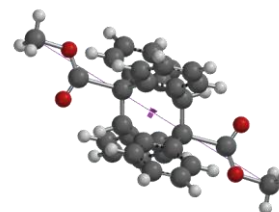
$F_{max}$	5.8 nN
$E_{max}$	557 kJ/mol
<b>Force-Bond Angle</b>	57.8°

**(i) Equilibrium Geometry**



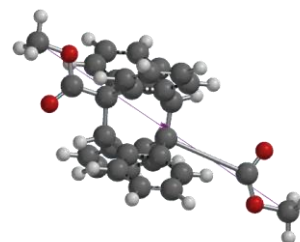
10.728 Å

**(ii) Immediately Prior to Bond Cleavage**

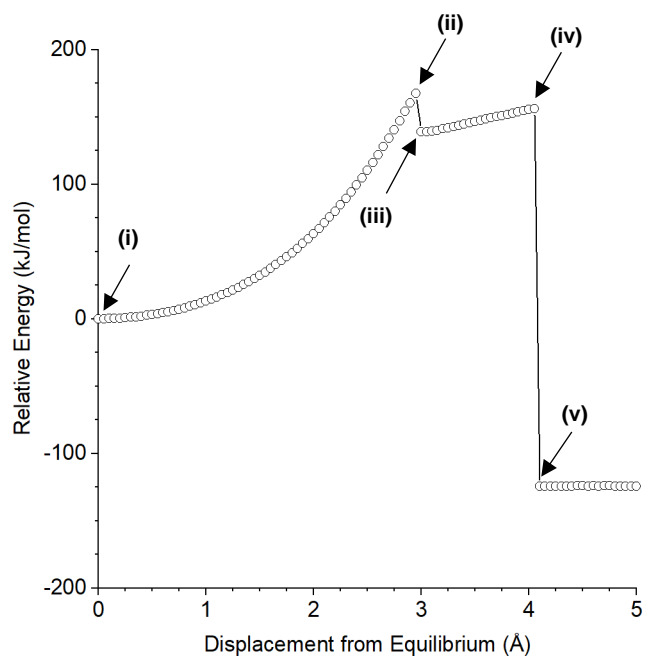
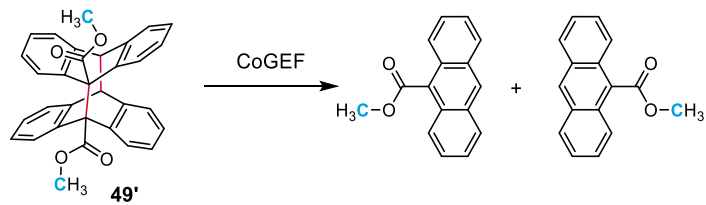


13.128 Å

**(iii) Immediately After Bond Cleavage**



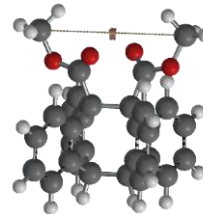
13.178 Å



#### Summary of CoGEF Results

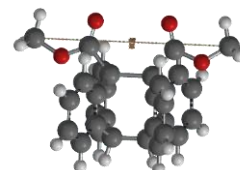
$F_{max}$	2.2 nN
$E_{max}$	167 kJ/mol
Force-Bond Angle	0.5°

#### (i) Equilibrium Geometry



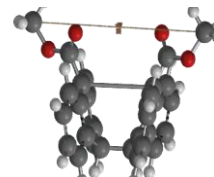
6.033 Å

#### (ii) Immediately Prior to First Bond Cleavage



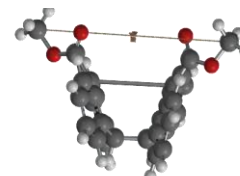
8.983 Å

#### (iii) Immediately After First Bond Cleavage



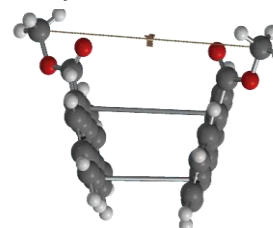
9.033 Å

#### (iv) Immediately Prior to Second Bond Cleavage

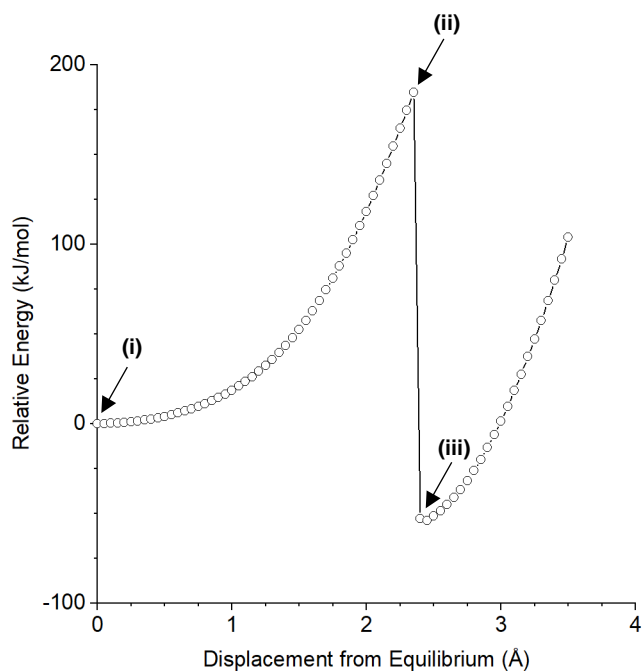
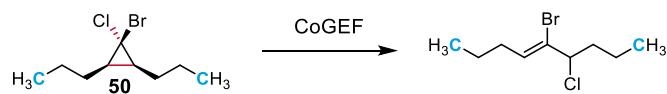


10.083 Å

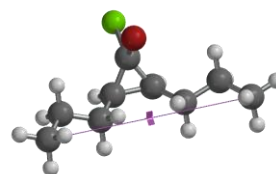
#### (v) Immediately After Second Bond Cleavage



10.133 Å

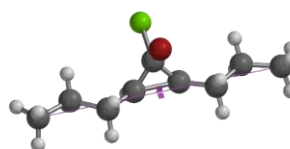


(i) Equilibrium Geometry



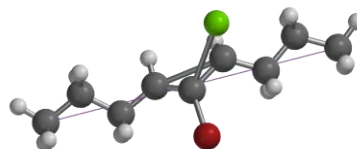
7.809 Å

(ii) Immediately Prior to Bond Cleavage



10.359 Å

(iii) Immediately After Bond Cleavage



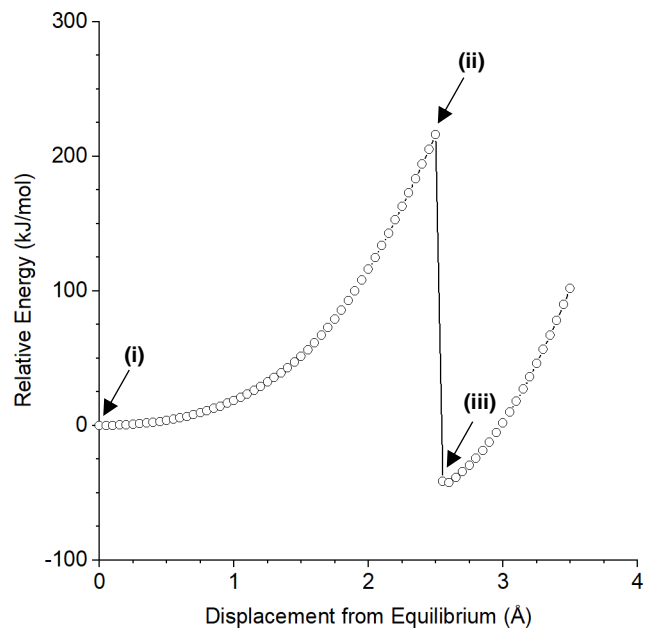
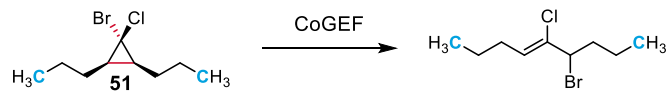
10.359 Å

**Summary of CoGEF Results**

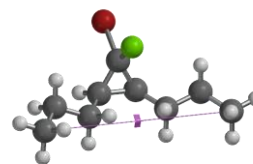
$F_{max}$  3.6 nN

$E_{max}$  216 kJ/mol

Force-Bond Angle 0.1°

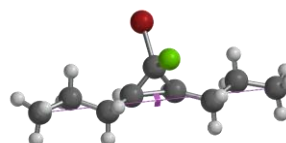


(i) Equilibrium Geometry



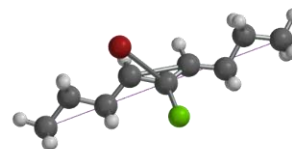
7.824 Å

(ii) Immediately Prior to Bond Cleavage



10.174 Å

(iii) Immediately After Bond Cleavage



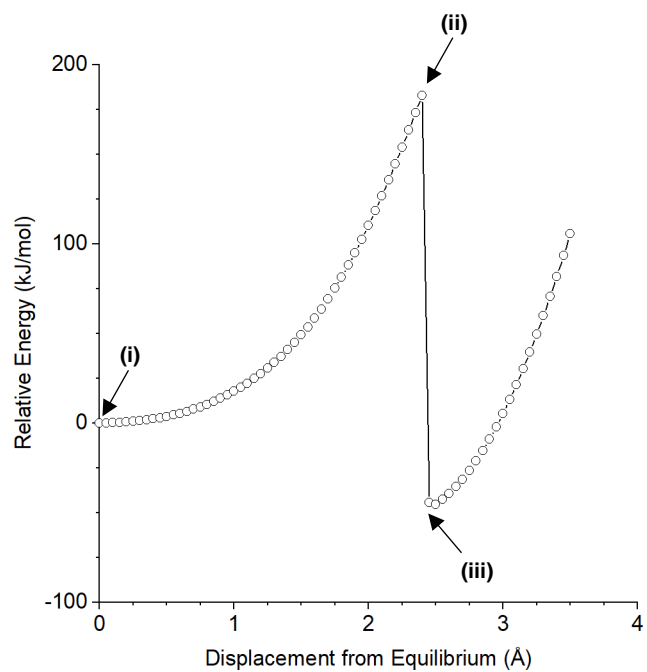
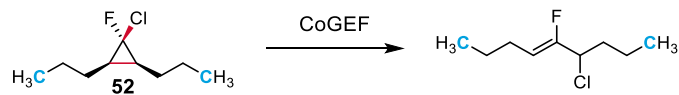
10.224 Å

**Summary of CoGEF Results**

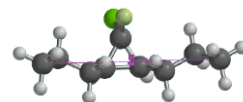
$F_{max}$  3.3 nN

$E_{max}$  184 kJ/mol

Force-Bond Angle 0.1°

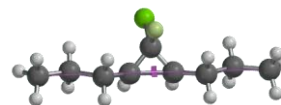


**(i) Equilibrium Geometry**



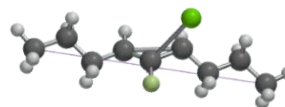
7.776 Å

**(ii) Immediately Prior to Bond Cleavage**



10.176 Å

**(iii) Immediately After Bond Cleavage**



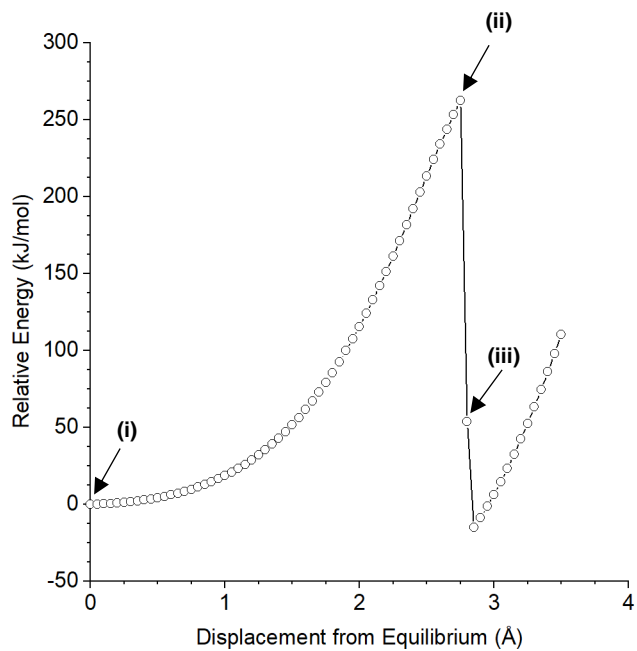
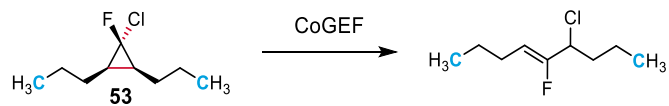
10.226 Å

**Summary of CoGEF Results**

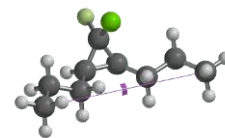
$F_{max}$  3.5 nN

$E_{max}$  262 kJ/mol

**Force-Bond Angle** 0.0°

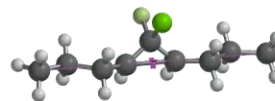


(i) Equilibrium Geometry



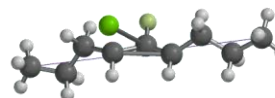
7.816 Å

(ii) Immediately Prior to Bond Cleavage



10.566 Å

(iii) Immediately After Bond Cleavage



10.616 Å

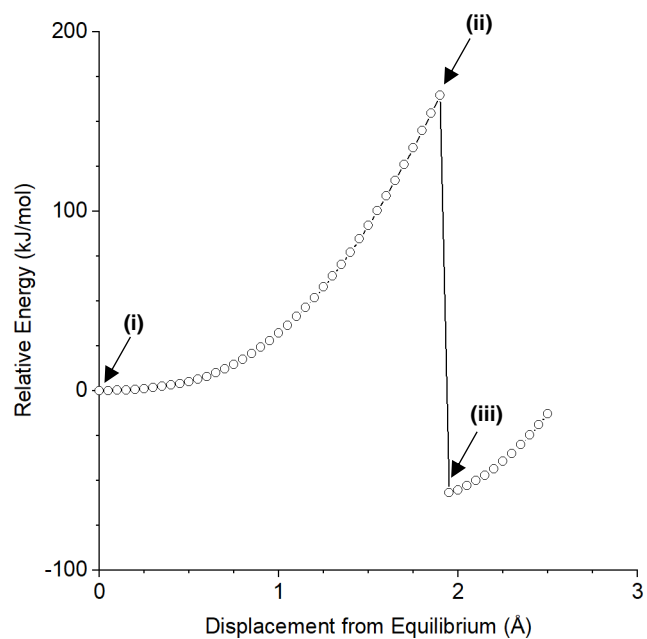
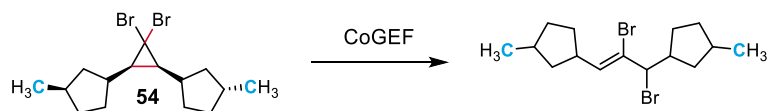
**Summary of CoGEF Results**

$F_{max}$  3.2 nN

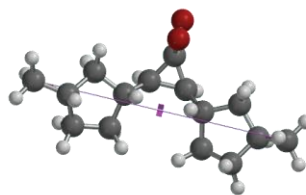
$E_{max}$  183 kJ/mol

**Force-Bond Angle** 0.1°



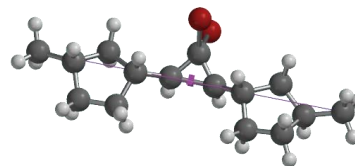


(i) Equilibrium Geometry



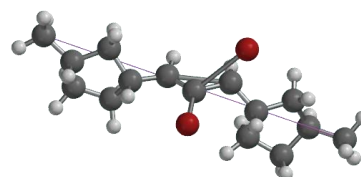
10.675 Å

(ii) Immediately Prior to Bond Cleavage



12.575 Å

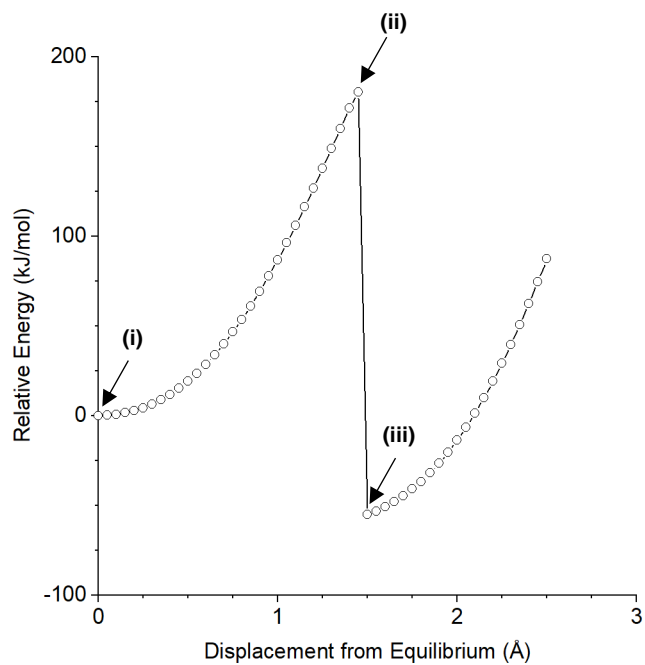
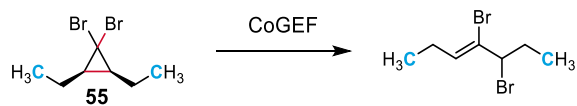
(iii) Immediately After Bond Cleavage



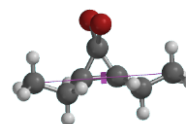
12.625 Å

**Summary of CoGEF Results**

$F_{max}$	3.3 nN
$E_{max}$	164 kJ/mol
<b>Force-Bond Angle</b>	0.3°

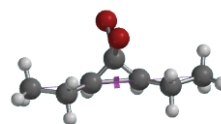


(i) Equilibrium Geometry



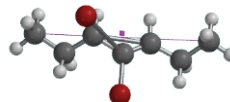
6.081 Å

(ii) Immediately Prior to Bond Cleavage



7.531 Å

(iii) Immediately After Bond Cleavage



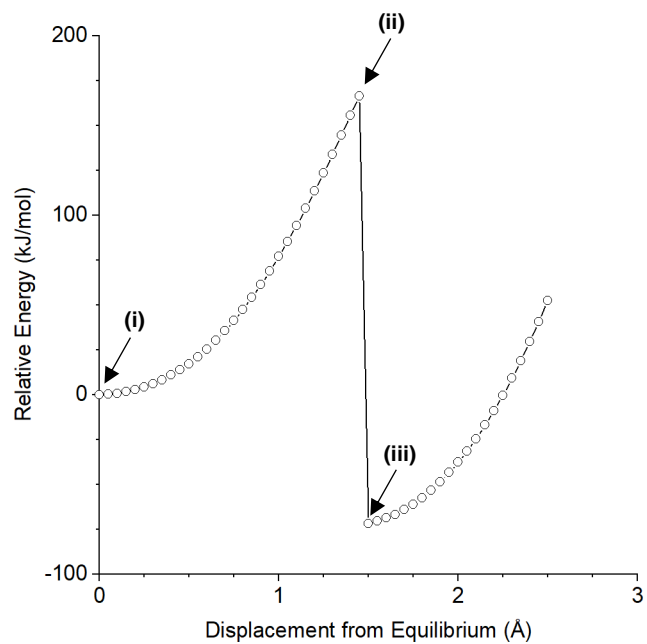
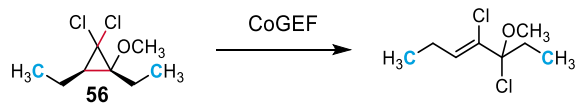
7.581 Å

**Summary of CoGEF Results**

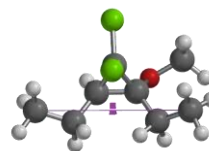
$F_{max}$  3.7 nN

$E_{max}$  180 kJ/mol

Force-Bond Angle 0.1°

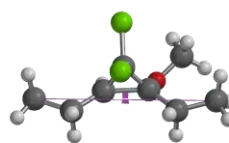


**(i) Equilibrium Geometry**



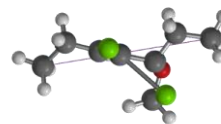
5.971 Å

**(ii) Immediately Prior to Bond Cleavage**



7.421 Å

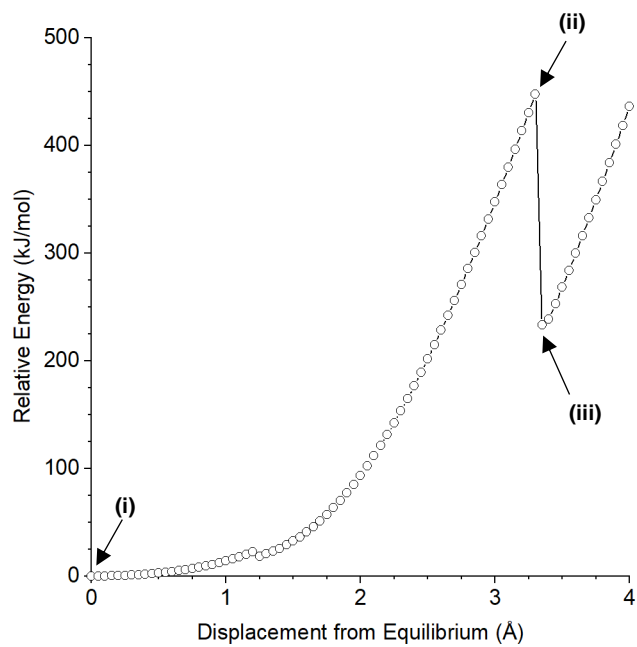
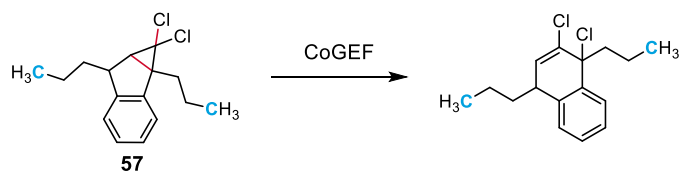
**(iii) Immediately After Bond Cleavage**



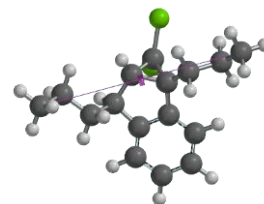
7.471 Å

**Summary of CoGEF Results**

$F_{max}$	3.6 nN
$E_{max}$	166 kJ/mol
<b>Force-Bond Angle</b>	3.8°

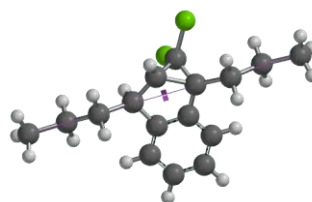


**(i) Equilibrium Geometry**



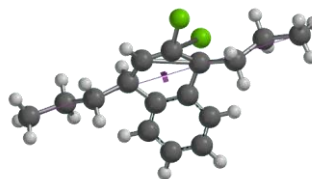
8.972 Å

**(ii) Immediately Prior to Bond Cleavage**



12.272 Å

**(iii) Immediately After Bond Cleavage**



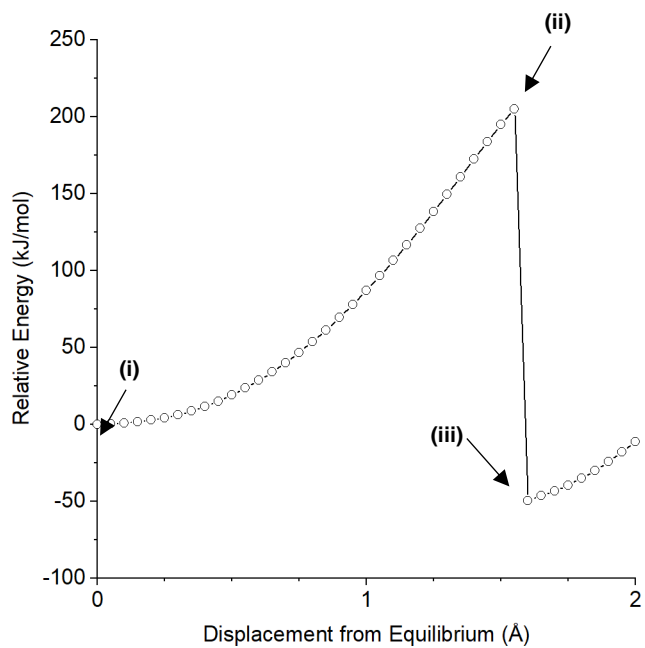
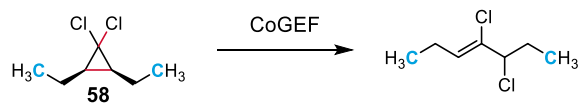
12.322 Å

**Summary of CoGEF Results**

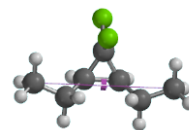
$F_{max}$  5.7 nN

$E_{max}$  448 kJ/mol

**Force-Bond Angle** 31°

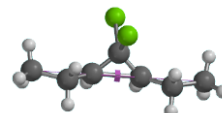


(i) Equilibrium Geometry



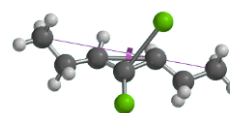
6.079 Å

(ii) Immediately Prior to Bond Cleavage



7.629 Å

(iii) Immediately After Bond Cleavage



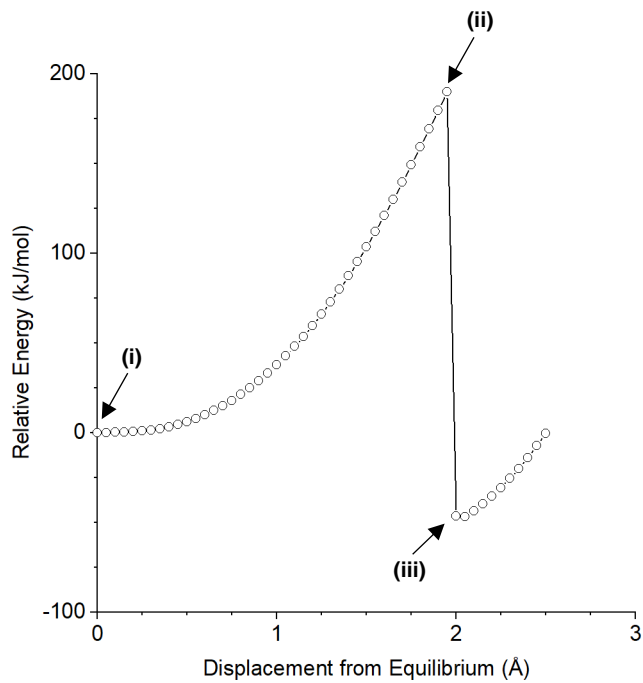
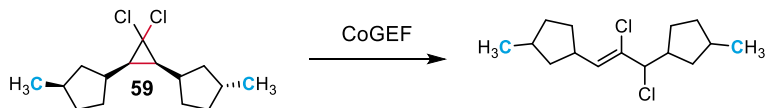
7.679 Å

**Summary of CoGEF Results**

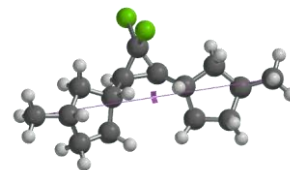
$F_{max}$  3.8 nN

$E_{max}$  205 kJ/mol

**Force-Bond Angle** 0.0°

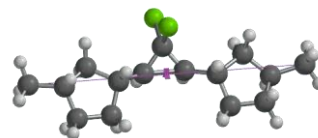


(i) Equilibrium Geometry



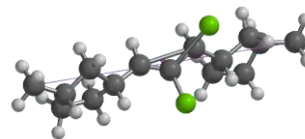
10.746 Å

(ii) Immediately Prior to Bond Cleavage



12.696 Å

(iii) Immediately After Bond Cleavage



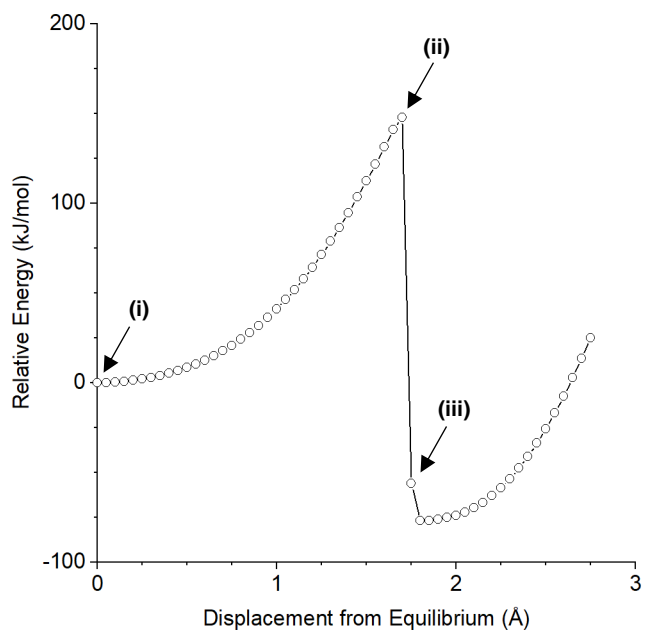
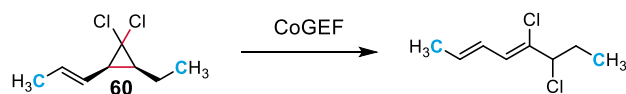
12.746 Å

**Summary of CoGEF Results**

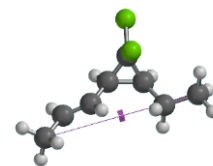
$F_{max}$  3.4 nN

$E_{max}$  190 kJ/mol

Force-Bond Angle 0.4°

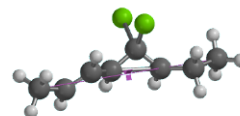


(i) Equilibrium Geometry



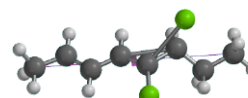
6.904 Å

(ii) Immediately Prior to Bond Cleavage



8.604 Å

(iii) Immediately After Bond Cleavage



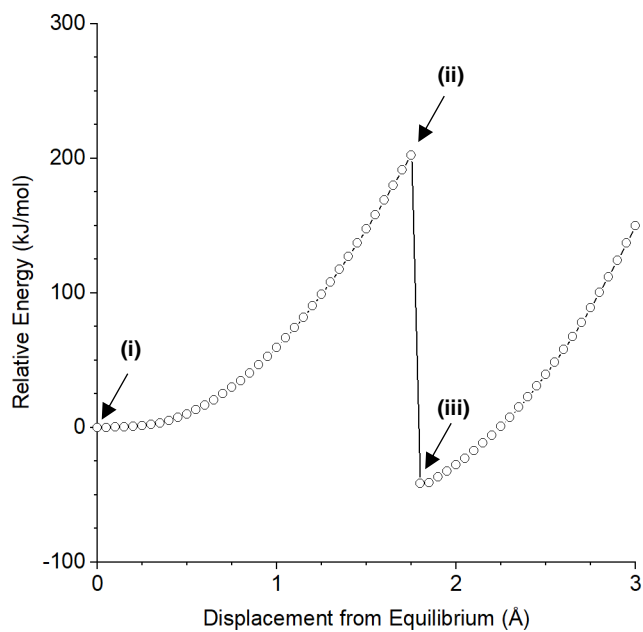
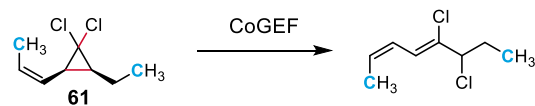
8.654 Å

**Summary of CoGEF Results**

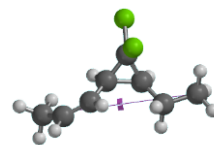
$F_{max}$  3.2 nN

$E_{max}$  148 kJ/mol

Force-Bond Angle 9.0°

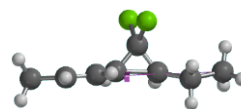


(i) Equilibrium Geometry



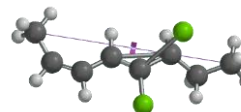
6.787 Å

(ii) Immediately Prior to Bond Cleavage



8.537 Å

(iii) Immediately After Bond Cleavage



8.587 Å

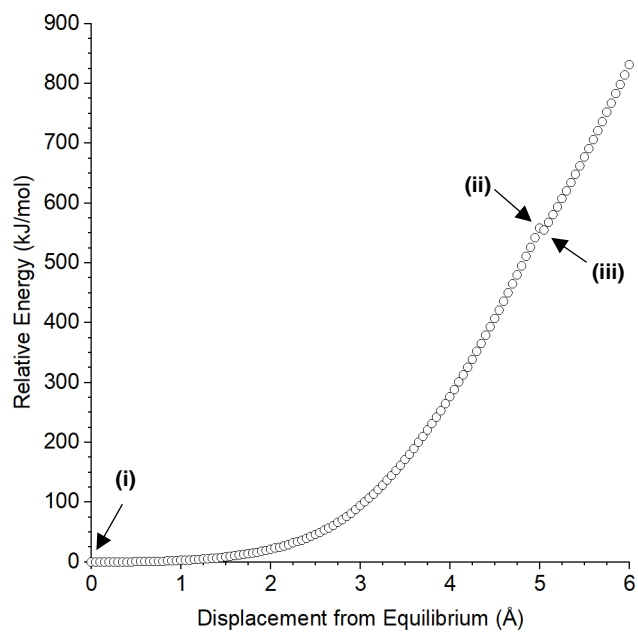
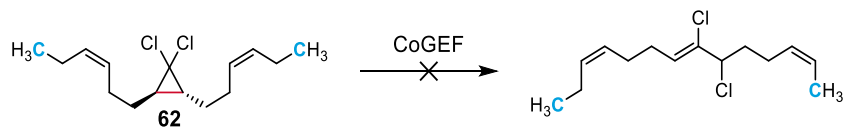
**Summary of CoGEF Results**

$F_{max}$  3.7 nN

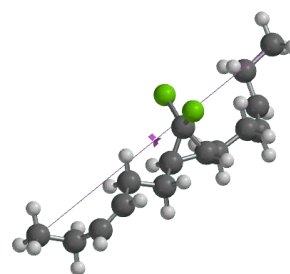
$E_{max}$  202 kJ/mol

Force-Bond Angle 3.9°



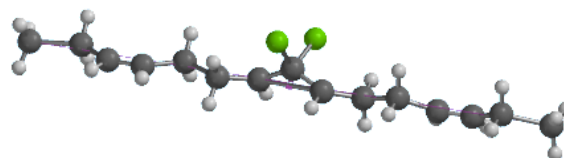


(i) Equilibrium Geometry



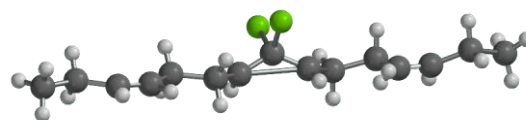
13.974 Å

(ii) Immediately Prior to Bond Cleavage



21.174 Å

(iii) Immediately After Bond Cleavage



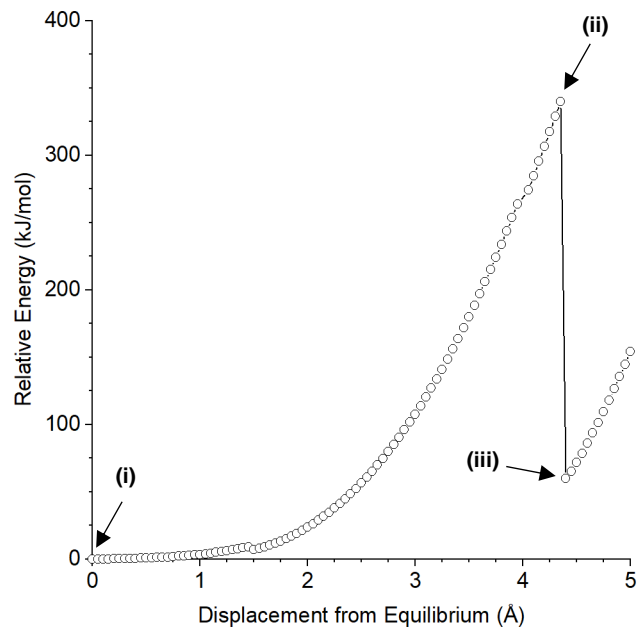
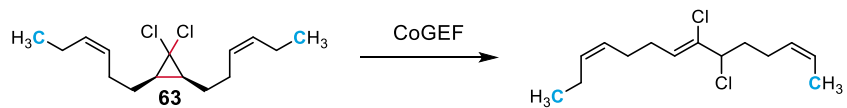
21.224 Å

**Summary of CoGEF Results**

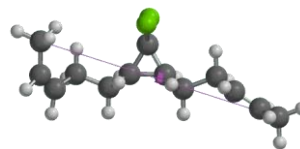
$F_{max}$  5.2 nN

$E_{max}$  557 kJ/mol

Force-Bond Angle 20°

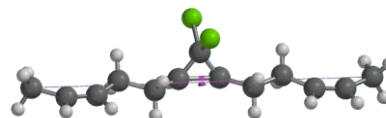


**(i) Equilibrium Geometry**



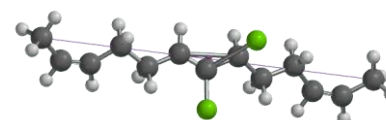
11.037 Å

**(i) Immediately Prior to Bond Cleavage**



15.337 Å

**(ii) Immediately After Bond Cleavage**



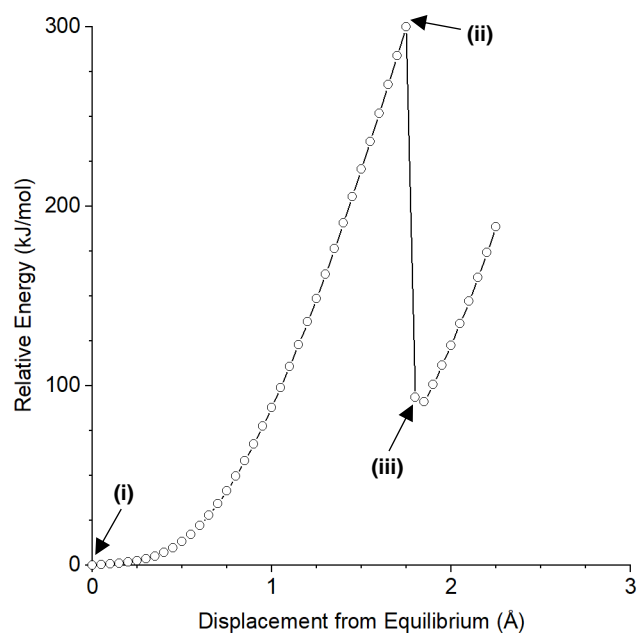
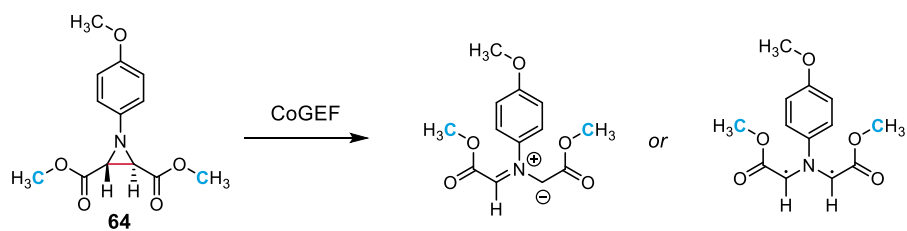
15.387 Å

**Summary of CoGEF Results**

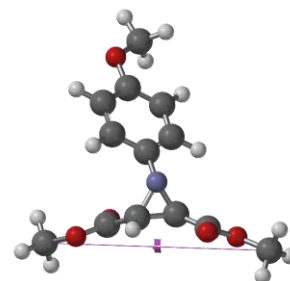
$F_{max}$  3.8 nN

$E_{max}$  340 kJ/mol

Force/Bond angle 0.1°

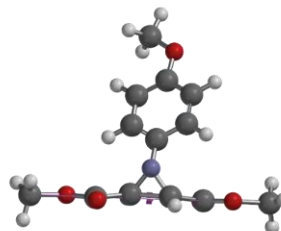


(i) Equilibrium Geometry



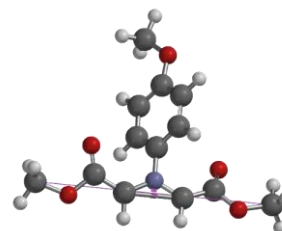
8.232 Å

(ii) Immediately Prior to Bond Cleavage



9.982 Å

(iii) Immediately After Bond Cleavage

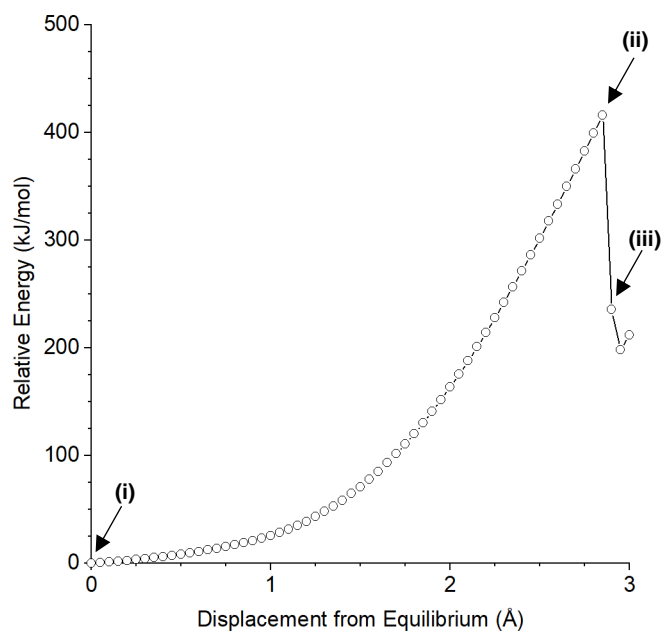
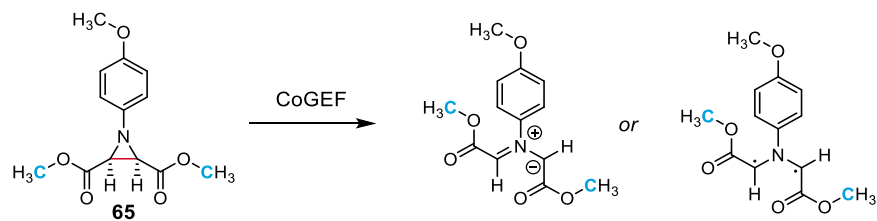


10.032 Å

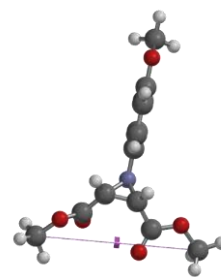
**Summary of CoGEF Results**

$F_{max}$  5.4 nN  
 $E_{max}$  300 kJ/mol

**Force-Bond Angle** 22°

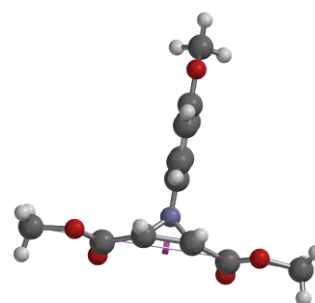


(i) Equilibrium Geometry



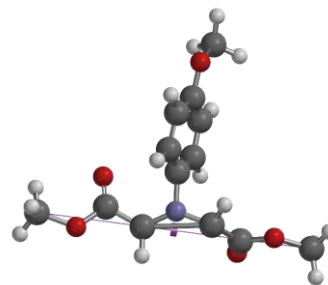
7.37 Å

(ii) Immediately Prior to Bond Cleavage



10.22 Å

(iii) Immediately After Bond Cleavage



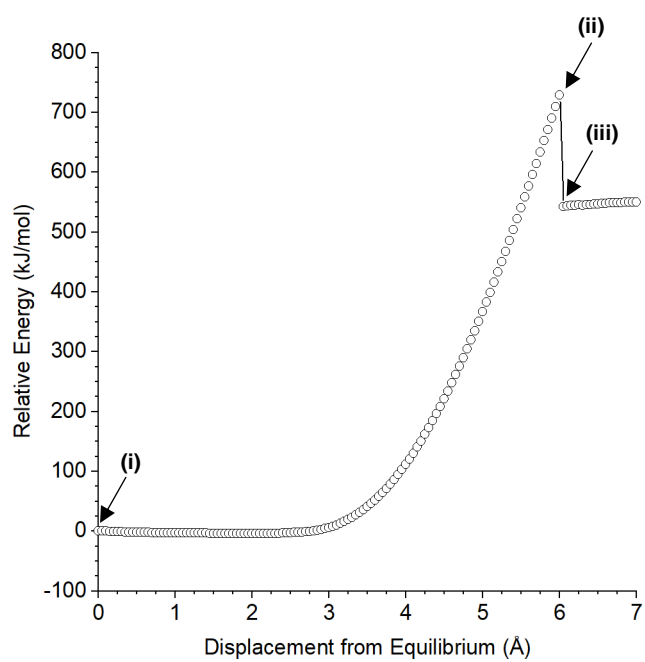
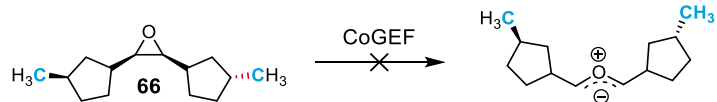
10.27 Å

**Summary of CoGEF Results**

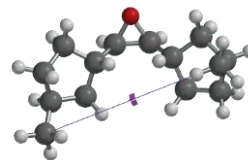
$F_{max}$  5.6 nN

$E_{max}$  416 kJ/mol

Force-Bond Angle 0.1°

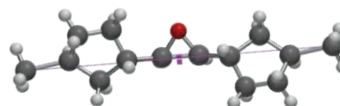


(i) Equilibrium Geometry



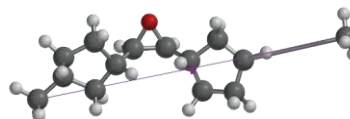
8.113 Å

(ii) Immediately Prior to Bond Cleavage



14.113 Å

(iii) Immediately After Bond Cleavage



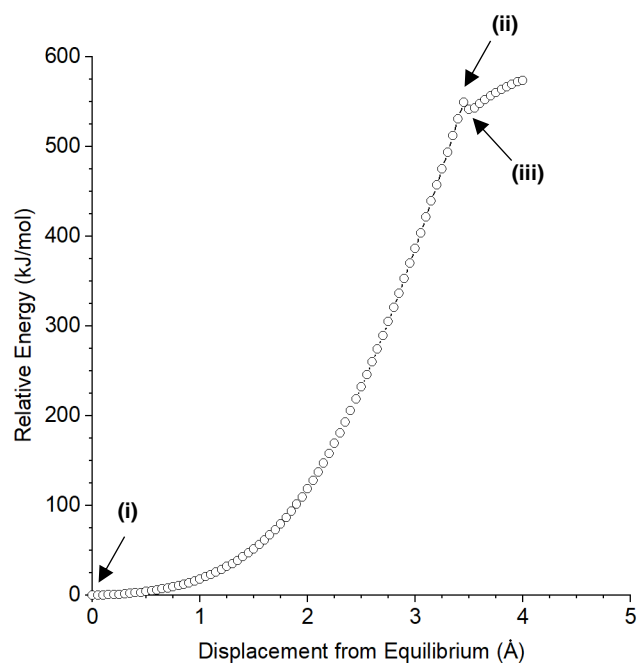
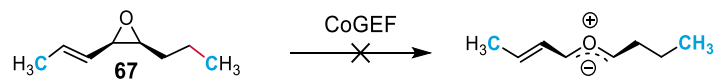
14.163 Å

**Summary of CoGEF Results**

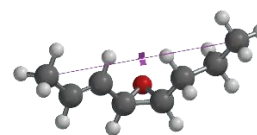
$F_{max}$  6.4 nN

$E_{max}$  729 kJ/mol

Force-Bond Angle 0.8°

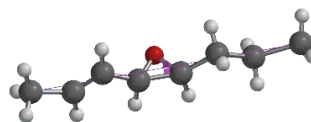


(i) Equilibrium Geometry



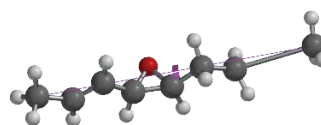
7.555 Å

(ii) Immediately Prior to Bond Cleavage



11.005 Å

(iii) Immediately After Bond Cleavage



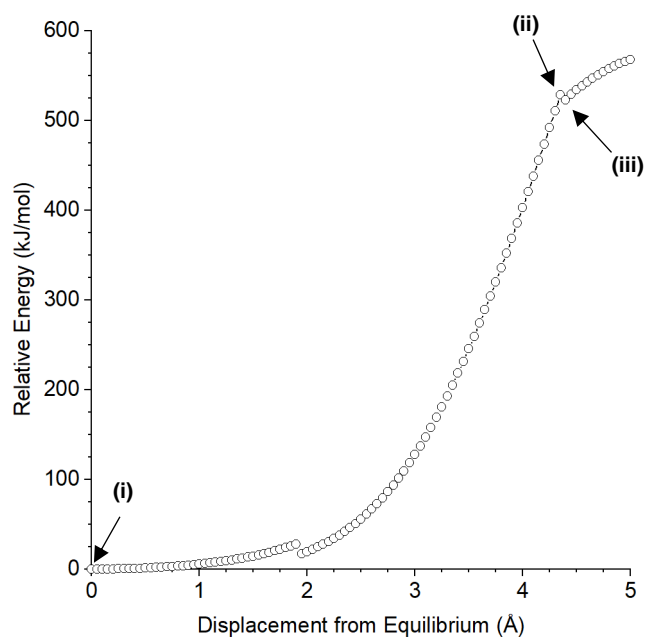
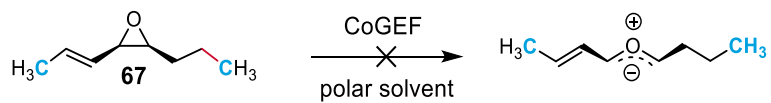
11.055 Å

**Summary of CoGEF Results**

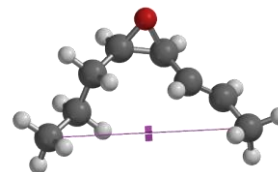
$F_{max}$  6.2 nN

$E_{max}$  549 kJ/mol

Force-Bond Angle 1.5°

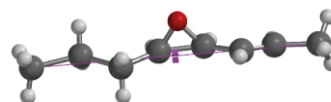


(i) Equilibrium Geometry



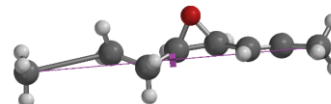
6.606 Å

(ii) Immediately Prior to Bond Cleavage



10.956 Å

(iii) Immediately After Bond Cleavage



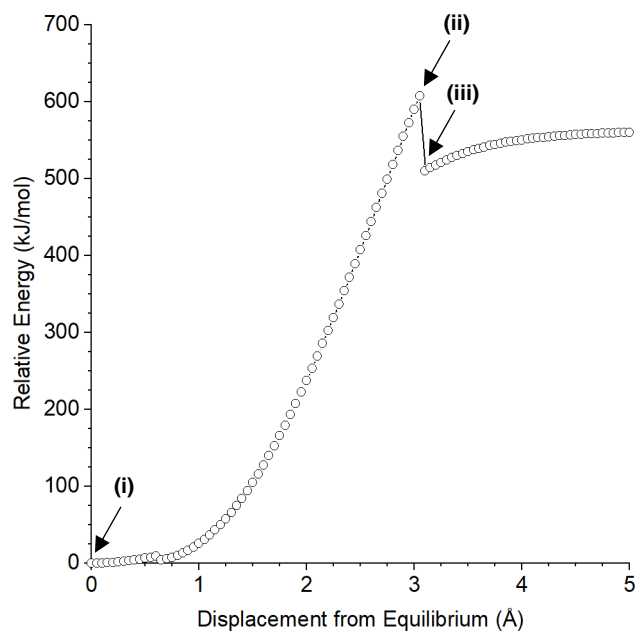
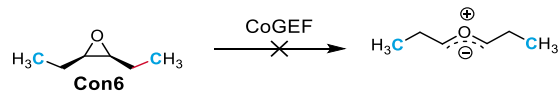
11.006 Å

**Summary of CoGEF Results**

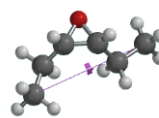
$F_{max}$  6.1 nN

$E_{max}$  529 kJ/mol

Force-Bond Angle 1.6°

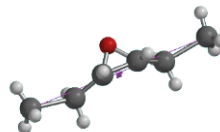


(i) Equilibrium Geometry



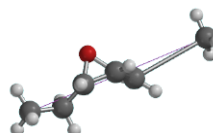
5.523 Å

(ii) Immediately Prior to Bond Cleavage



8.573 Å

(iii) Immediately After Bond Cleavage



8.623 Å

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**Summary of CoGEF Results**

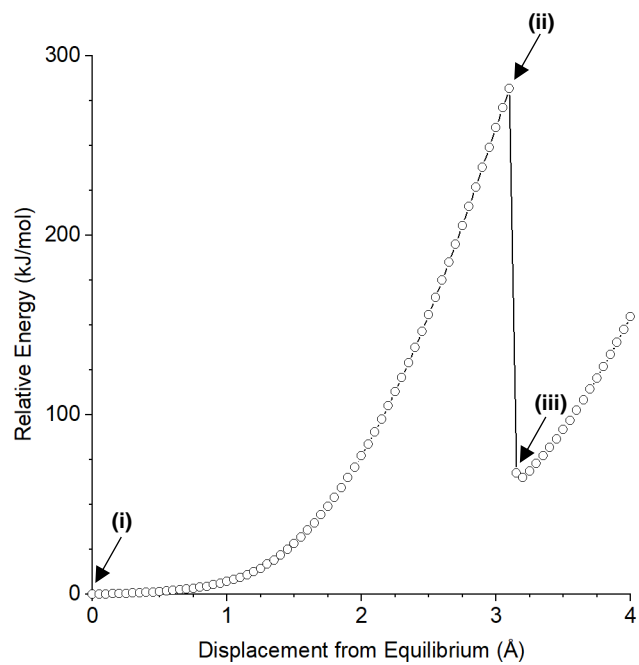
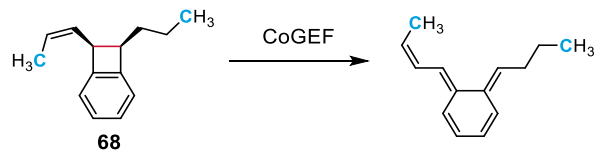
---

$F_{max}$  6.2 nN

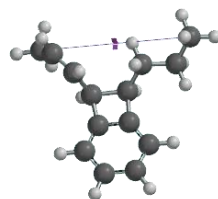
$E_{max}$  607 kJ/mol

**Force-Bond Angle** 0.0°



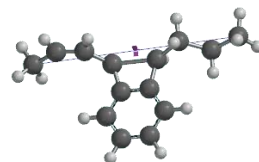


(i) Equilibrium Geometry



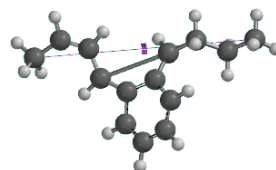
7.067 Å

(ii) Immediately Prior to Bond Cleavage



10.167 Å

(iii) Immediately After Bond Cleavage



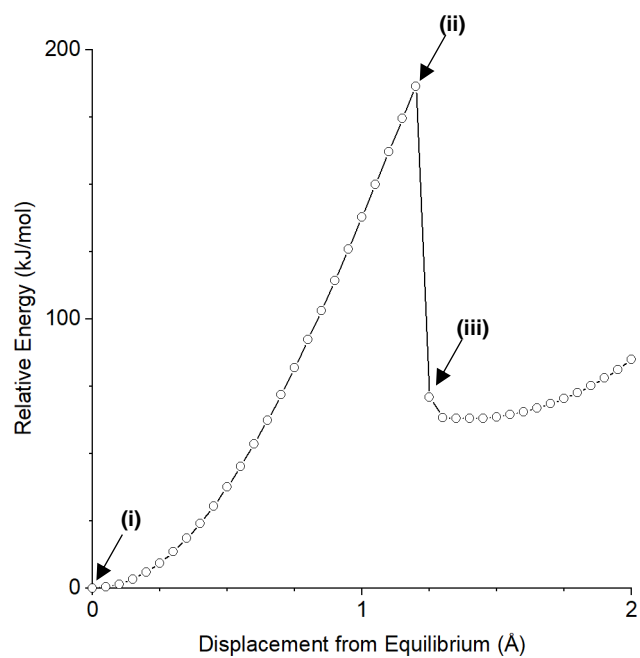
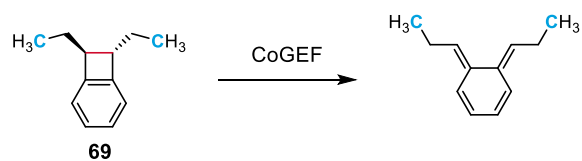
10.217 Å

**Summary of CoGEF Results**

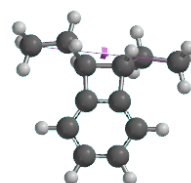
$F_{max}$  3.7 nN

$E_{max}$  282 kJ/mol

Force/Bond angle 3.2°

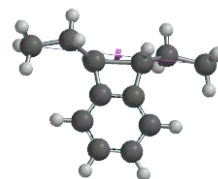


**(i) Equilibrium Geometry**



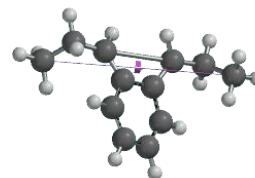
6.463 Å

**(ii) Immediately Prior to Bond Cleavage**



7.663 Å

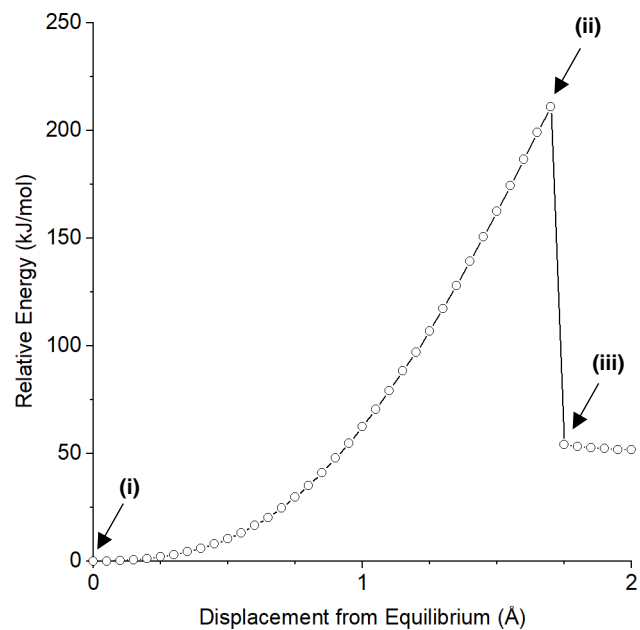
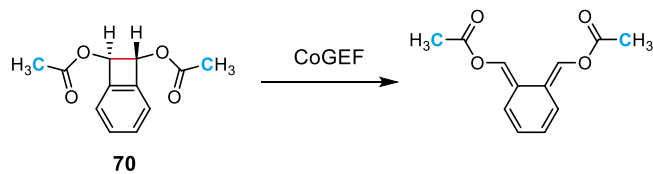
**(iii) Immediately After Bond Cleavage**



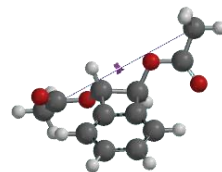
7.713 Å

**Summary of CoGEF Results**

$F_{max}$	4.1 nN
$E_{max}$	186 kJ/mol
Force/Bond angle	17°

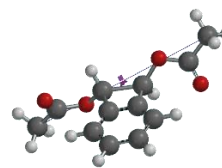


**(i) Equilibrium Geometry**



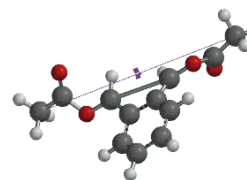
7.936 Å

**(ii) Immediately Prior to Bond Cleavage**



9.636 Å

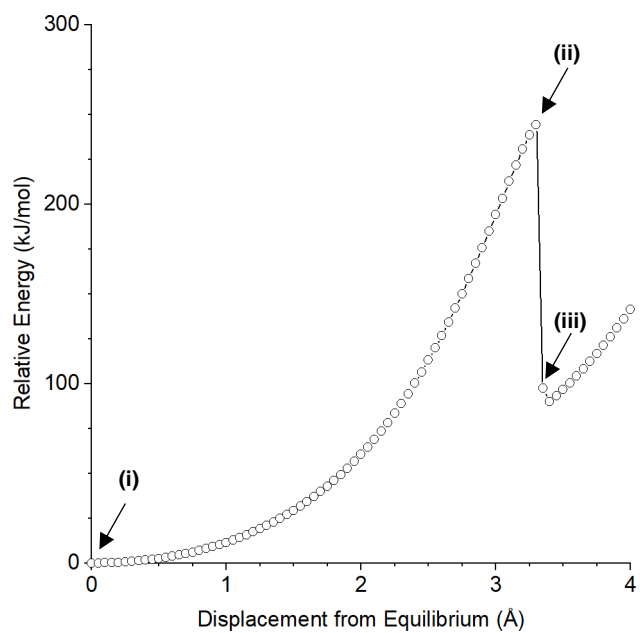
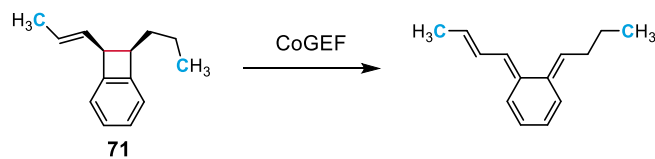
**(iii) Immediately After Bond Cleavage**



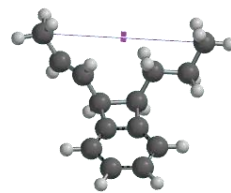
9.686 Å

**Summary of CoGEF Results**

$F_{max}$	4.1 nN
$E_{max}$	211 kJ/mol
<b>Force-Bond Angle</b>	25°

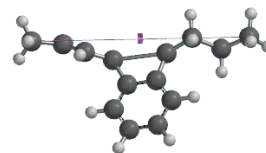


(i) Equilibrium Geometry



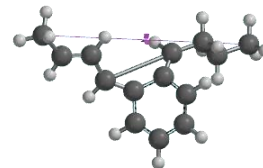
7.011 Å

(ii) Immediately Prior to Bond Cleavage



10.161 Å

(iii) Immediately After Bond Cleavage



10.211 Å

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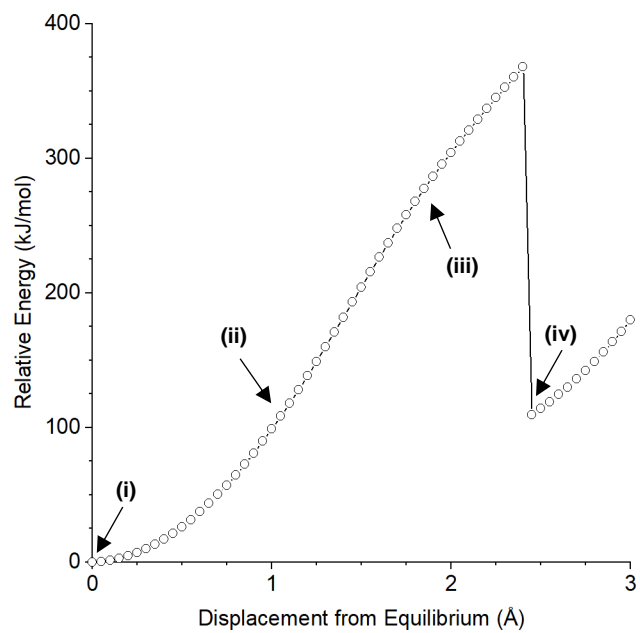
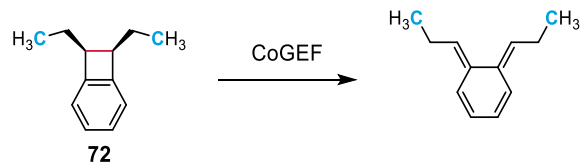
**Summary of CoGEF Results**

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$F_{max}$  3.1 nN

$E_{max}$  244 kJ/mol

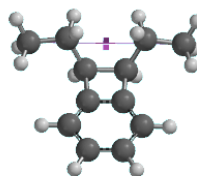
**Force-Bond Angle** 2.8°



**Summary of CoGEF Results**

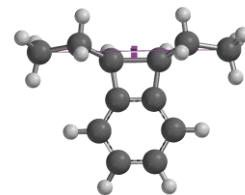
$F_{max}$	3.7 nN
$E_{max}$	367 kJ/mol
Force/Bond angle	0.0°

**(i) Equilibrium Geometry**



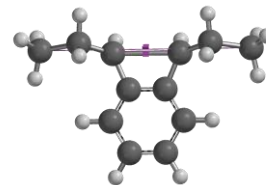
6.123 Å

**(ii) Prior to Bond Cleavage**



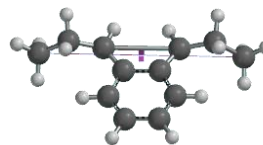
7.273 Å

**(iii) After Bond Cleavage**

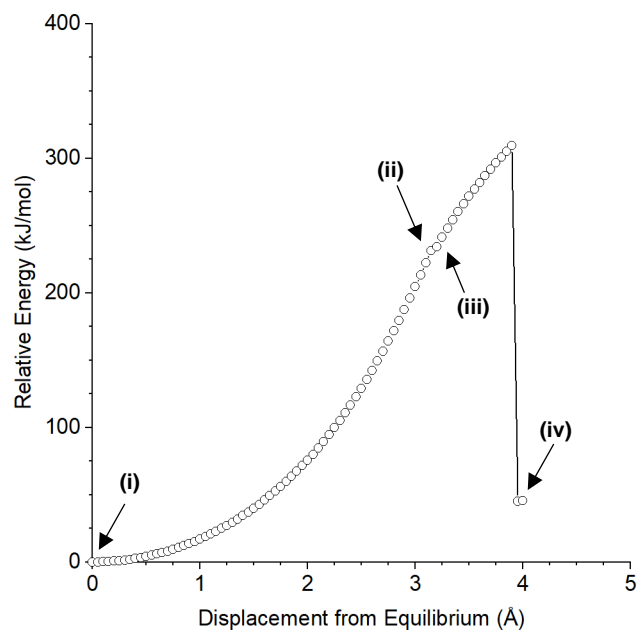
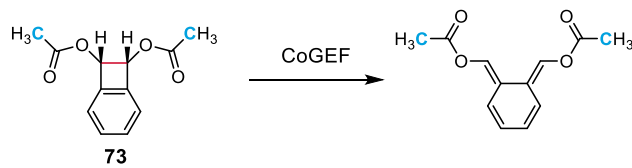


8.123

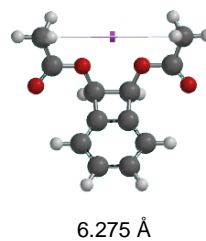
**(iv) After Formation of Double Bonds**



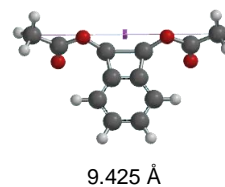
8.573 Å



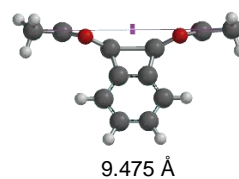
**(i) Equilibrium Geometry**



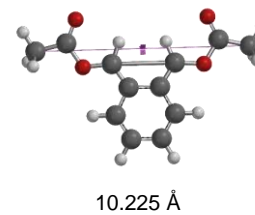
**(ii) Immediately Prior to Bond Cleavage**



**(iii) Immediately After Bond Cleavage**



**(iv) After Formation of Double Bonds**

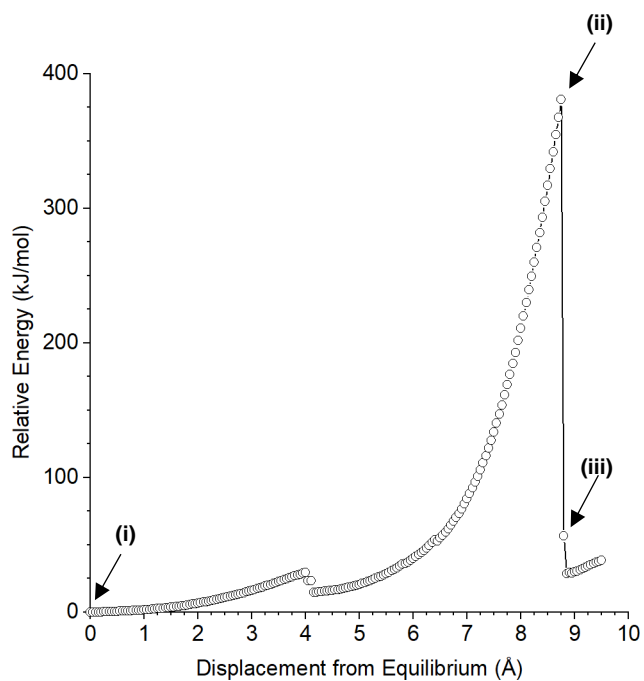
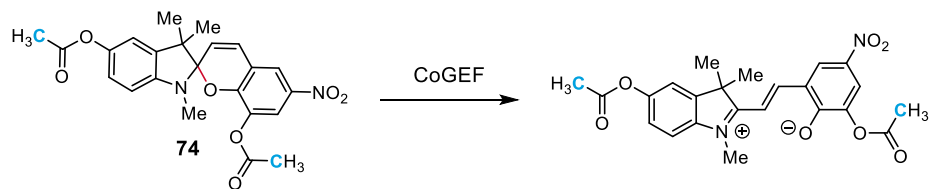


**Summary of CoGEF Results**

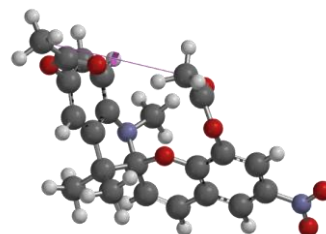
$F_{max}$  3.0 nN

$E_{max}$  310 kJ/mol

Force-Bond Angle 0.0°

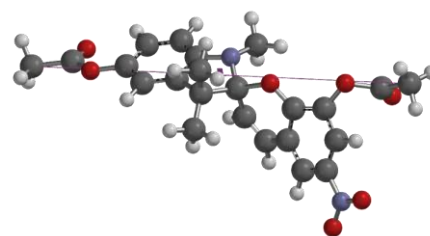


(i) Equilibrium Geometry



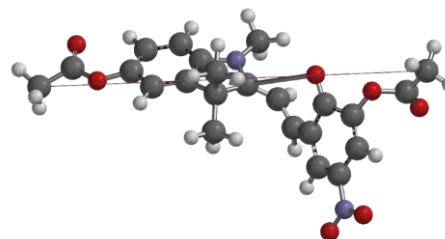
6.048 Å

(ii) Immediately Prior to Bond Cleavage



16.648 Å

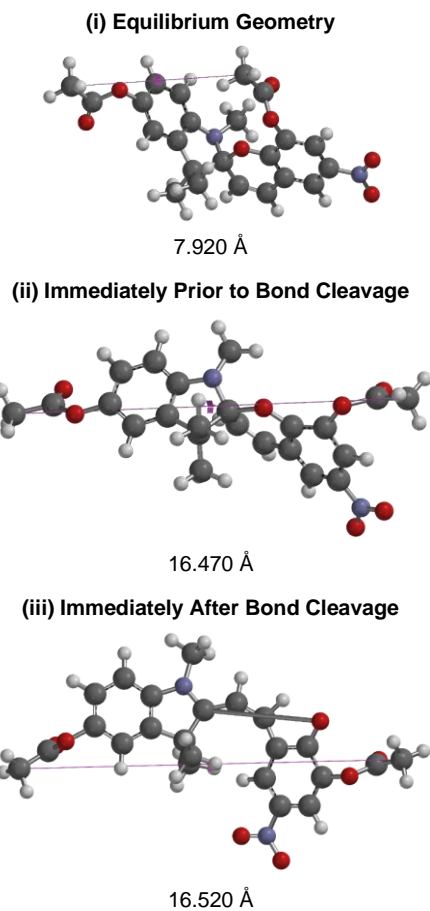
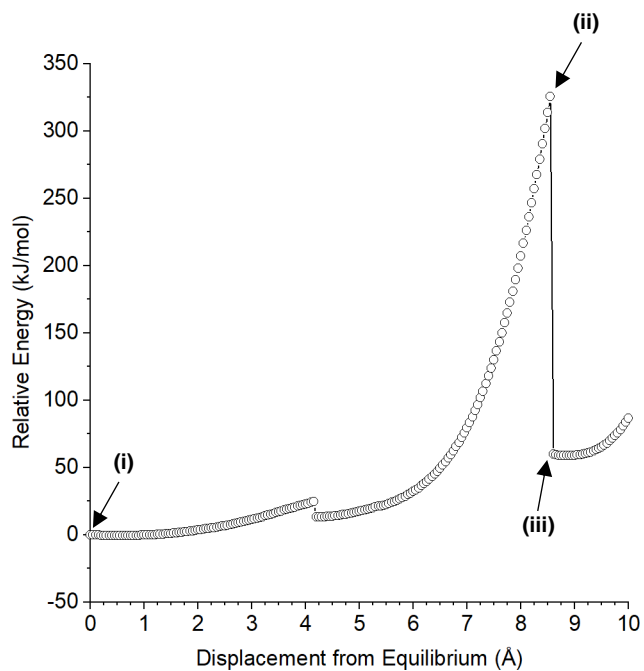
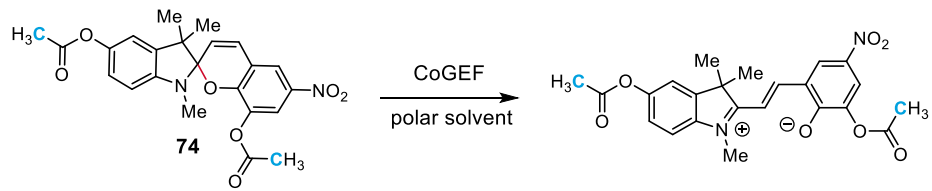
(iii) Immediately After Bond Cleavage



16.698 Å

**Summary of CoGEF Results**

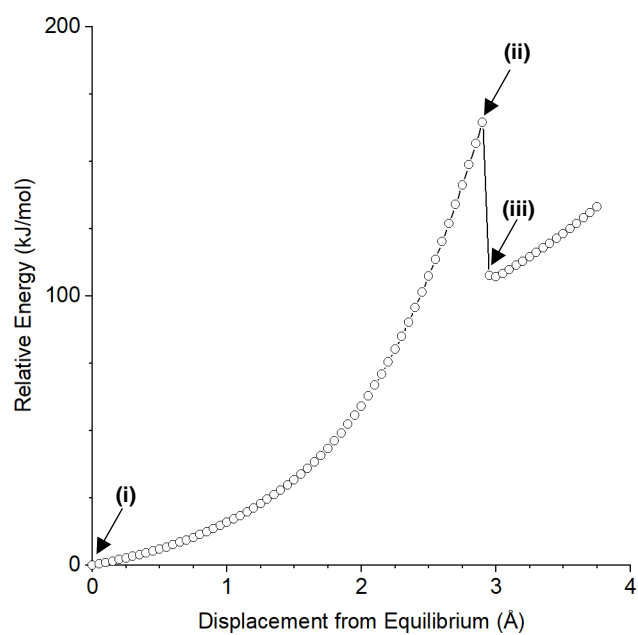
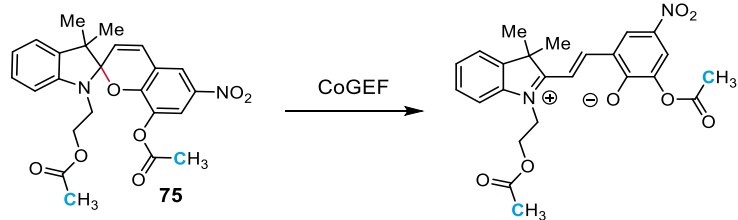
$F_{max}$	4.4 nN
$E_{max}$	381 kJ/mol
<b>Force-Bond Angle</b>	14°



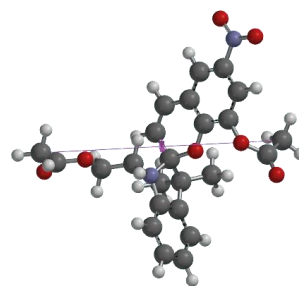
**Summary of CoGEF Results**

$F_{max}$	4.0 nN
$E_{max}$	325 kJ/mol
<b>Force-Bond Angle</b>	14°



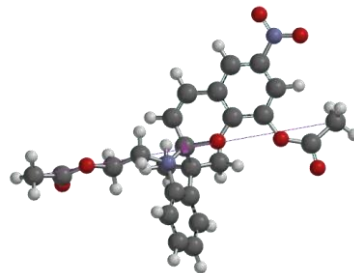


(i) Equilibrium Geometry



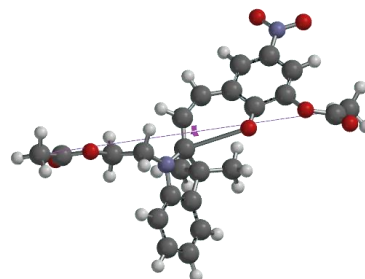
11.600 Å

(ii) Immediately Prior to Bond Cleavage



14.500 Å

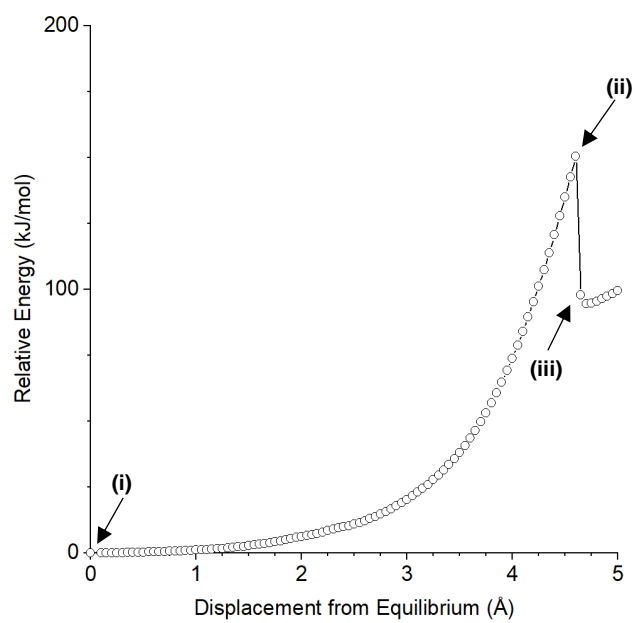
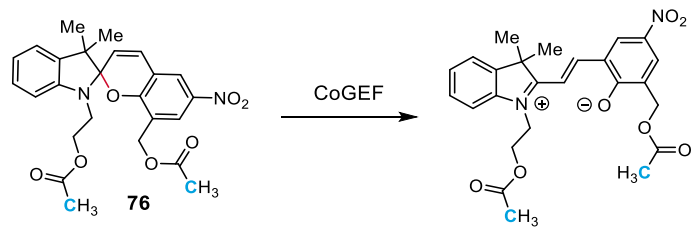
(iii) Immediately After Bond Cleavage



14.550 Å

**Summary of CoGEF Results**

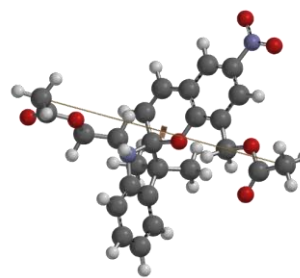
$F_{max}$	2.7 nN
$E_{max}$	165 kJ/mol
Force-Bond Angle	29°



**Summary of CoGEF Results**

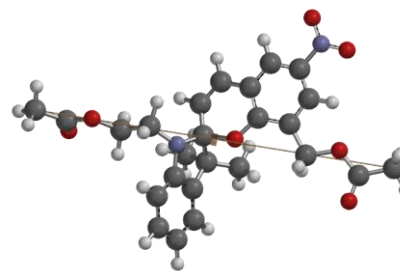
$F_{max}$	2.6 nN
$E_{max}$	150 kJ/mol
Force-Bond Angle	27°

**(i) Equilibrium Geometry**



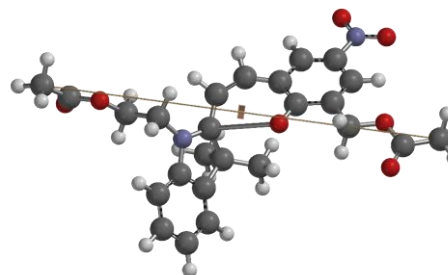
11.322 Å

**(ii) Immediately Prior to Bond Cleavage**

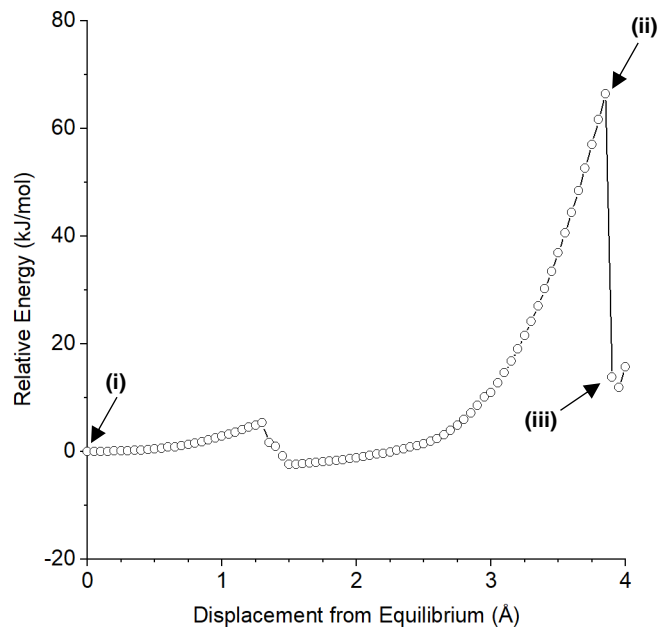
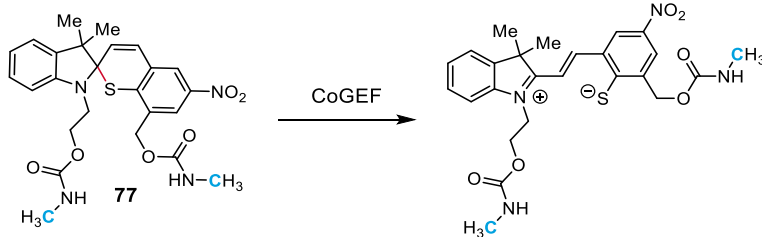


15.922 Å

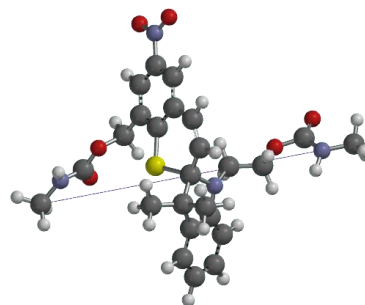
**(iii) Immediately After Bond Cleavage**



15.972 Å

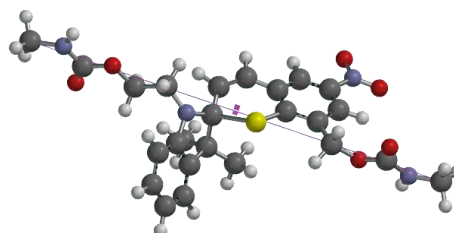


(i) Equilibrium Geometry



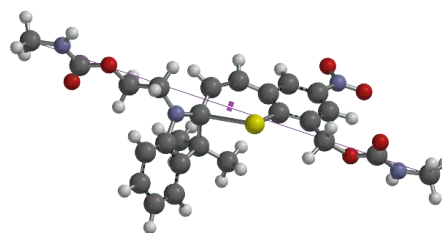
14.303 Å

(ii) Immediately Prior to Bond Cleavage



18.803 Å

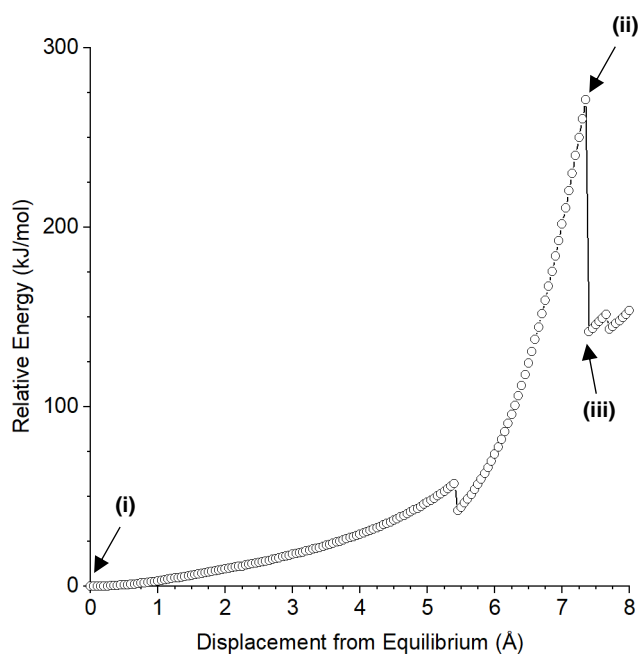
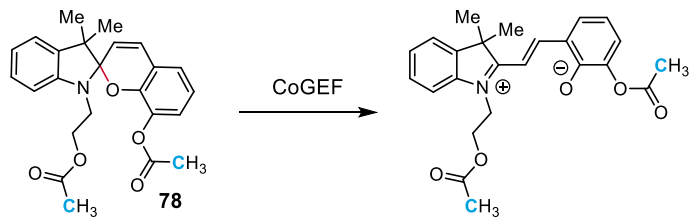
(iii) Immediately After Bond Cleavage



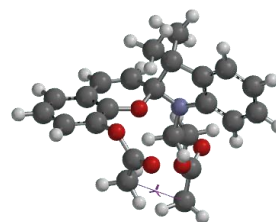
18.853 Å

**Summary of CoGEF Results**

$F_{max}$	2.0 nN
$E_{max}$	74 kJ/mol
Force-Bond Angle	31°

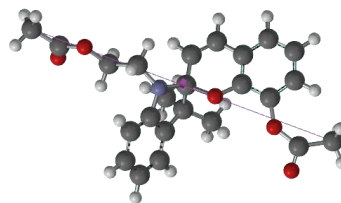


**(i) Equilibrium Geometry**



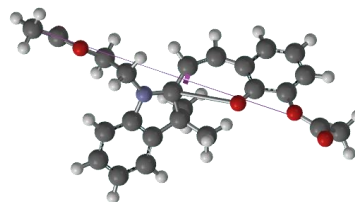
7.625 Å

**(ii) Immediately Prior to Bond Cleavage**



14.975 Å

**(iii) Immediately After Bond Cleavage**



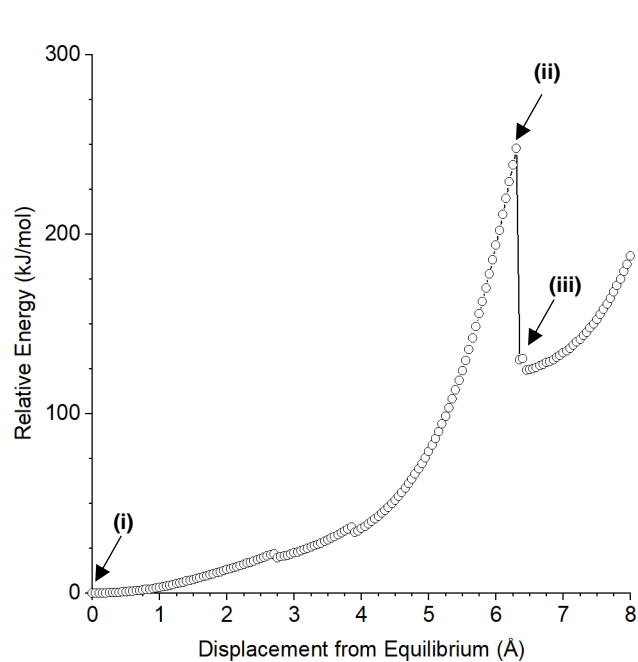
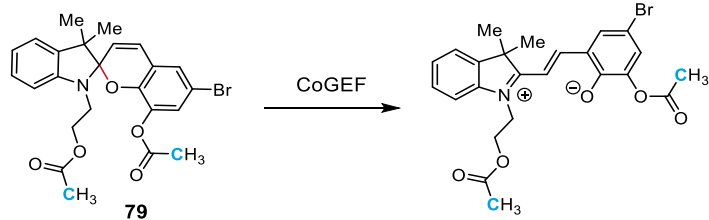
15.025 Å

**Summary of CoGEF Results**

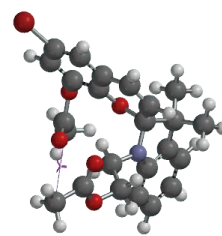
$F_{max}$  3.5 nN

$E_{max}$  271 kJ/mol

**Force-Bond Angle** 28°

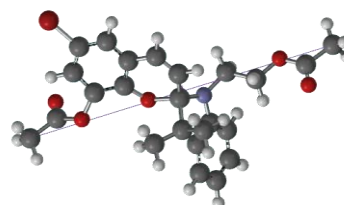


**(i) Equilibrium Geometry**



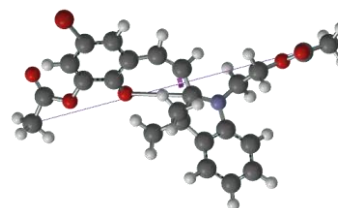
8.544 Å

**(ii) Immediately Prior to Bond Cleavage**



14.844 Å

**(iii) Immediately After Bond Cleavage**



14.894 Å

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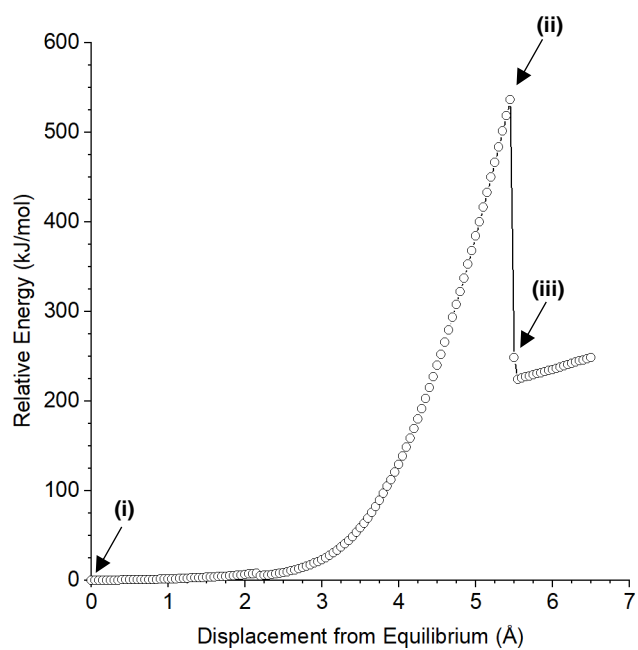
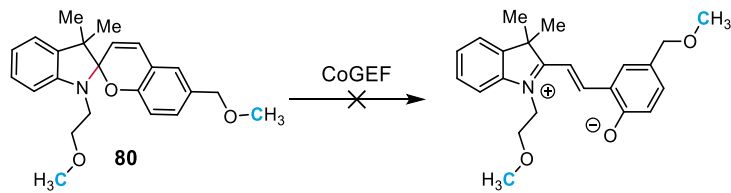
**Summary of CoGEF Results**

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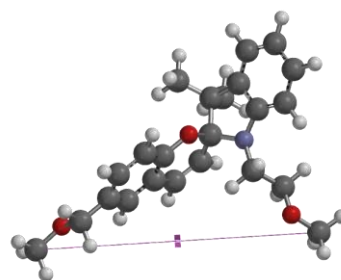
$F_{max}$  3.2 nN

$E_{max}$  248 kJ/mol

**Force-Bond Angle** 27°

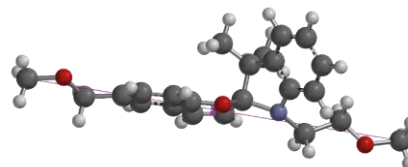


(i) Equilibrium Geometry



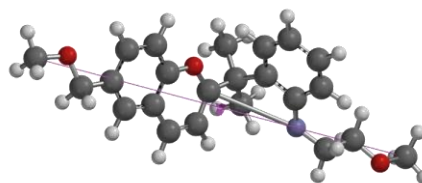
11.447 Å

(ii) Immediately Prior to Bond Cleavage



16.897 Å

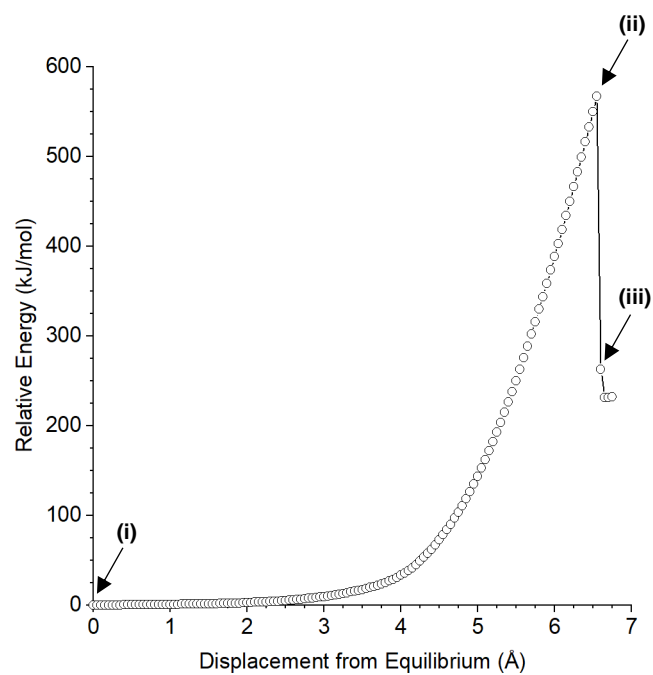
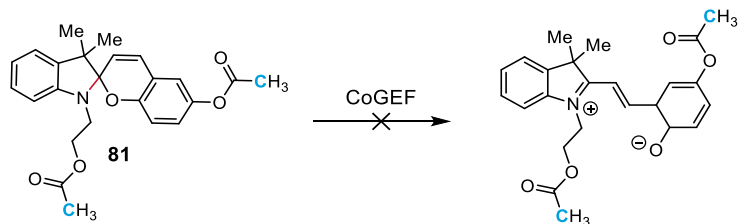
(iii) Immediately After Bond Cleavage



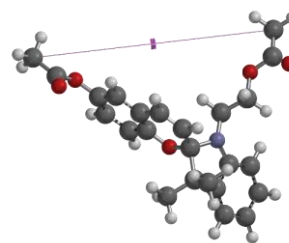
16.947 Å

**Summary of CoGEF Results**

$F_{max}$	5.9 nN
$E_{max}$	536 kJ/mol
Force-Bond Angle	47°

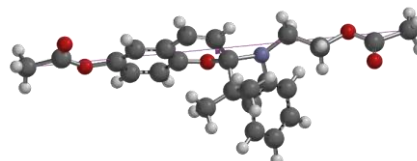


**(i) Equilibrium Geometry**



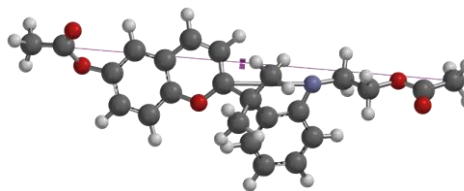
11.638 Å

**(ii) Immediately Prior to Bond Cleavage**



18.188 Å

**(iii) Immediately After Bond Cleavage**



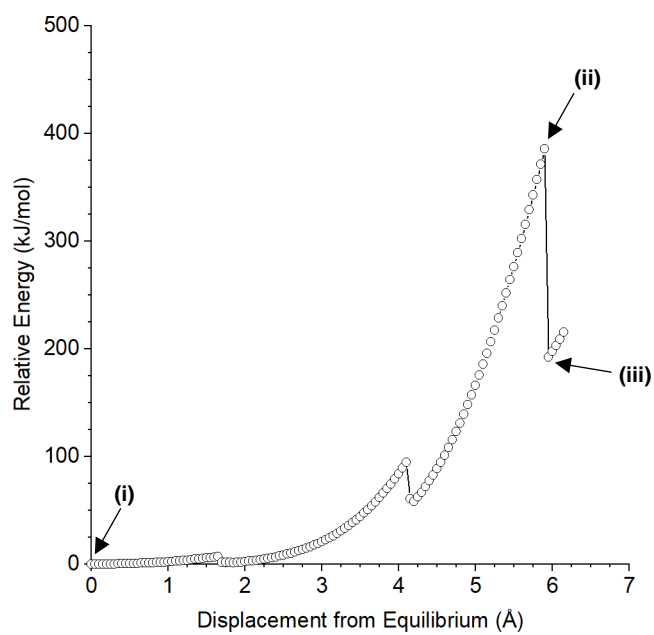
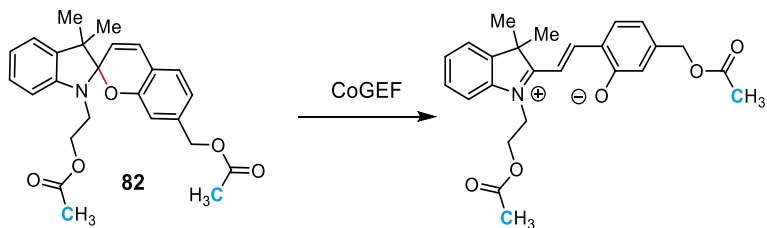
18.238 Å

**Summary of CoGEF Results**

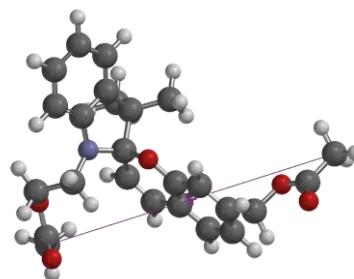
$F_{max}$  5.7 nN

$E_{max}$  567 kJ/mol

**Force-Bond Angle** 49°

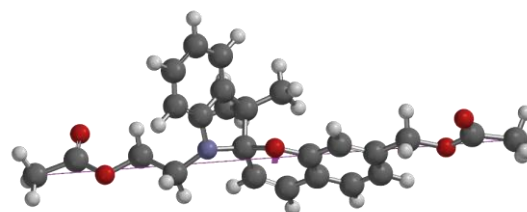


**(i) Equilibrium Geometry**



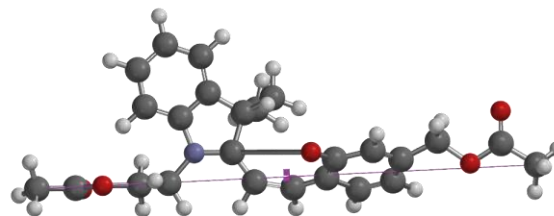
12.787 Å

**(ii) Immediately Prior to Bond Cleavage**



18.687 Å

**(iii) Immediately After Bond Cleavage**



18.737 Å

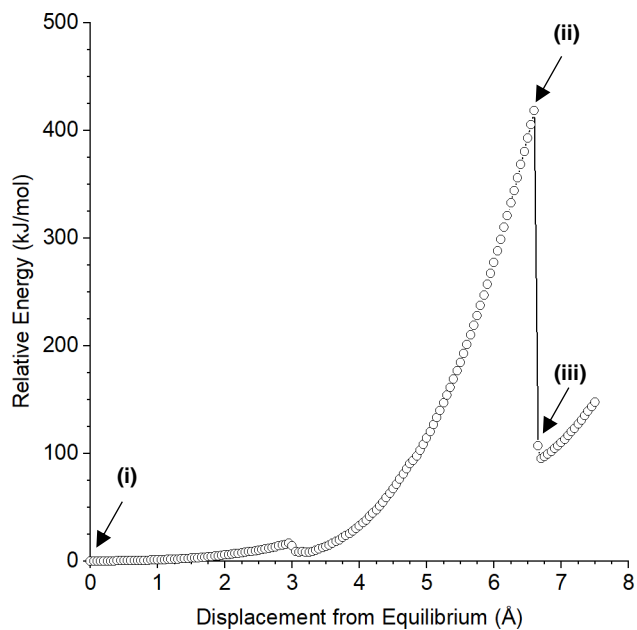
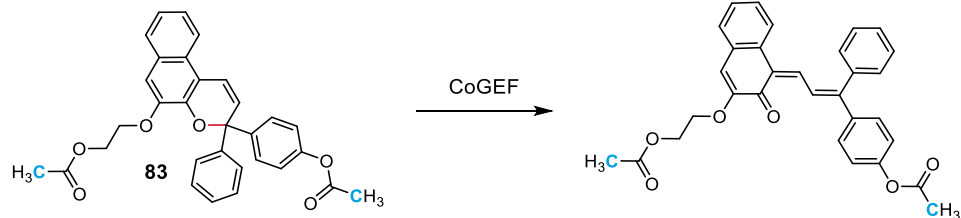
**Summary of CoGEF Results**

$F_{max}$  4.8 nN

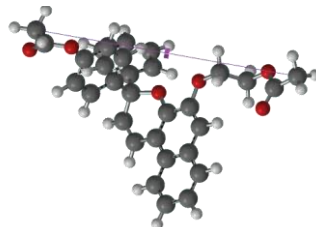
$E_{max}$  386 kJ/mol

Force-Bond Angle 35°



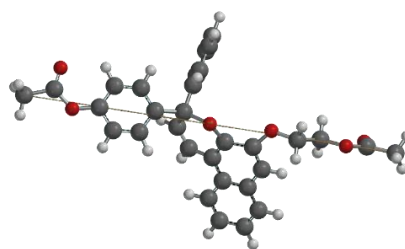


(i) Equilibrium Geometry



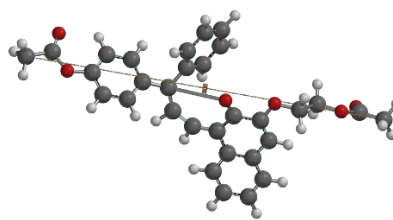
13.325 Å

(ii) Immediately Prior to Bond Cleavage



19.925 Å

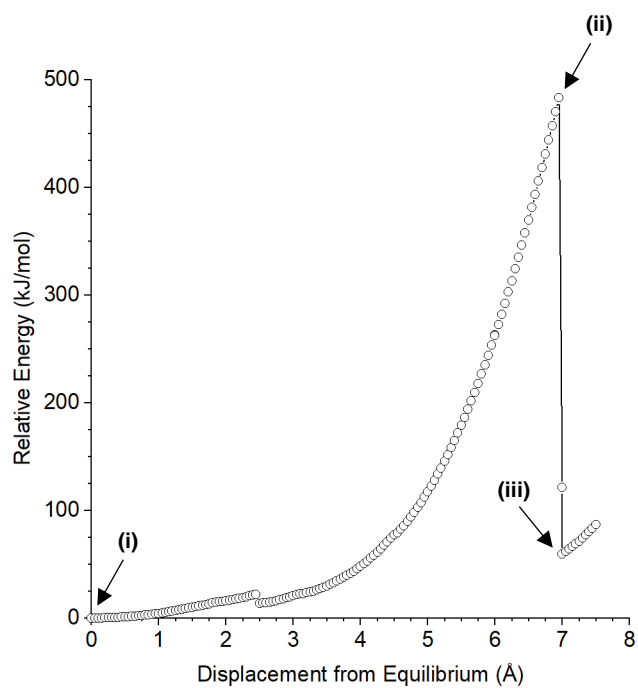
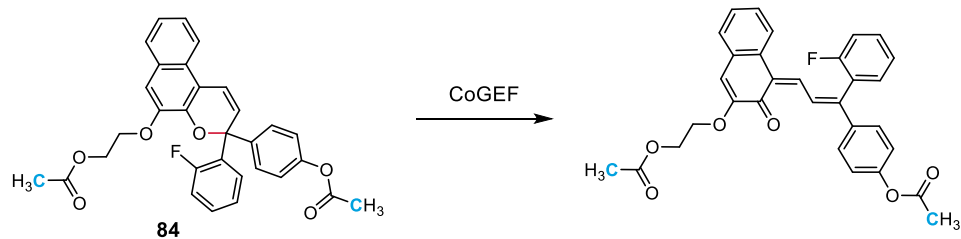
(iii) Immediately After Bond Cleavage



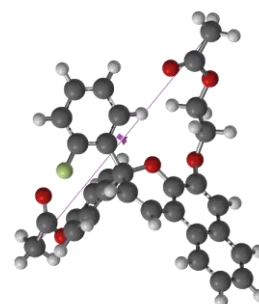
19.975 Å

**Summary of CoGEF Results**

$F_{max}$	4.3 nN
$E_{max}$	418 kJ/mol
Force-Bond Angle	29°

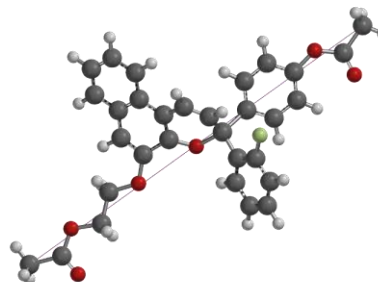


(i) Equilibrium Geometry



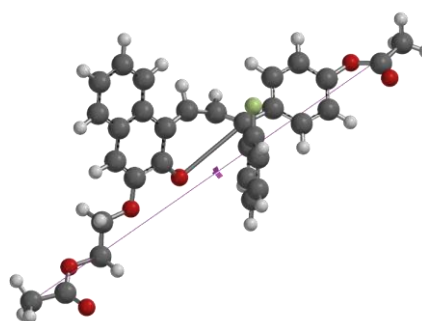
13.160 Å

(ii) Immediately Prior to Bond Cleavage



20.110 Å

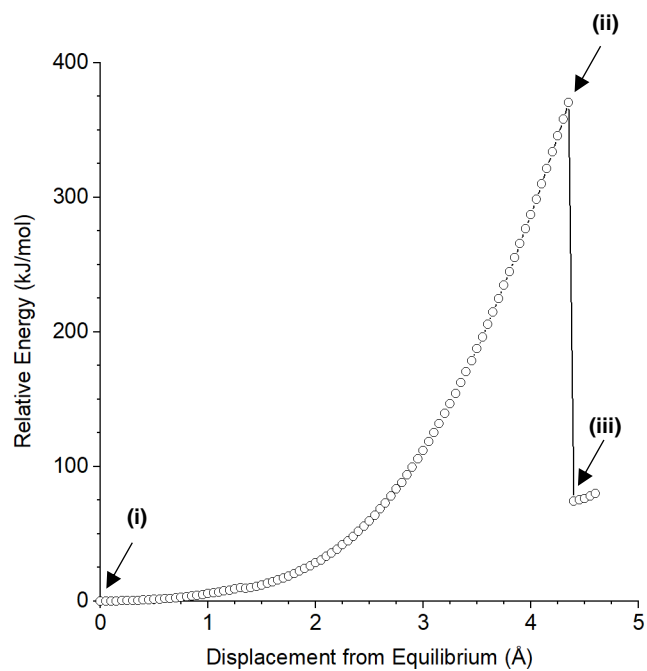
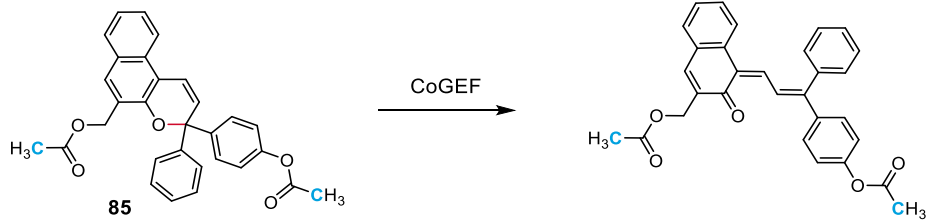
(iii) Immediately After Bond Cleavage



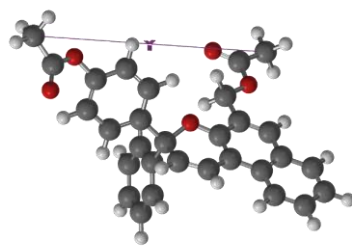
20.160 Å

**Summary of CoGEF Results**

$F_{max}$	4.4 nN
$E_{max}$	483 kJ/mol
Force-Bond Angle	26°

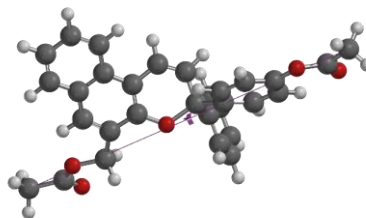


(i) Equilibrium Geometry



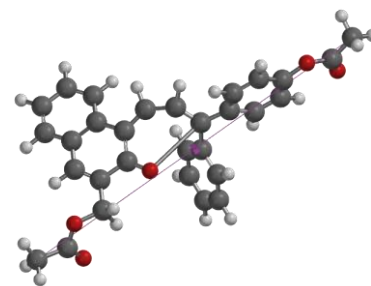
13.153 Å

(ii) Immediately Prior to Bond Cleavage



17.503 Å

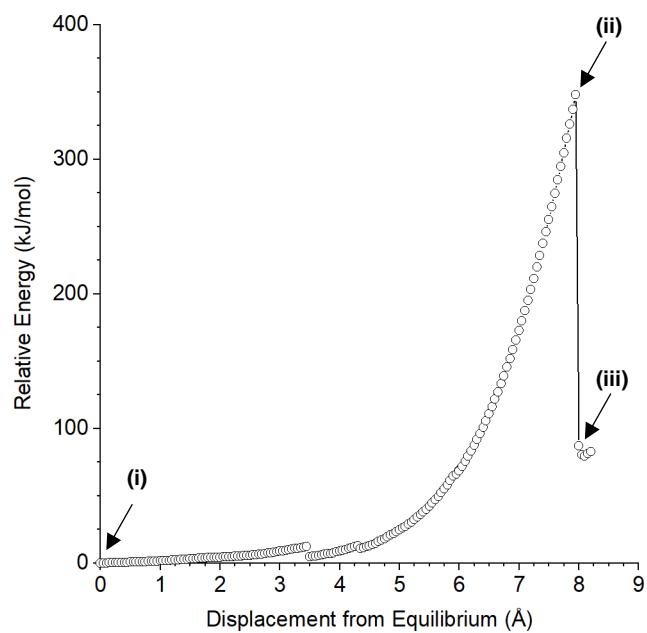
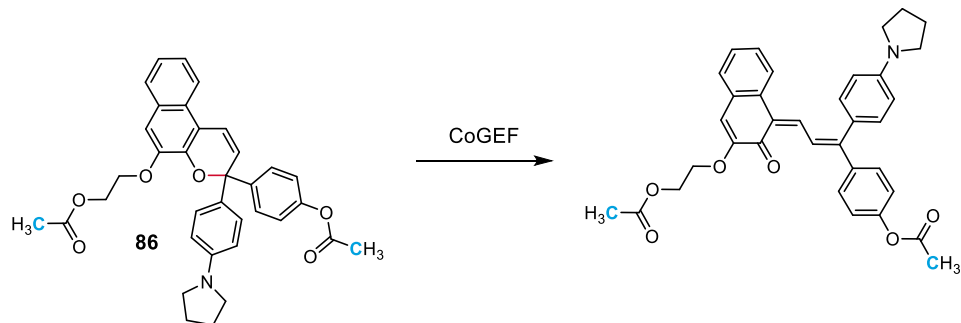
(iii) Immediately After Bond Cleavage



17.553 Å

**Summary of CoGEF Results**

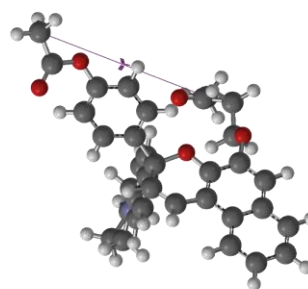
$F_{max}$	4.1 nN
$E_{max}$	370 kJ/mol
Force-Bond Angle	29°



**Summary of CoGEF Results**

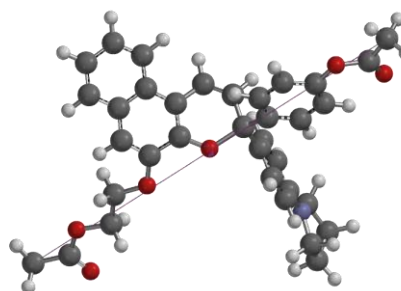
$F_{max}$	3.7 nN
$E_{max}$	348 kJ/mol
Force-Bond Angle	30°

**(i) Equilibrium Geometry**



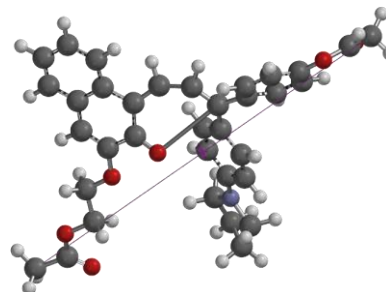
11.651 Å

**(ii) Immediately Prior to Bond Cleavage**

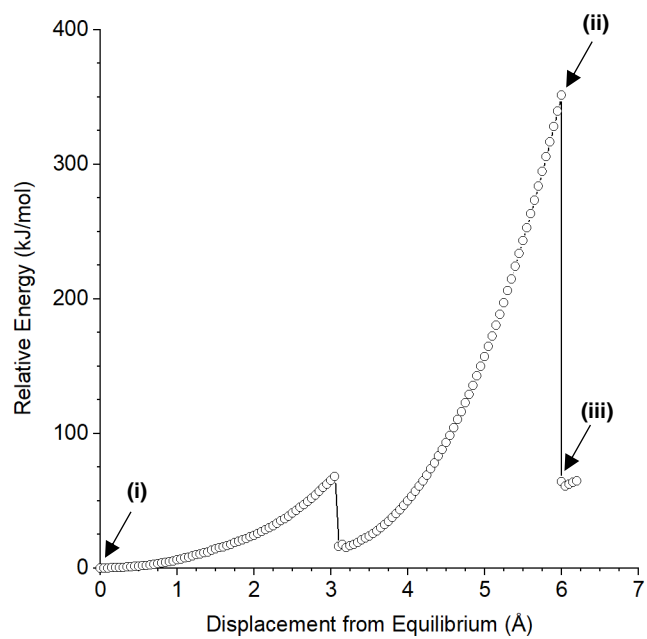
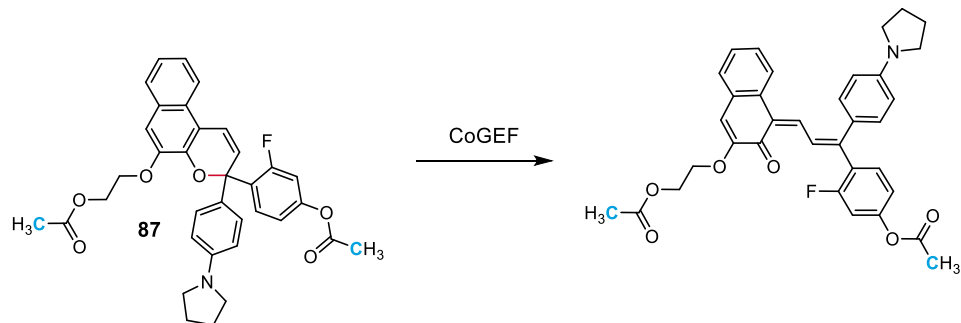


19.601 Å

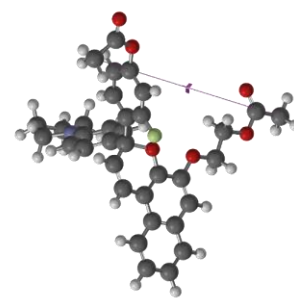
**(iii) Immediately After Bond Cleavage**



19.651 Å

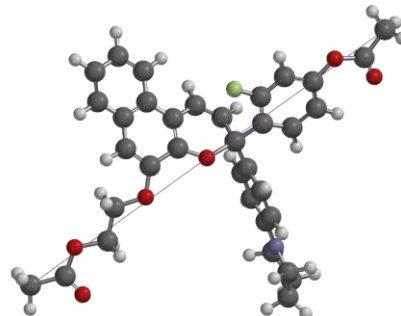


(i) Equilibrium Geometry



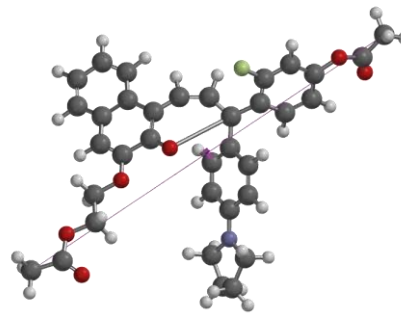
11.190 Å

(ii) Immediately Prior to Bond Cleavage



19.590 Å

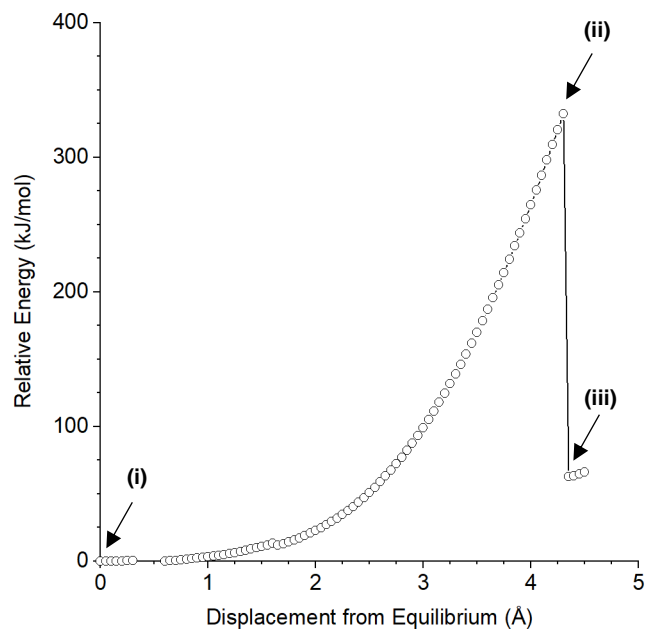
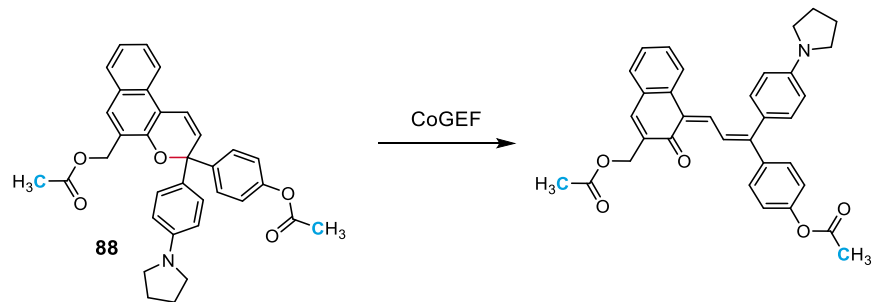
(iii) Immediately After Bond Cleavage



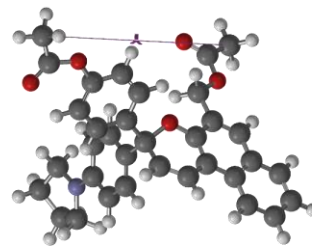
19.640 Å

**Summary of CoGEF Results**

$F_{max}$	3.7 nN
$E_{max}$	334 kJ/mol
Force-Bond Angle	33°

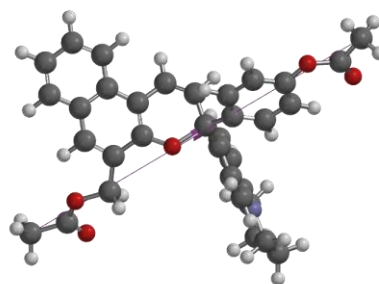


(i) Equilibrium Geometry



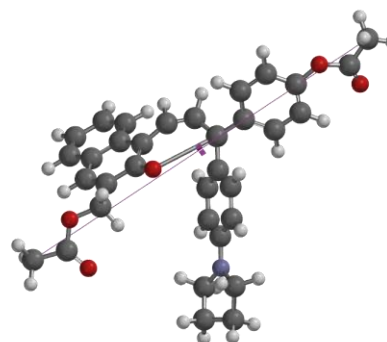
13.054 Å

(ii) Immediately Prior to Bond Cleavage



17.354 Å

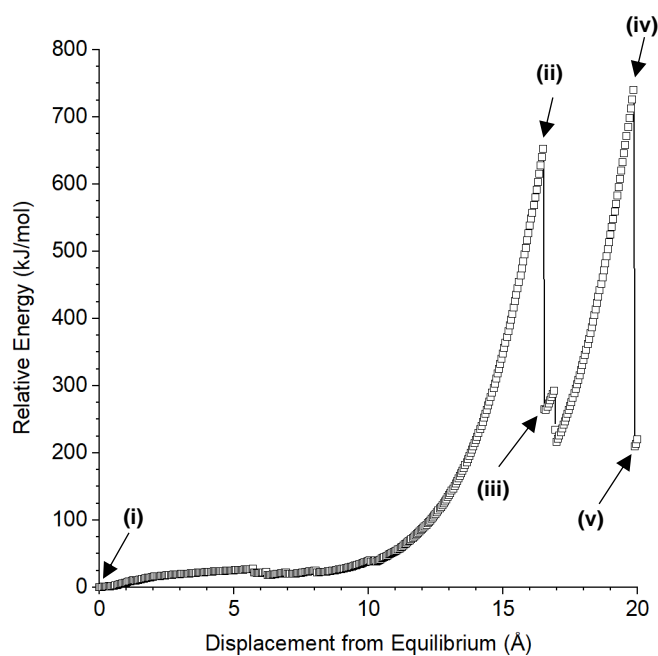
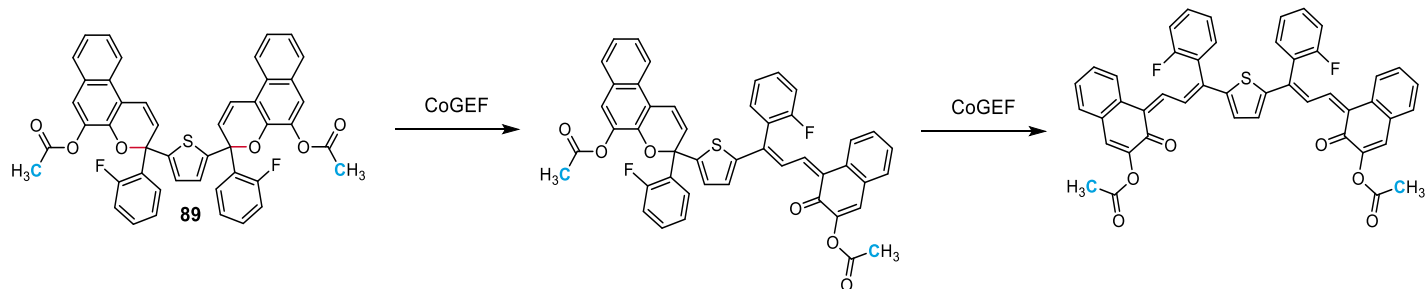
(iii) Immediately After Bond Cleavage



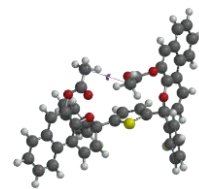
17.404 Å

**Summary of CoGEF Results**

$F_{max}$	3.9 nN
$E_{max}$	332 kJ/mol
Force-Bond Angle	30°

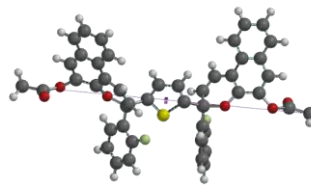


(i) Equilibrium Geometry



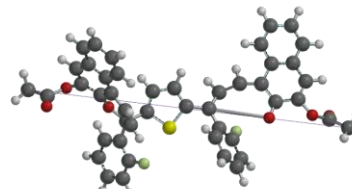
4.159 Å

(ii) Immediately Prior to First Bond Cleavage



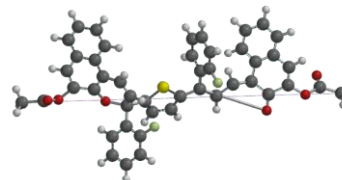
20.659 Å

(iii) Immediately After Bond First Cleavage



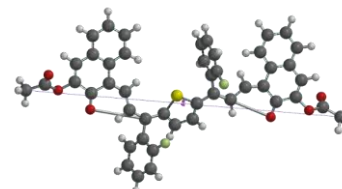
20.709 Å

(iv) Immediately Prior to Second Bond Cleavage



24.009 Å

(v) Immediately After Bond Second Cleavage



24.059 Å

#### Summary of CoGEF Results (S,S)

$F_{max}$  4.1 nN (first)  
4.6 nN (second)

$E_{max}$  652 kJ/mol (first)  
740 kJ/mol (second)

**Force-Bond Angle** 25° (first), 27° (second)

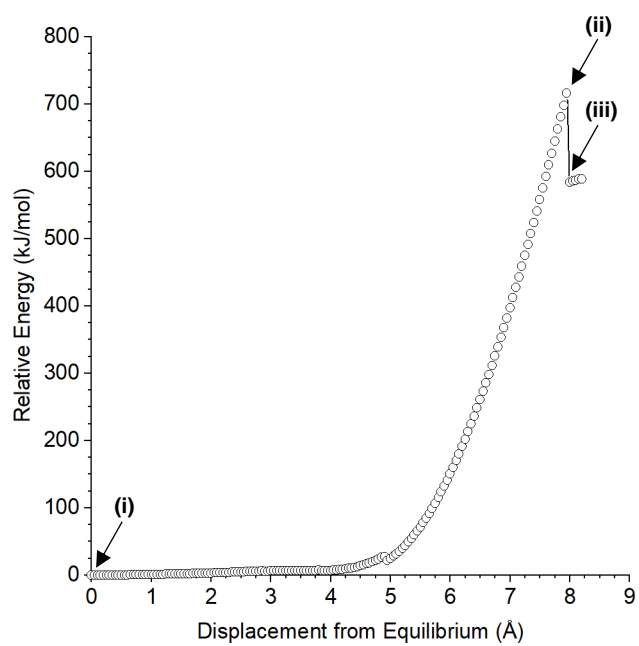
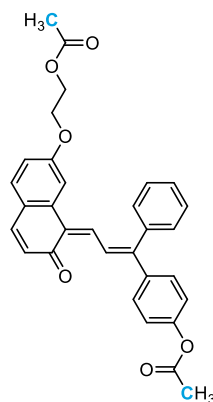
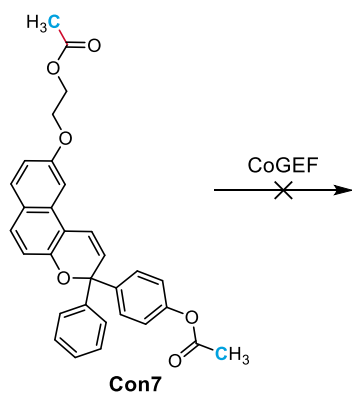
The results presented here correspond to the (S,S)-isomer of compound **82**. The CoGEF results for the (R,S)-isomer are similar:

#### Summary of CoGEF Results (R,S)

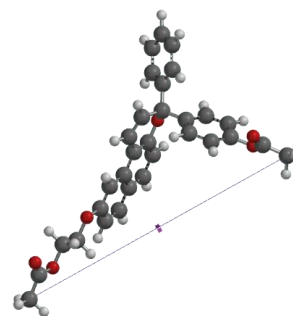
$F_{max}$  4.1 nN (first)  
4.5 nN (second)

$E_{max}$  644 kJ/mol (first)  
727 kJ/mol (second)

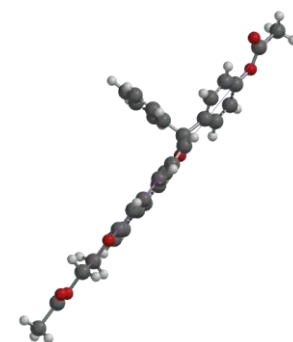
**Force-Bond Angle** 24° (first), 26° (second)



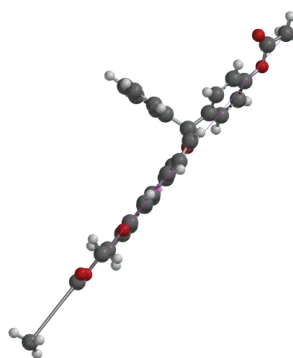
(i) Equilibrium Geometry



(ii) Immediately Prior to Bond Cleavage



(iii) Immediately After Bond Cleavage



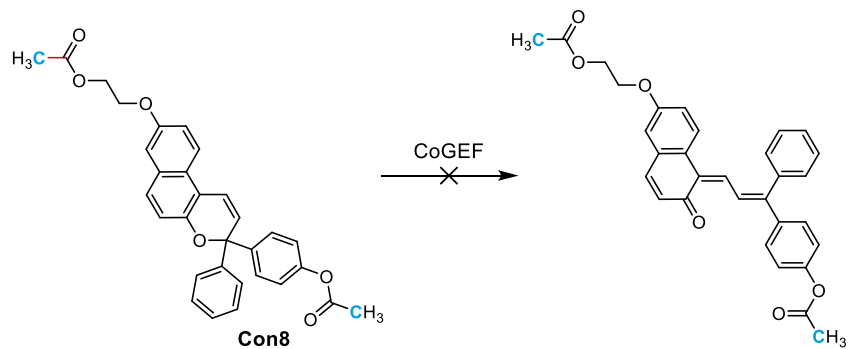
**Summary of CoGEF Results**

$F_{max}$  6.0 nN

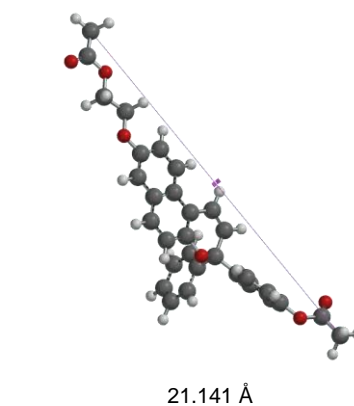
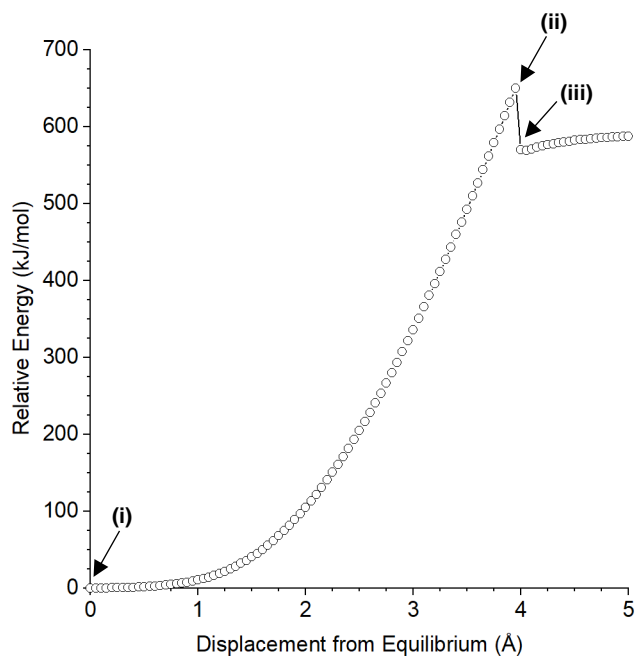
$E_{max}$  716 kJ/mol

Force-Bond Angle 63°

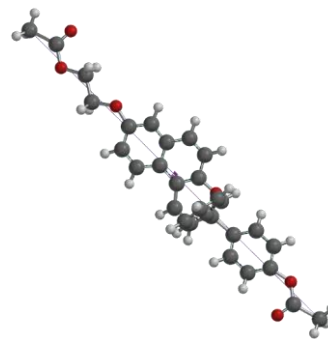




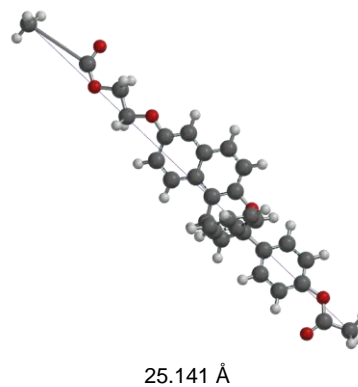
(i) Equilibrium Geometry



(ii) Immediately Prior to Bond Cleavage

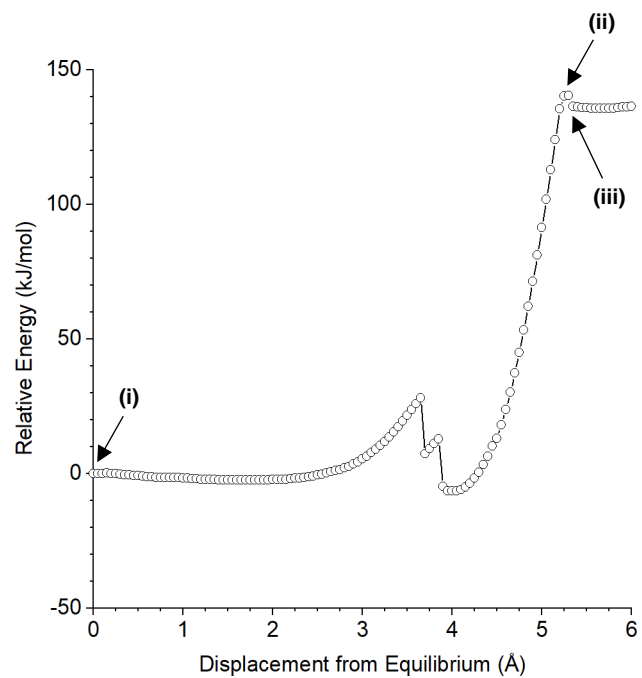
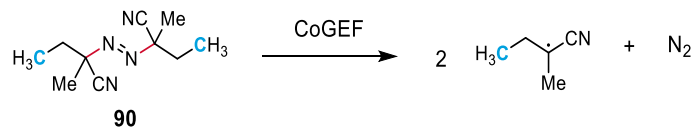


(iii) Immediately After Bond Cleavage

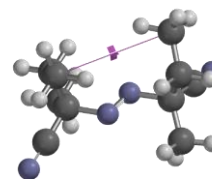


**Summary of CoGEF Results**

$F_{max}$	6.0 nN
$E_{max}$	650 kJ/mol
Force-Bond Angle	56°

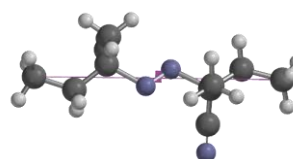


**(i) Equilibrium Geometry**



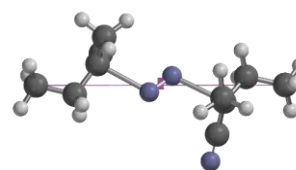
4.452 Å

**(ii) Immediately Prior to Bond Cleavage**



9.652 Å

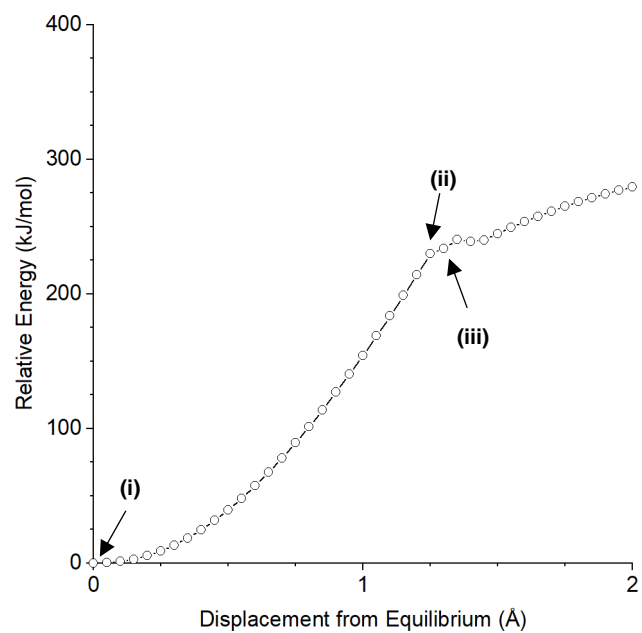
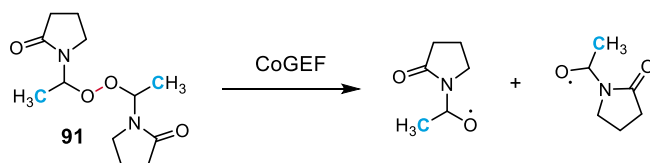
**(iii) Immediately After Bond Cleavage**



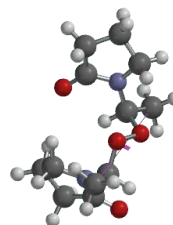
9.702 Å

**Summary of CoGEF Results**

$F_{max}$	3.7 nN
$E_{max}$	140 kJ/mol
<b>Force-Bond Angle</b>	29°

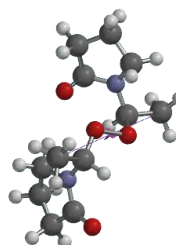


(i) Equilibrium Geometry



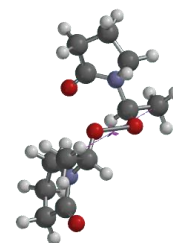
5.818 Å

(ii) Immediately Prior to Bond Cleavage



7.068 Å

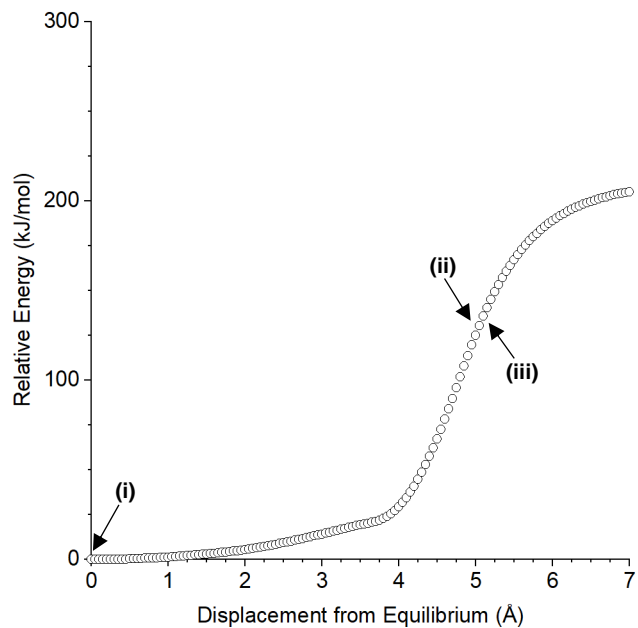
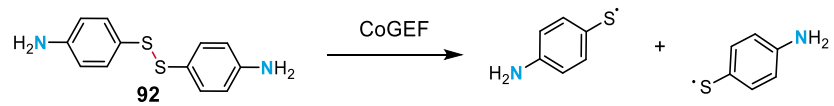
(iii) Immediately After Bond Cleavage



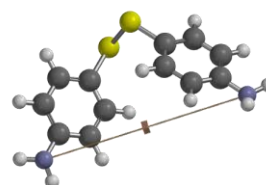
7.118 Å

**Summary of CoGEF Results**

$F_{max}$	5.2 nN
$E_{max}$	230 kJ/mol
<b>Force-Bond Angle</b>	28°



(i) Equilibrium Geometry



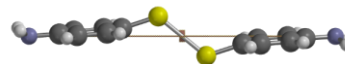
9.023 Å

(ii) Immediately Prior to Bond Cleavage



13.923 Å

(iii) Immediately After Bond Cleavage



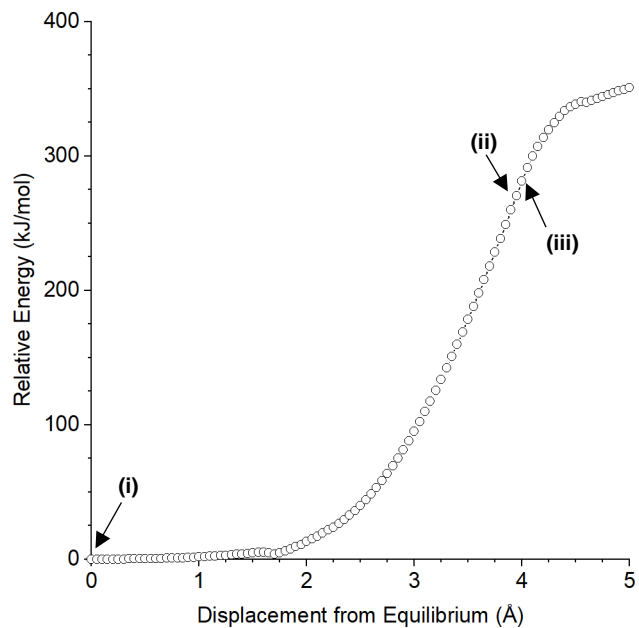
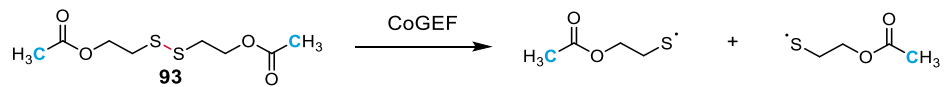
13.973 Å

**Summary of CoGEF Results**

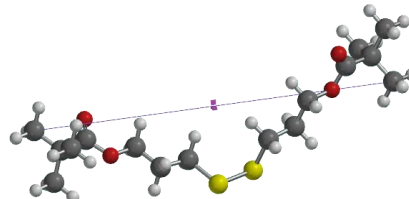
$F_{max}$  2.0 nN

$E_{max}$  114 kJ/mol

Force-Bond Angle 45°

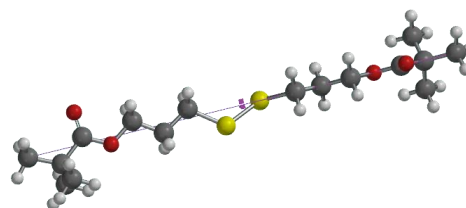


(i) Equilibrium Geometry



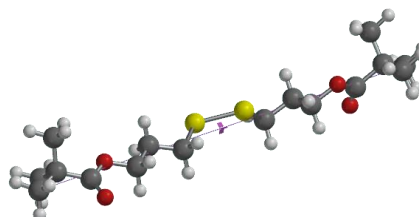
11.920 Å

(ii) Immediately Prior to Bond Cleavage



15.920 Å

(iii) Immediately After Bond Cleavage



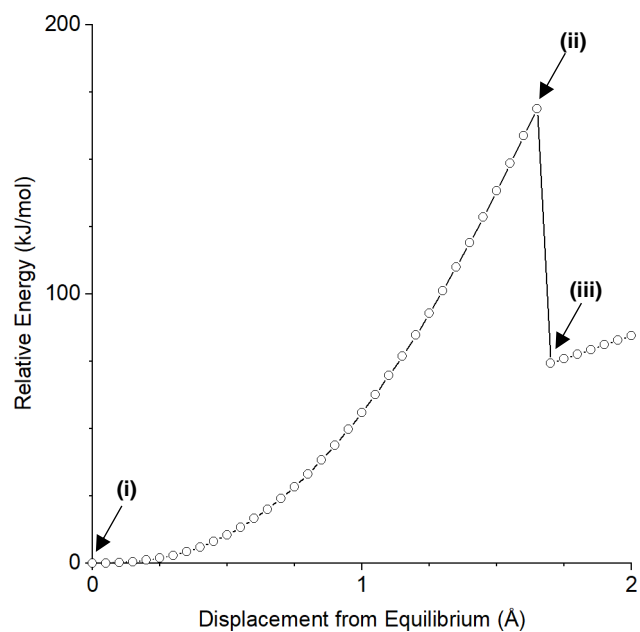
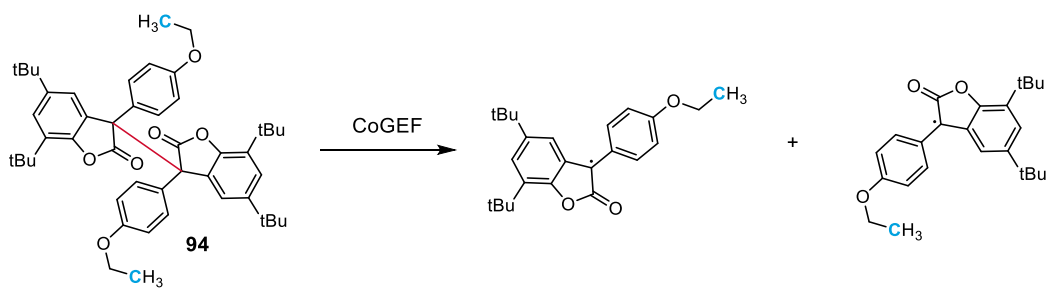
15.970 Å

**Summary of CoGEF Results**

$F_{max}$  3.6 nN

$E_{max}$  271 kJ/mol

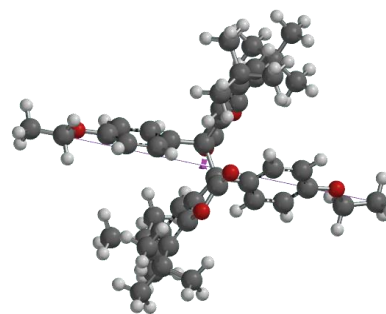
Force-Bond Angle 29°



**Summary of CoGEF Results**

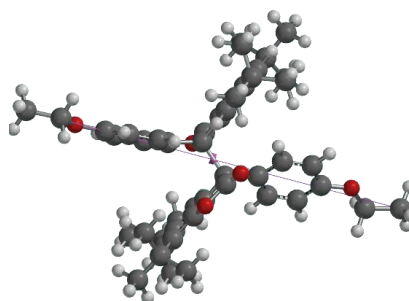
$F_{max}$	3.5 nN
$E_{max}$	169 kJ/mol
Force-Bond Angle	44°

**(i) Equilibrium Geometry**



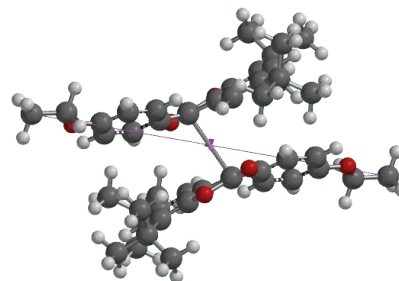
16.559 Å

**(ii) Immediately Prior to Bond Cleavage**

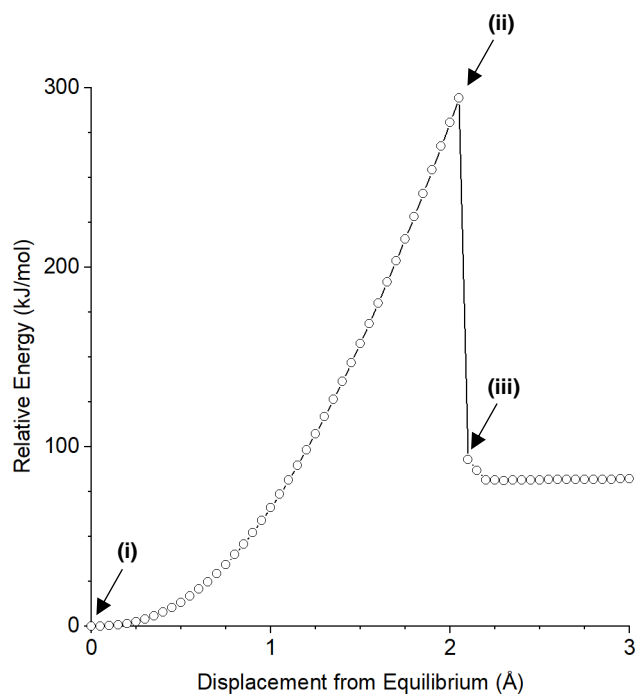
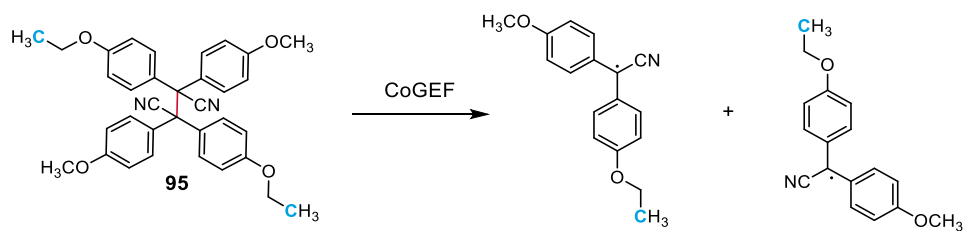


18.209 Å

**(iii) Immediately After Bond Cleavage**



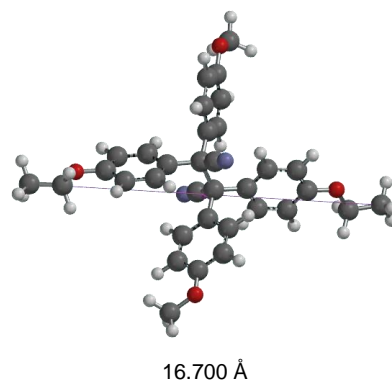
18.259 Å



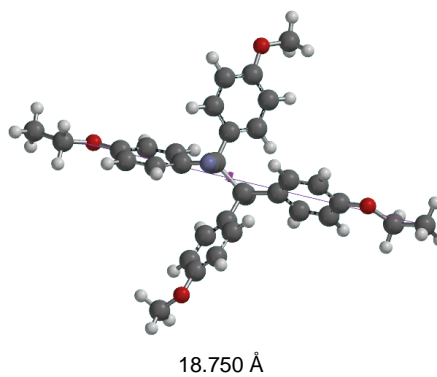
**Summary of CoGEF Results**

$F_{max}$	4.5 nN
$E_{max}$	294 kJ/mol
Force-Bond Angle	41°

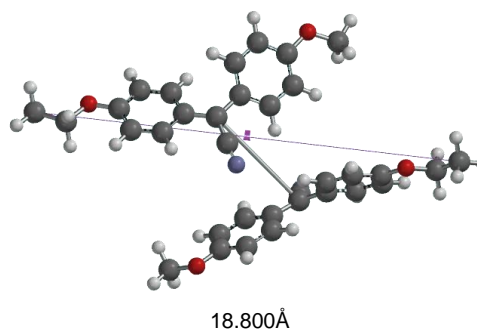
**(i) Equilibrium Geometry**

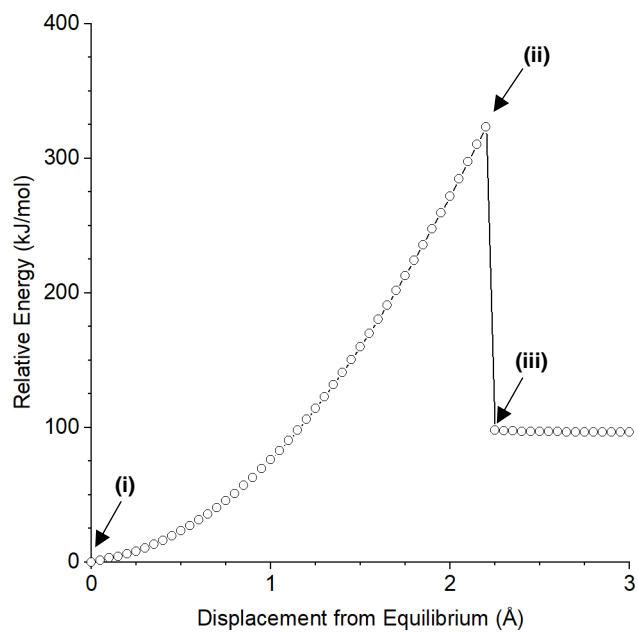
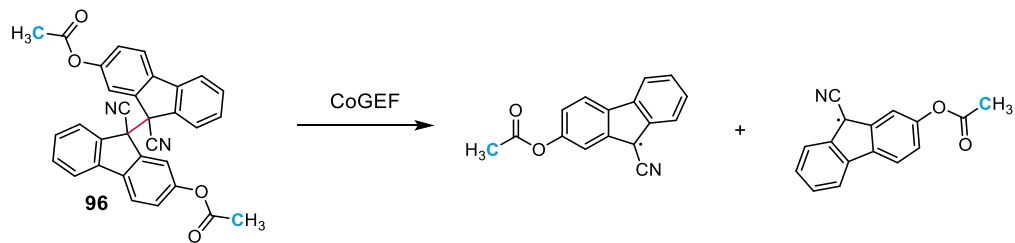


**(ii) Immediately Prior to Bond Cleavage**

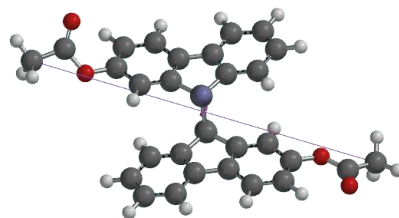


**(iii) Immediately After Bond Cleavage**



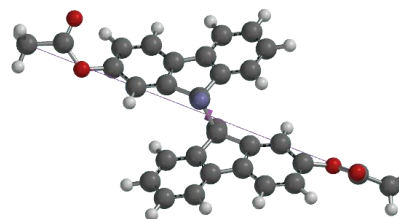


(i) Equilibrium Geometry



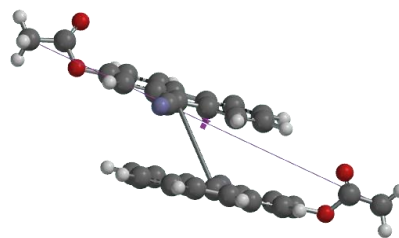
15.307 Å

(ii) Immediately Prior to Bond Cleavage



17.507 Å

(iii) Immediately After Bond Cleavage



17.557 Å

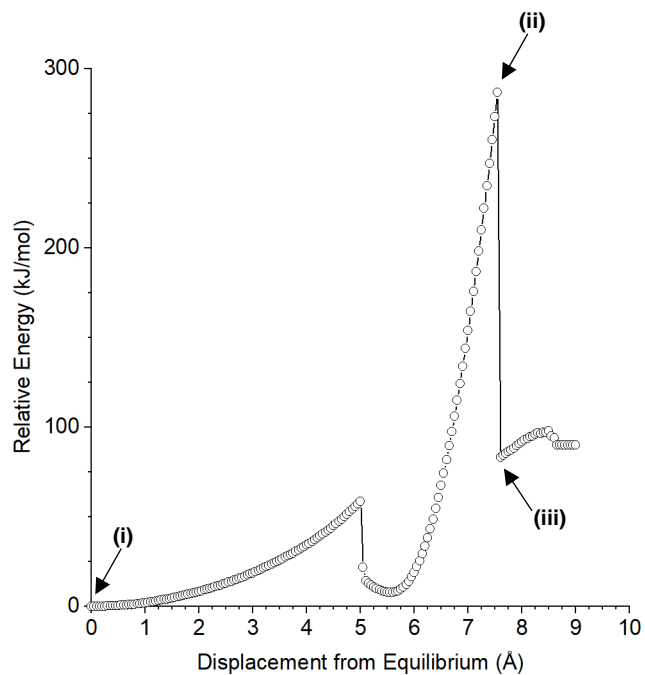
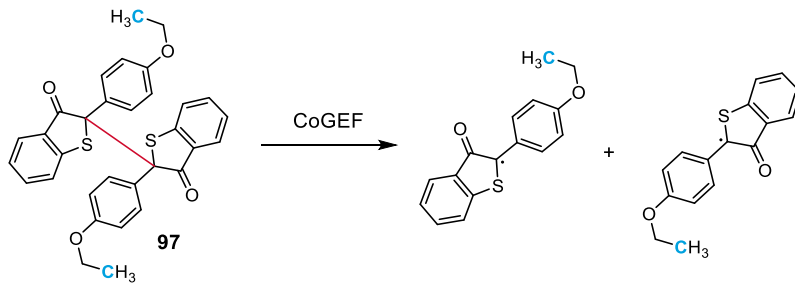
**Summary of CoGEF Results**

$F_{max}$  4.3 nN

$E_{max}$  326 kJ/mol

Force-Bond Angle 46°

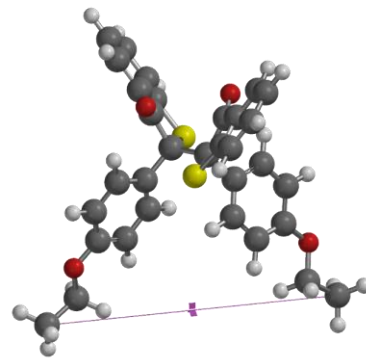




**Summary of CoGEF Results**

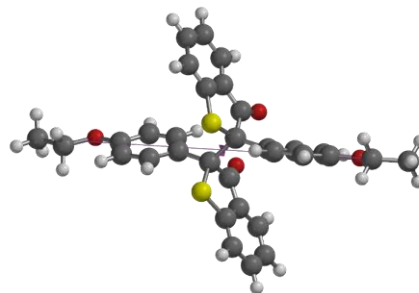
$F_{max}$	4.4 nN
$E_{max}$	287 kJ/mol
<b>Force-Bond Angle</b>	41°

**(i) Equilibrium Geometry**



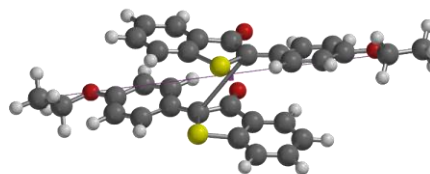
11.109 Å

**(ii) Immediately Prior to Bond Cleavage**

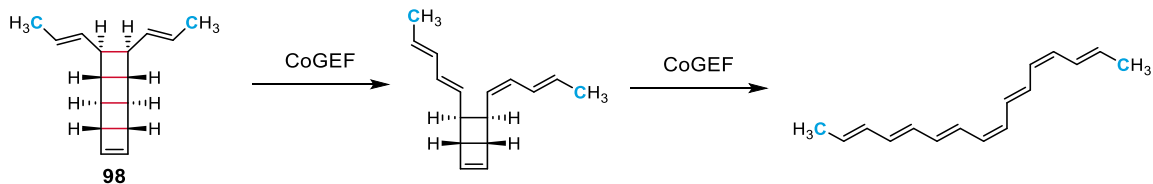


18.659 Å

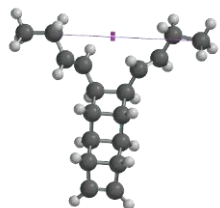
**(iii) Immediately After Bond Cleavage**



18.709 Å

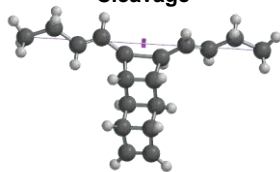


(i) Equilibrium Geometry



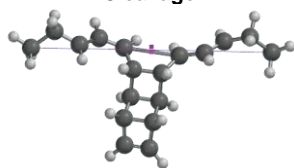
6.269 Å

(ii) Immediately Prior to First Bond Cleavage



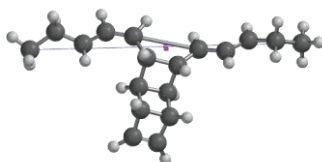
10.019 Å

(iii) Immediately After First Bond Cleavage



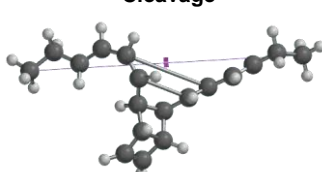
10.069 Å

(iv) Immediately Prior to Second Bond Cleavage



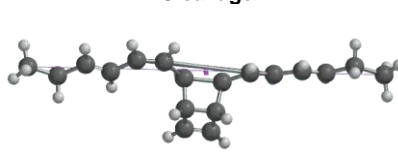
10.169 Å

(v) Immediately After Second Bond Cleavage



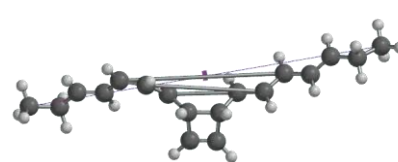
10.219 Å

(vi) Immediately Prior to Third Bond Cleavage



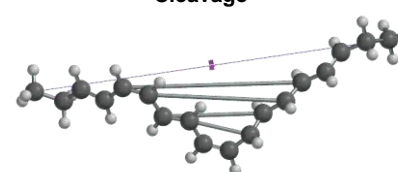
15.219 Å

(vii) Immediately After Third Bond Cleavage

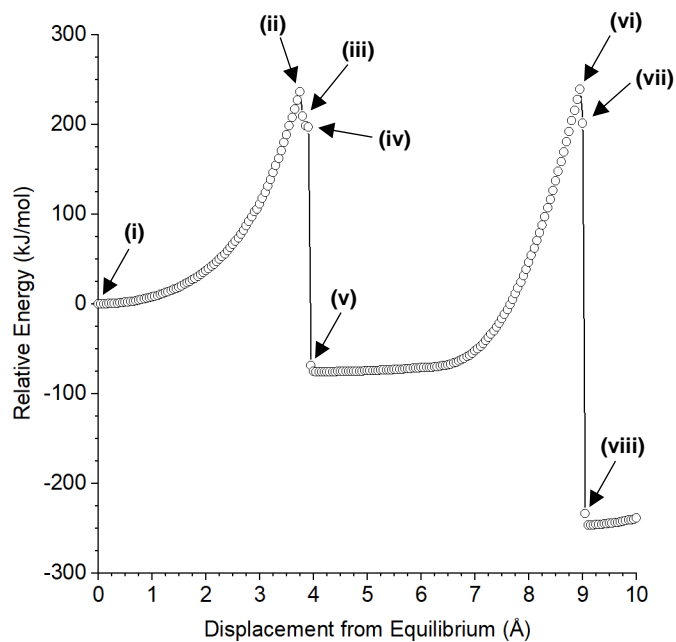


15.269 Å

(viii) Immediately After Fourth Bond Cleavage

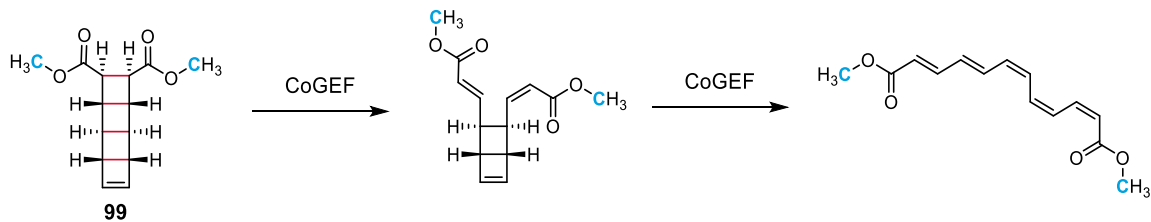


15.319 Å

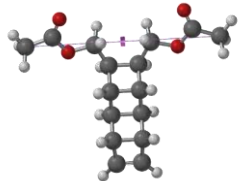


#### Summary of CoGEF Results

$F_{max}$	3.2 nN (first) 3.9 nN (second)
$E_{max}$	236 kJ/mol (first) 239 kJ/mol (second)
<b>Force-Bond Angle</b>	0.1° (first), 4.4° (second)

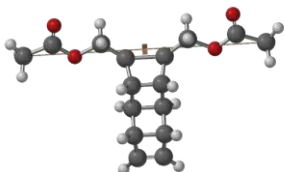


(i) Equilibrium Geometry



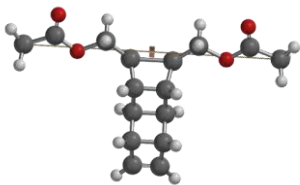
10.304 Å

(ii) Immediately Prior to First Bond Cleavage



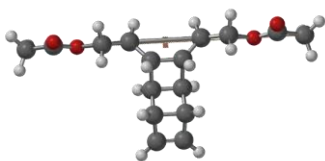
12.554 Å

(iii) Immediately After First Bond Cleavage



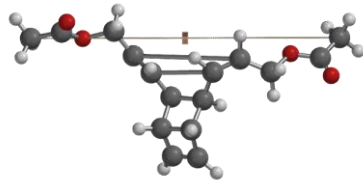
12.604 Å

(iv) Immediately Prior to Second Bond Cleavage



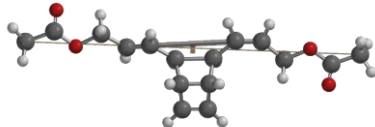
13.754 Å

(v) Immediately After Second Bond Cleavage



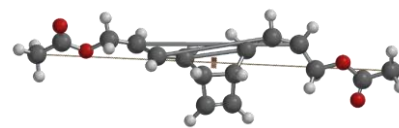
13.804 Å

(vi) Immediately Prior to Third Bond Cleavage



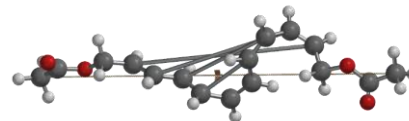
17.554 Å

(vii) Immediately After Third Bond Cleavage

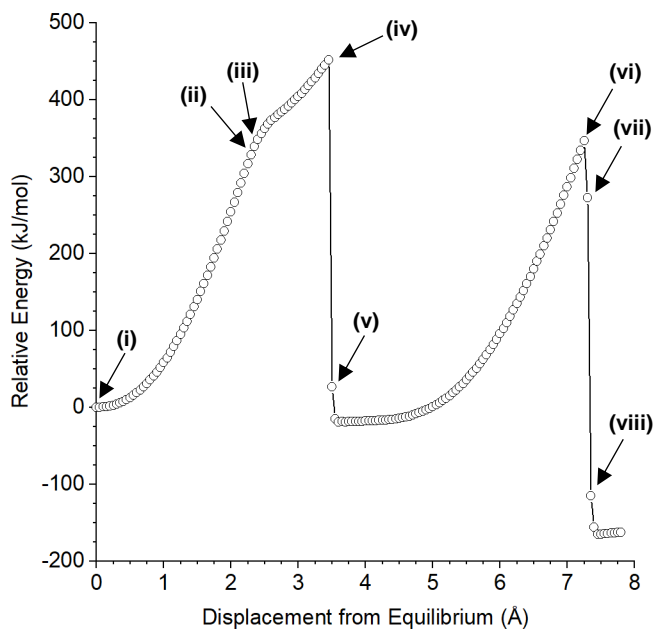


17.604 Å

(viii) Immediately After Fourth Bond Cleavage

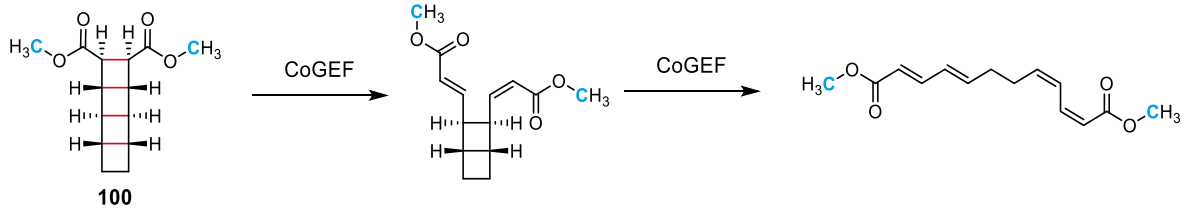


17.654 Å

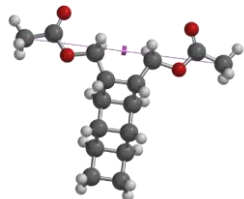


**Summary of CoGEF Results**

$F_{max}$	4.2 nN
	4.0 nN
$E_{max}$	451 kJ/mol
	346 kJ/mol
Force-Bond Angle	0.2° (first)
	3.4° (second)

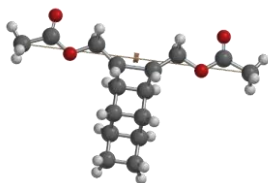


(i) Equilibrium Geometry



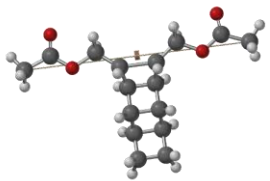
10.308 Å

(ii) Immediately Prior to First Bond Cleavage



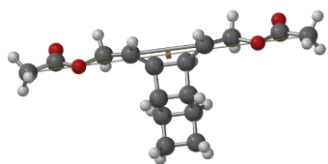
12.458 Å

(iii) Immediately After First Bond Cleavage



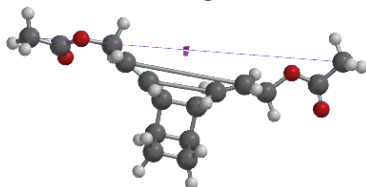
12.508 Å

(iv) Immediately Prior to Second Bond Cleavage



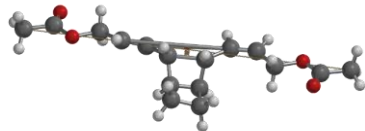
14.208 Å

(v) Immediately After Second Bond Cleavage



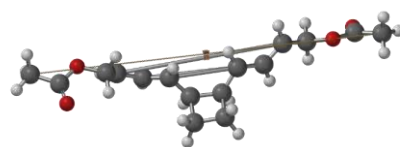
14.258 Å

(vi) Immediately Prior to Third Bond Cleavage



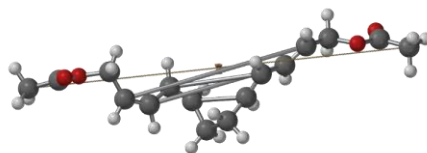
17.508 Å

(vii) Immediately After Third Bond Cleavage

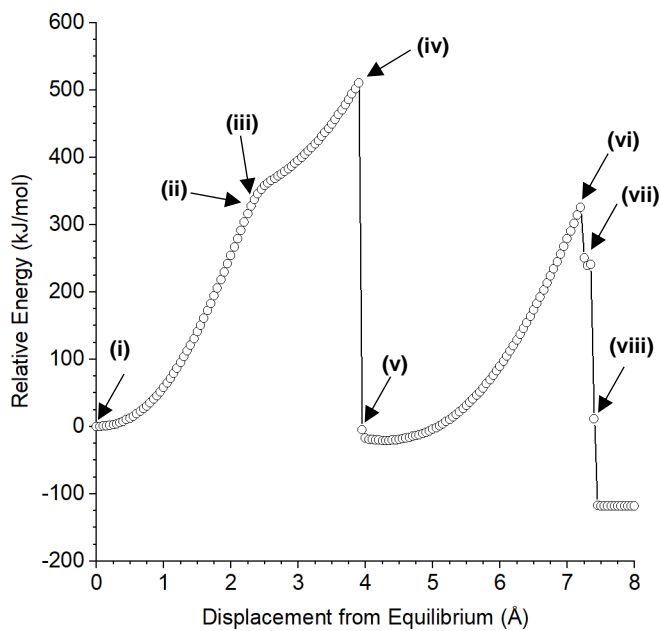


17.558 Å

(viii) Immediately After Fourth Bond Cleavage

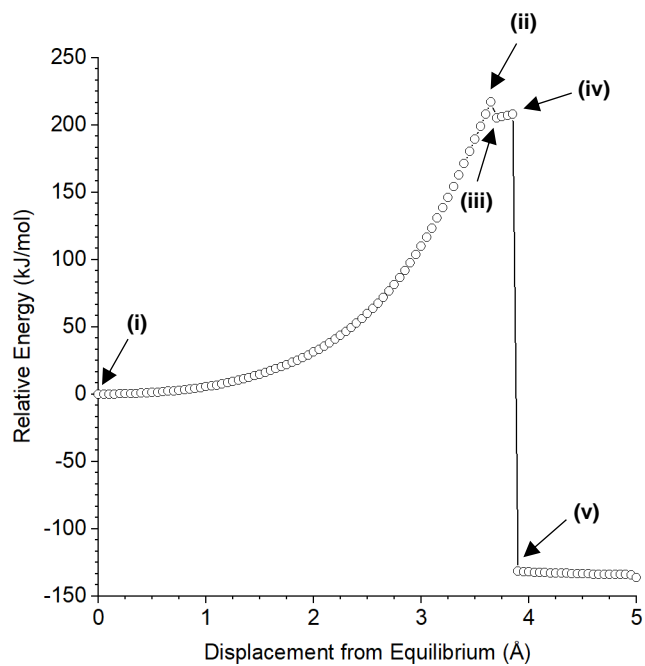
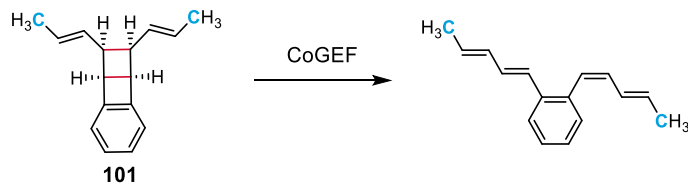


17.708 Å



#### Summary of CoGEF Results

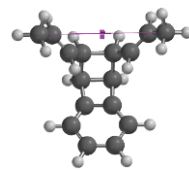
$F_{max}$	4.2 nN (first)
	3.9 nN (second)
$E_{max}$	511 kJ/mol (first)
	326 kJ/mol (second)
Force-Bond Angle	0.5° (first)
	4.0° (second)



**Summary of CoGEF Results**

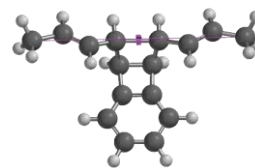
$F_{max}$	3.1 nN
$E_{max}$	207 kJ/mol
Force-Bond Angle	0.1°

**(i) Equilibrium Geometry**



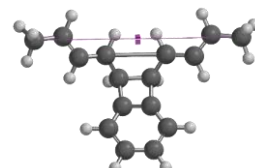
6.368 Å

**(ii) Immediately Prior to First Bond Cleavage**



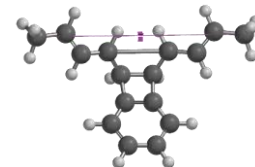
10.018 Å

**(iii) Immediately After First Bond Cleavage**



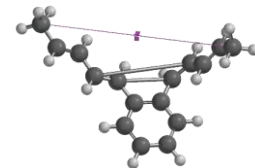
10.068 Å

**(iv) Immediately Prior to Second Bond Cleavage**

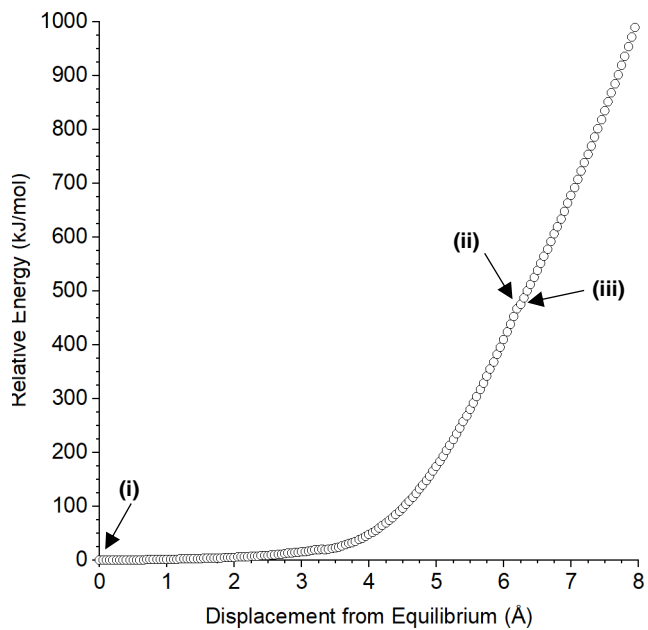
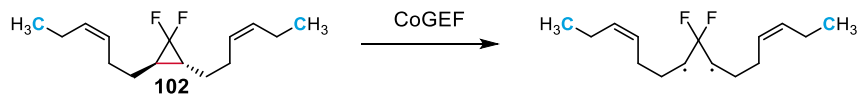


10.218 Å

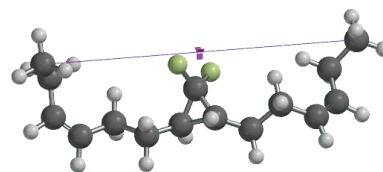
**(v) Immediately After Second Bond Cleavage**



10.268 Å

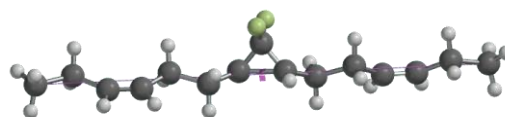


(i) Equilibrium Geometry



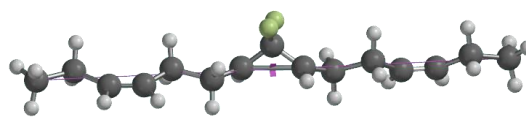
12.504 Å

(ii) Immediately Prior to Bond Cleavage



18.704 Å

(iii) Immediately After Bond Cleavage



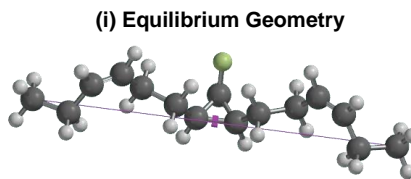
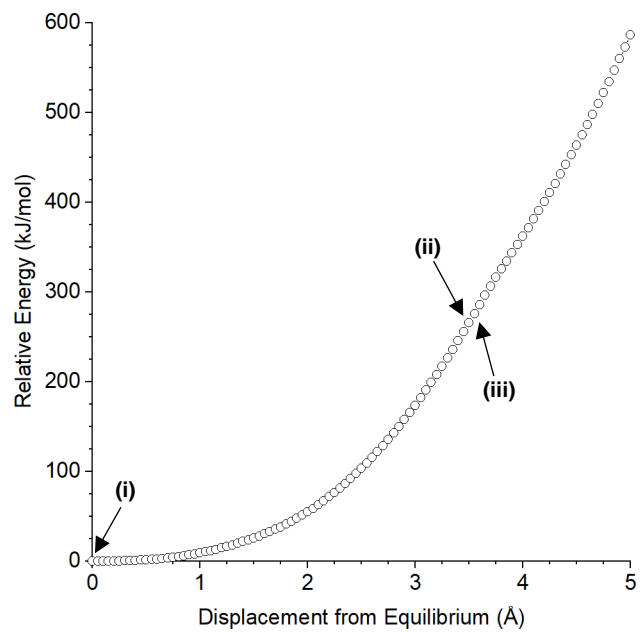
18.754 Å

**Summary of CoGEF Results**

$F_{max}$  4.8 nN

$E_{max}$  466 kJ/mol

Force-Bond Angle 21°



14.312 Å



17.912 Å



17.962 Å

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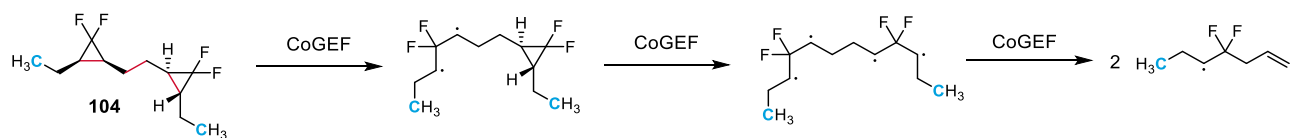
**Summary of CoGEF Results**

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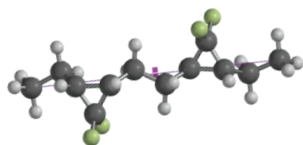
$F_{max}$  3.4 nN

$E_{max}$  292 kJ/mol

Force-Bond Angle 0.0°

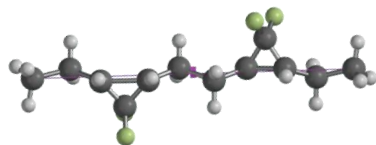


(i) Equilibrium Geometry



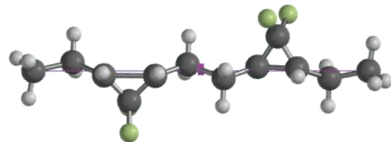
10.904 Å

(ii) Immediately Prior to First Bond Cleavage

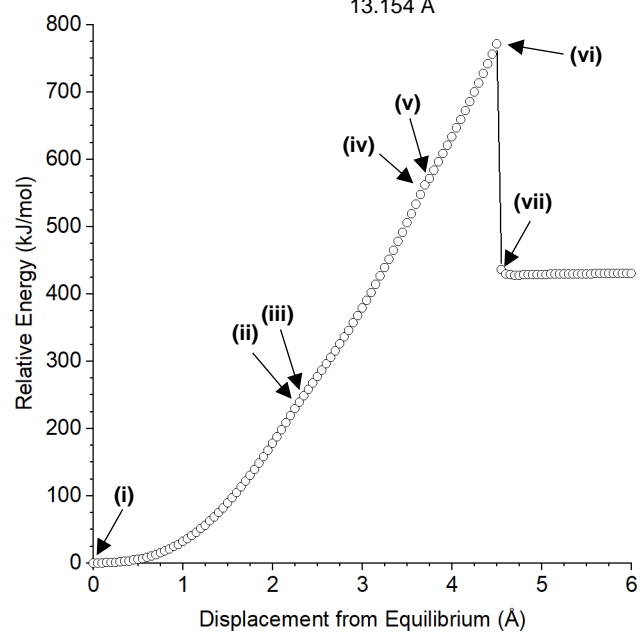


13.104 Å

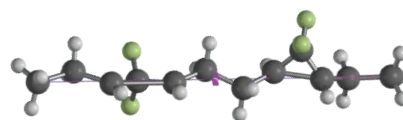
(iii) Immediately After First Bond Cleavage



13.154 Å

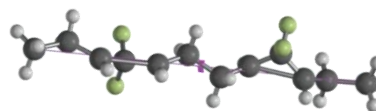


(iv) Immediately Prior to Second Bond Cleavage



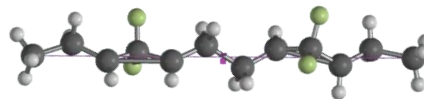
14.604 Å

(v) Immediately After Second Bond Cleavage



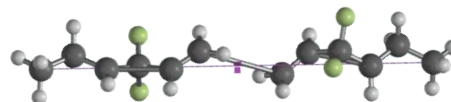
14.654 Å

(vi) Immediately Prior to Disproportionation



15.404 Å

(vii) Immediately After Disproportionation



15.454 Å

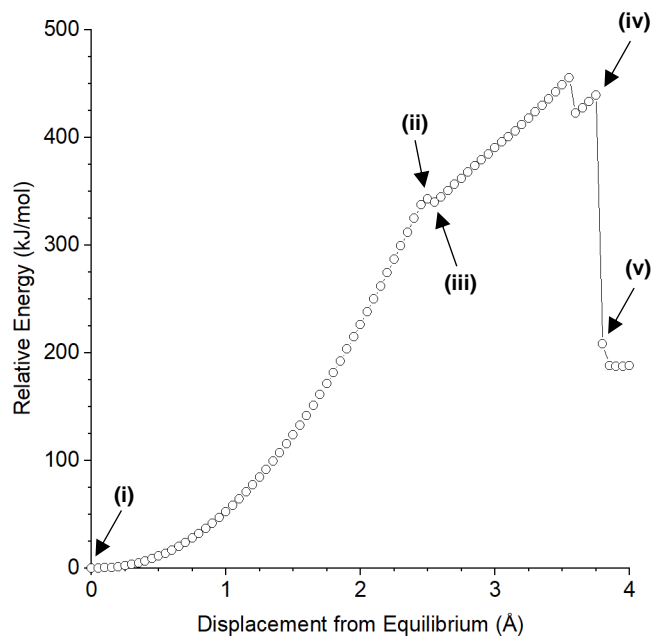
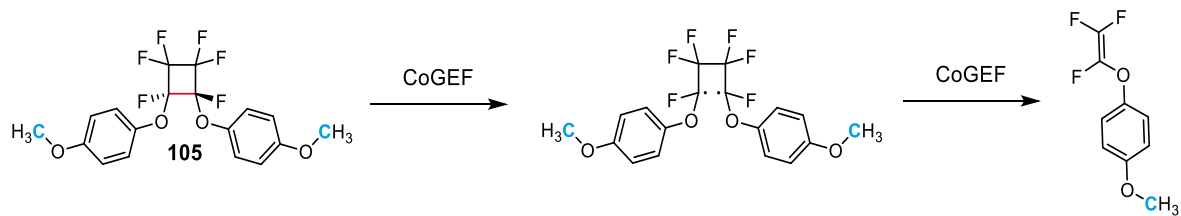
#### Summary of CoGEF Results

$F_{max}$  4.9 nN

$E_{max}$  771 kJ/mol

Force-Bond Angle 1.3°

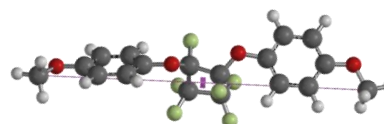




**Summary of CoGEF Results**

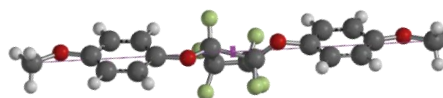
$F_{max}$	4.2 nN
$E_{max}$	455 kJ/mol
Force-Bond Angle	17°

**(i) Equilibrium Geometry**



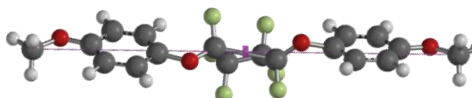
15.764 Å

**(ii) Immediately Prior to First Bond Cleavage**



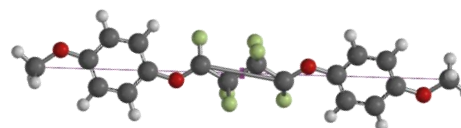
18.214 Å

**(iii) Immediately After First Bond Cleavage**



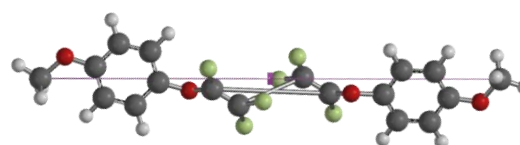
18.264 Å

**(iv) Immediately Before Second Bond Cleavage**

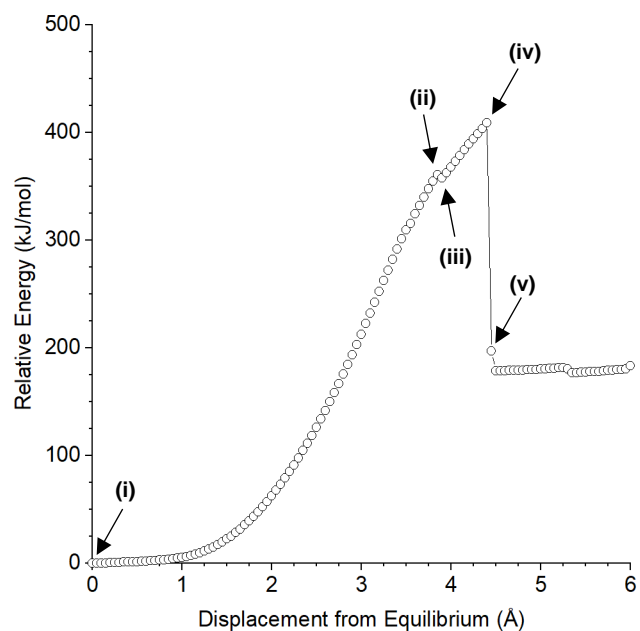
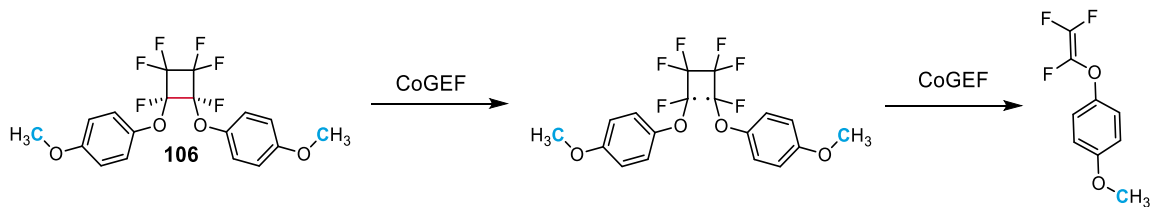


19.514 Å

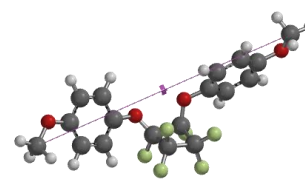
**(v) Immediately After Second Bond Cleavage**



19.562 Å

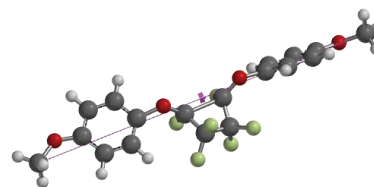


(i) Equilibrium Geometry



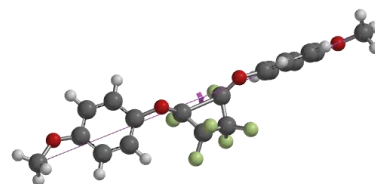
14.522 Å

(ii) Immediately Prior to First Bond Cleavage



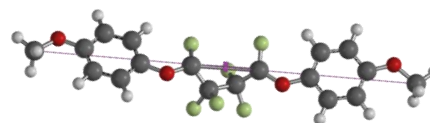
17.772 Å

(iii) Immediately After First Bond Cleavage



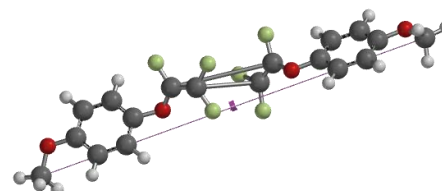
17.822 Å

(iv) Immediately Before Second Bond Cleavage



18.922 Å

(v) Immediately After Second Bond Cleavage



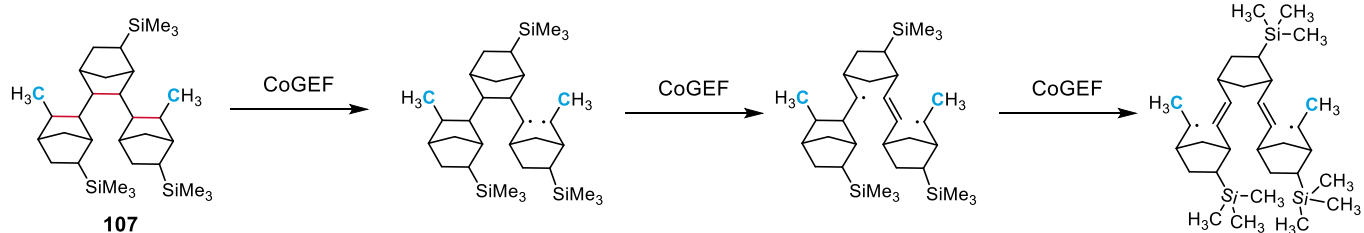
18.972 Å

**Summary of CoGEF Results**

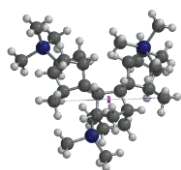
$F_{max}$  3.4 nN

$E_{max}$  409 kJ/mol

Force-Bond Angle 5.9°

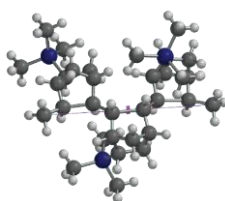


(i) Equilibrium Geometry



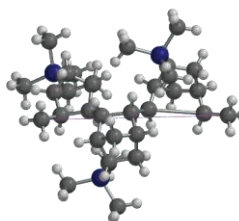
8.084 Å

(ii) Immediately Prior to First Bond Cleavage



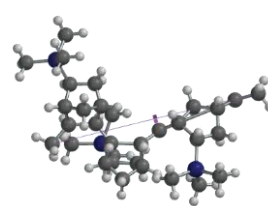
10.534 Å

(iii) Immediately After First Bond Cleavage



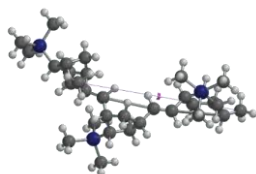
10.584 Å

(iv) Immediately Prior to Second Bond Cleavage



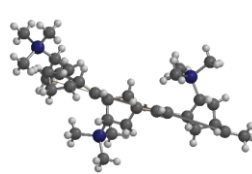
13.234 Å

(v) Immediately After Second Bond Cleavage



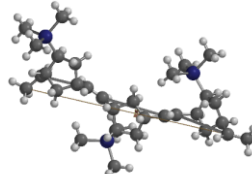
13.284 Å

(vi) Immediately Prior to Third Bond Cleavage

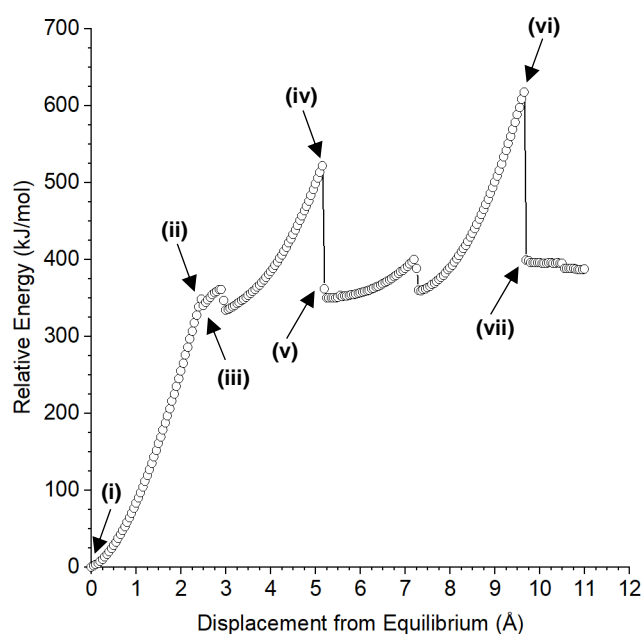


17.734 Å

(vii) Immediately After Third Bond Cleavage

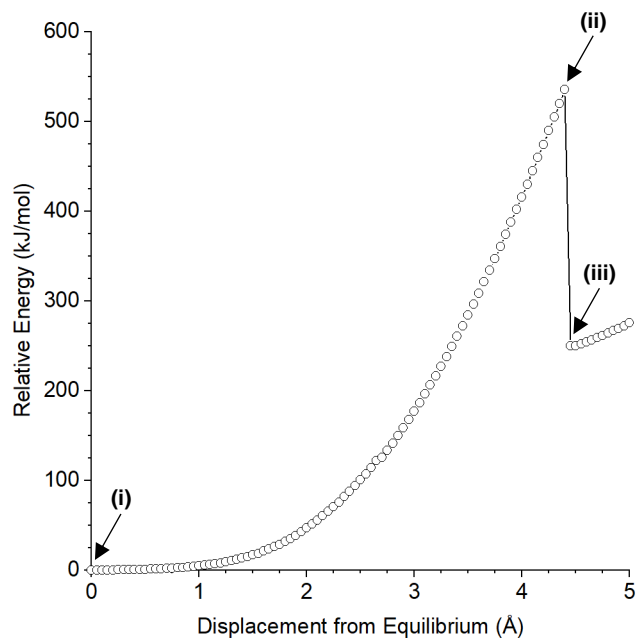
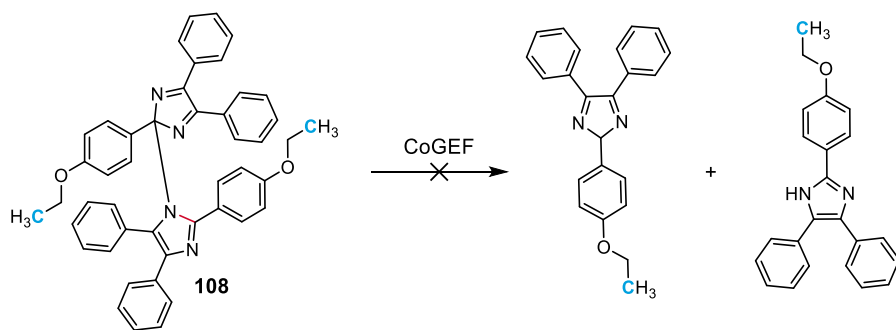


17.784 Å



#### Summary of CoGEF Results

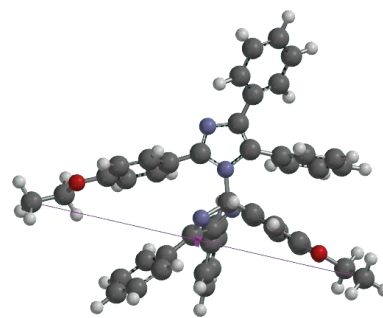
$F_{max}$	3.5 nN (first)
	2.6 nN (second)
	3.5 nN (third)
$E_{max}$	348 kJ/mol (first)
	521 kJ/mol (second)
	617 kJ/mol (third)
Force-Bond Angle	7.5° (first)
	16° (second)
	7.0° (third)



#### Summary of CoGEF Results

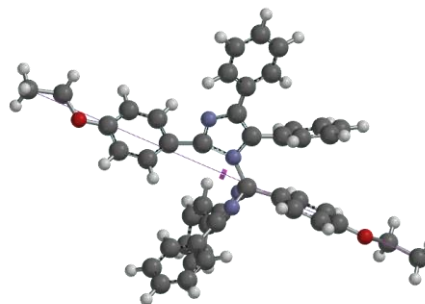
$F_{max}$	5.1 nN
$E_{max}$	536 kJ/mol
Force-Bond Angle	43°

#### (i) Equilibrium Geometry



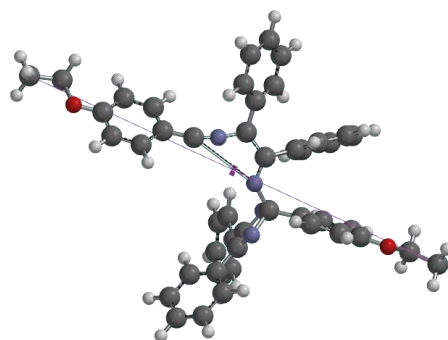
15.861 Å

#### (ii) Immediately Prior to Bond Cleavage

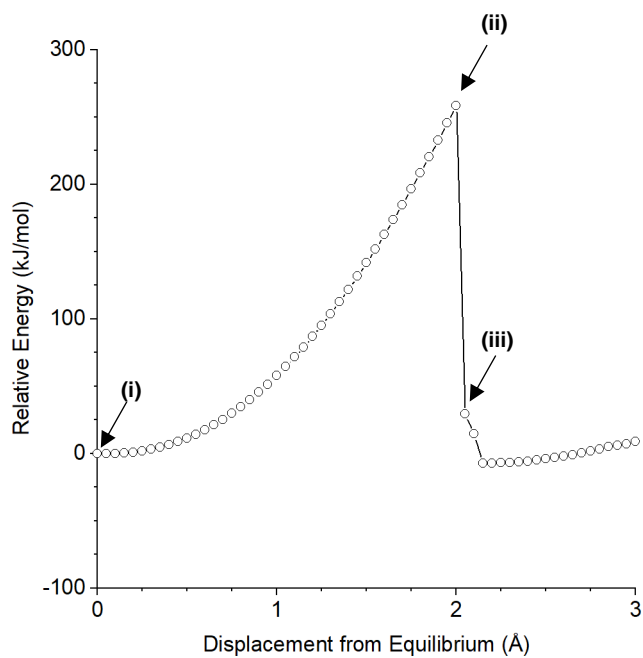
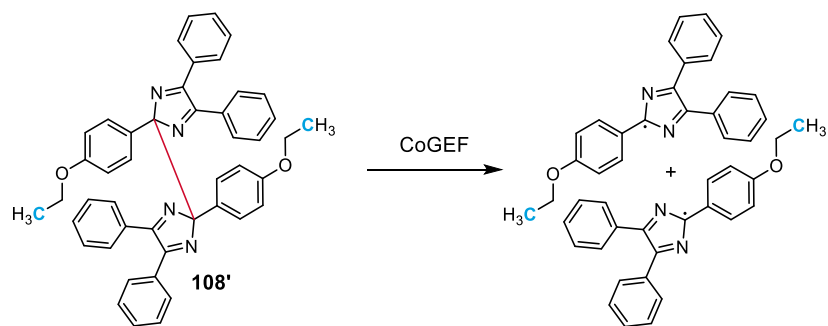


20.261 Å

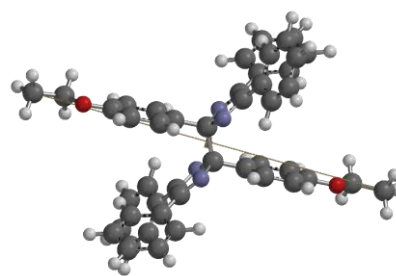
#### (iii) Immediately After Bond Cleavage



20.311 Å

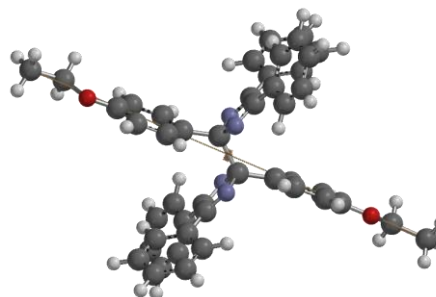


**(i) Equilibrium Geometry**



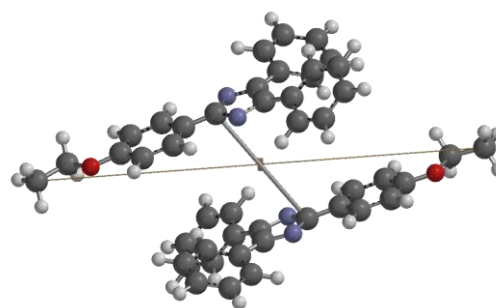
16.537 Å

**(ii) Immediately Prior to Bond Cleavage**



18.537 Å

**(iii) Immediately After Bond Cleavage**



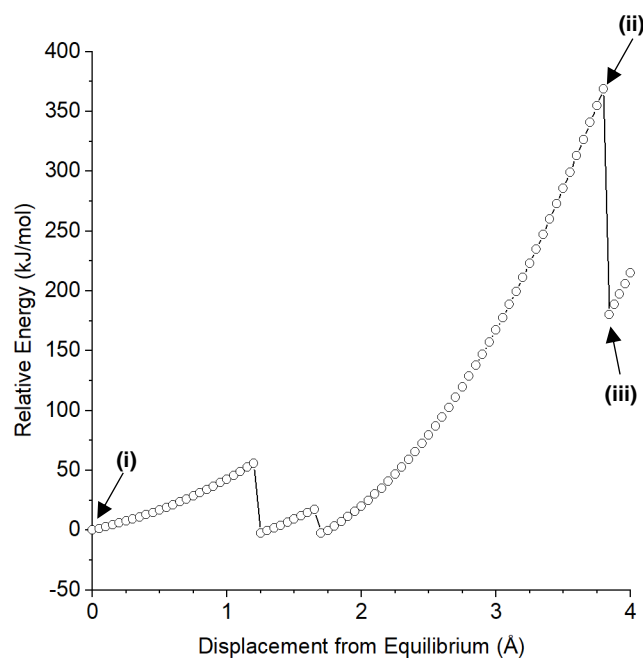
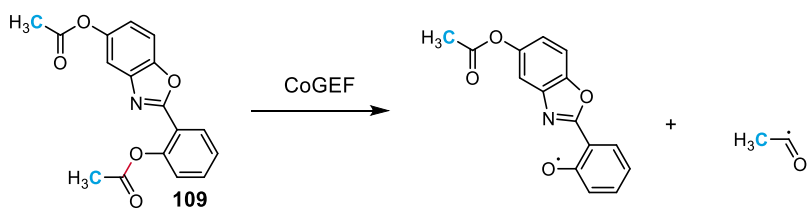
18.587 Å

**Summary of CoGEF Results**

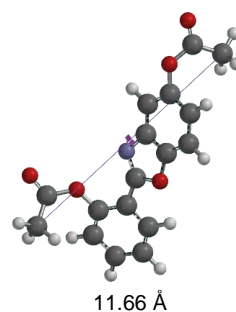
$F_{max}$  4.3 nN

$E_{max}$  258 kJ/mol

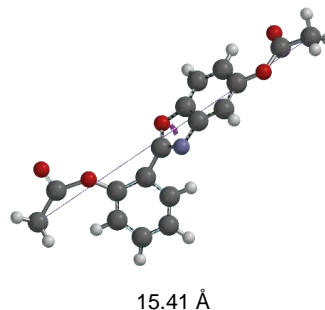
**Force-Bond Angle** 40°



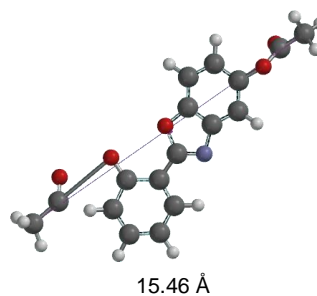
(i) Equilibrium Geometry



(ii) Immediately Prior to Bond Cleavage

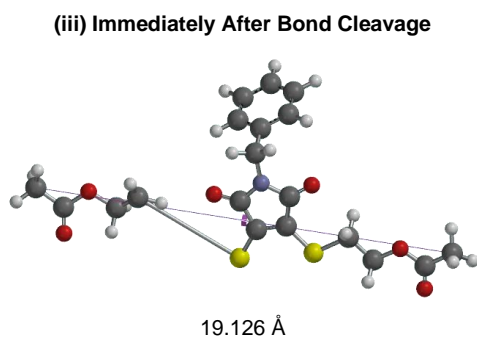
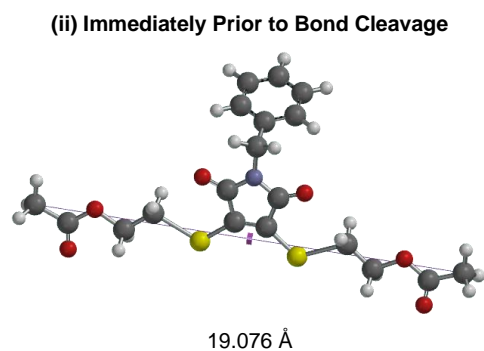
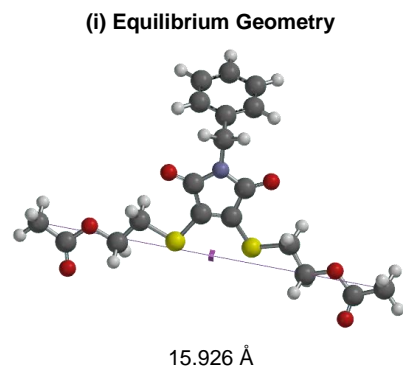
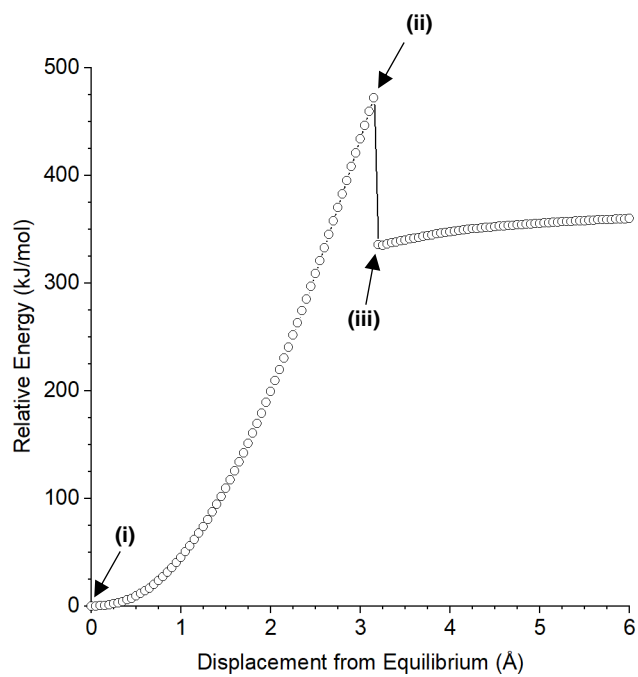
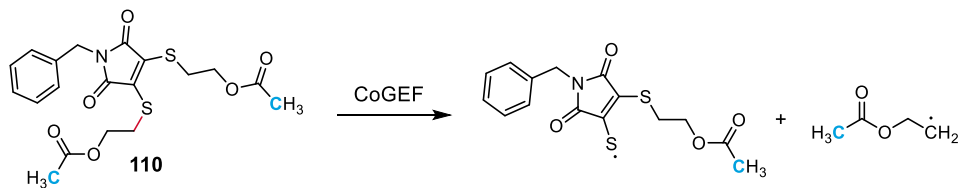


(iii) Immediately After Bond Cleavage



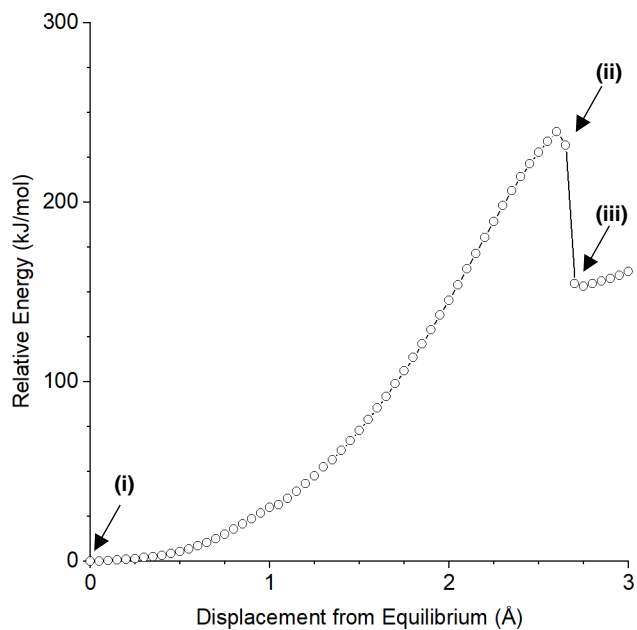
**Summary of CoGEF Results**

$F_{max}$	4.7 nN
$E_{max}$	369 kJ/mol
<b>Force-Bond Angle</b>	15°

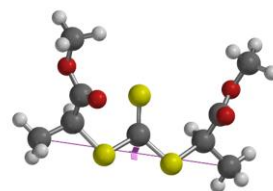


**Summary of CoGEF Results**

$F_{max}$	4.3 nN
$E_{max}$	472 kJ/mol
<b>Force-Bond Angle</b>	24°

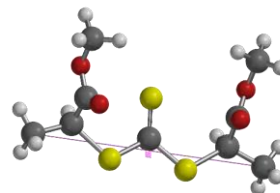


**(i) Equilibrium Geometry**



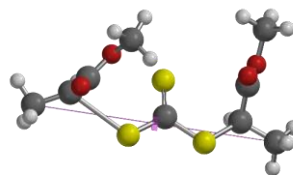
8.199 Å

**(ii) Immediately Prior to Bond Cleavage**



9.699 Å

**(iii) Immediately After Bond Cleavage**



9.749 Å

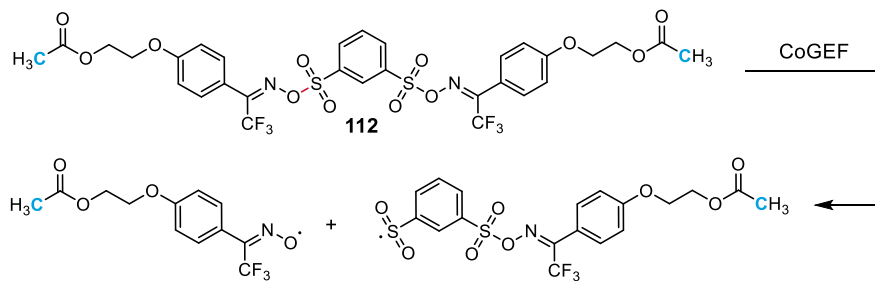
**Summary of CoGEF Results**

$F_{max}$  4.3 nN

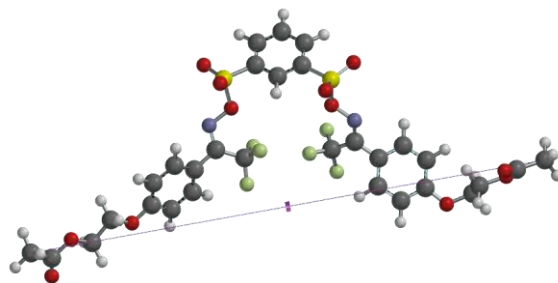
$E_{max}$  227 kJ/mol

**Force-Bond Angle** 35°



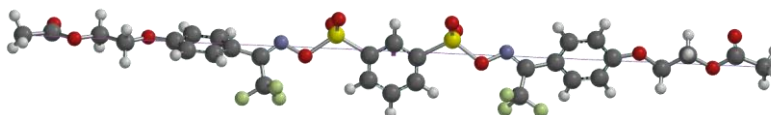


(i) Equilibrium Geometry



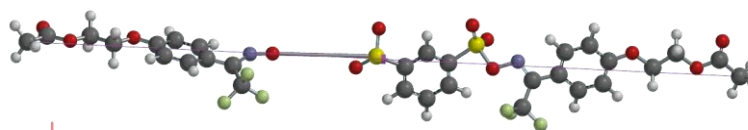
26.482 Å

(ii) Immediately Prior to Bond Cleavage

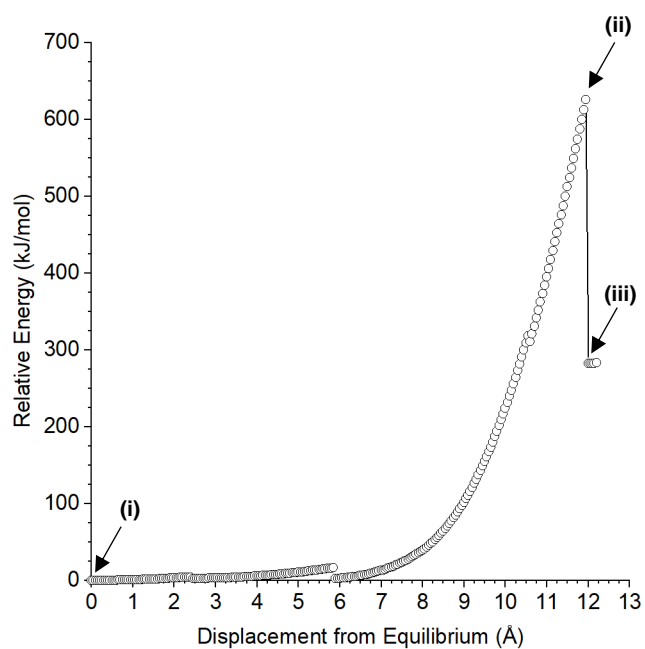


38.432 Å

(iii) Immediately After Bond Cleavage

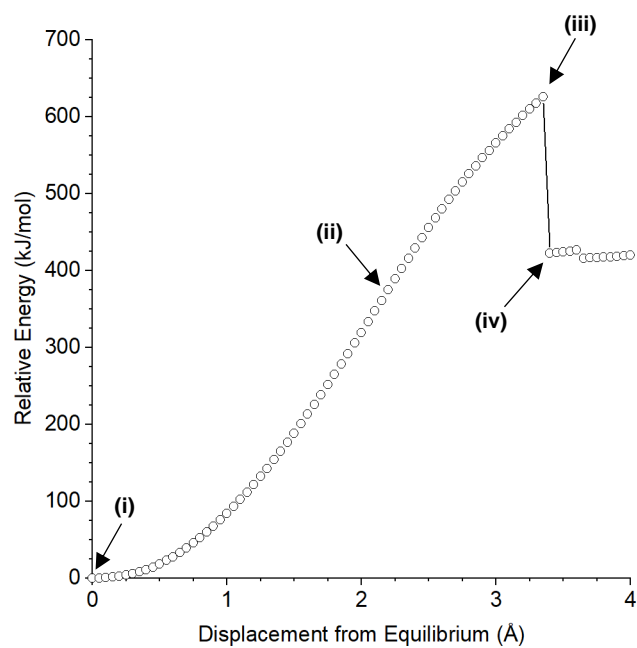


38.482 Å

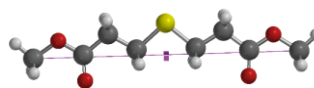


**Summary of CoGEF Results**

$F_{max}$	4.3 nN
$E_{max}$	625 kJ/mol
<b>Force-Bond Angle</b>	28°

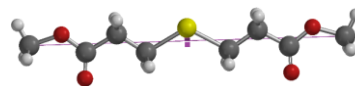


**(i) Equilibrium Geometry**



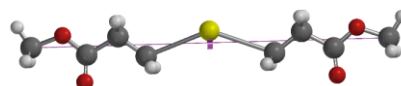
12.527 Å

**(ii) At  $F_{max}$**



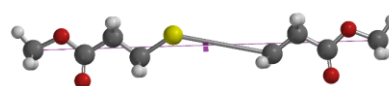
14.677 Å

**(iii) Immediately Prior to Bond Cleavage**



15.877 Å

**(iv) Immediately After Bond Cleavage**



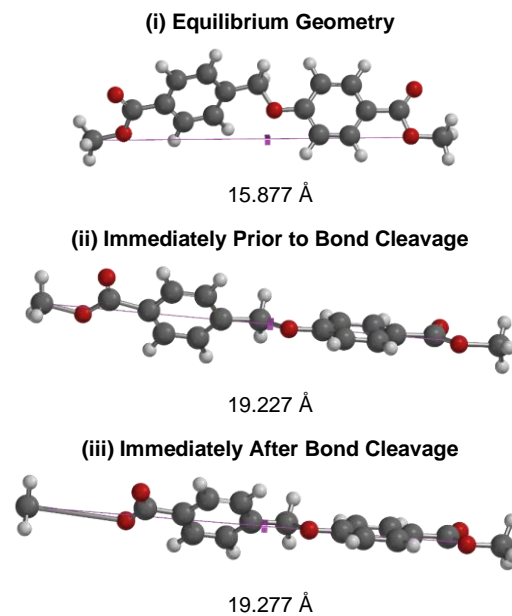
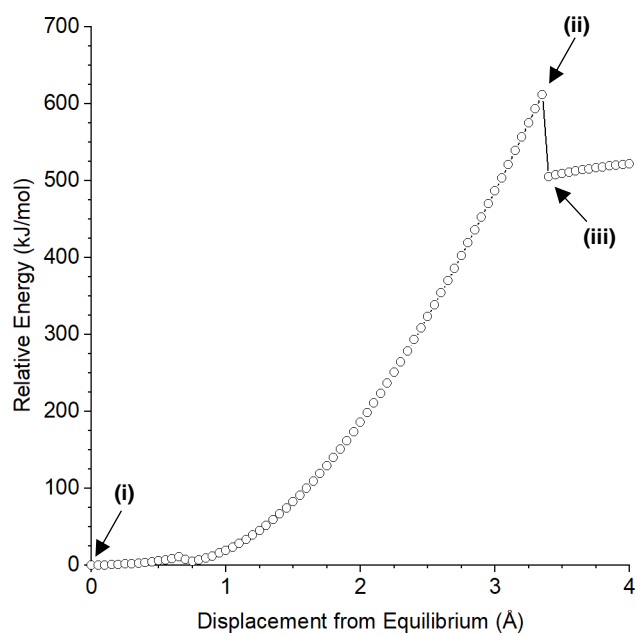
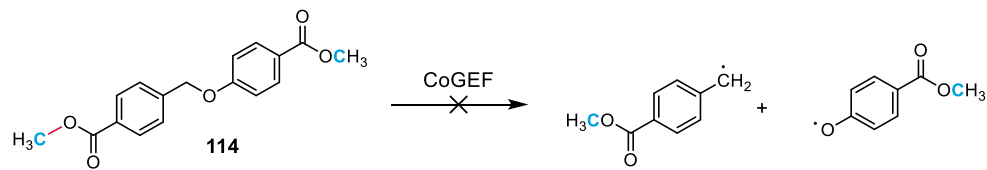
15.927 Å

**Summary of CoGEF Results**

$F_{max}$  4.6 nN

$E_{max}$  626 kJ/mol

**Force-Bond Angle** 20°

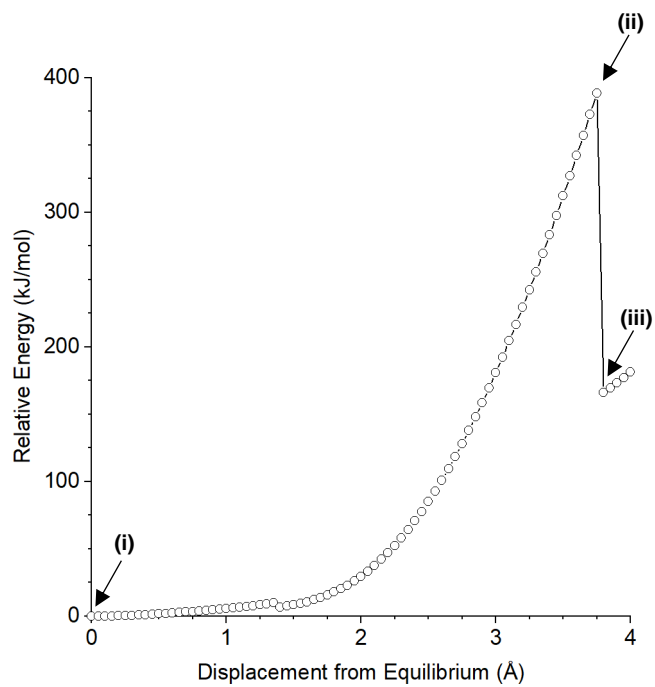
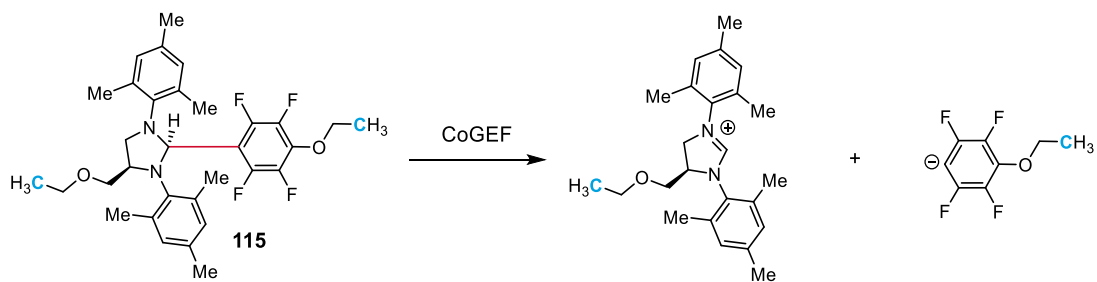


**Summary of CoGEF Results**

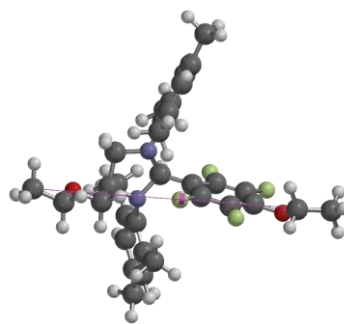
$F_{max}$  6.1 nN

$E_{max}$  611 kJ/mol

**Force-Bond Angle** 37°

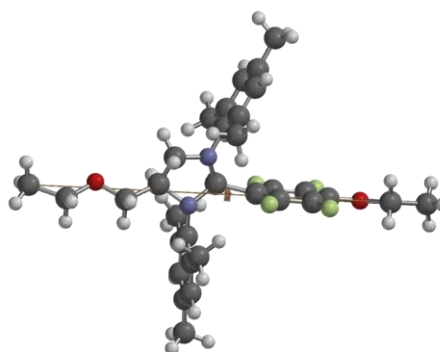


(i) Equilibrium Geometry



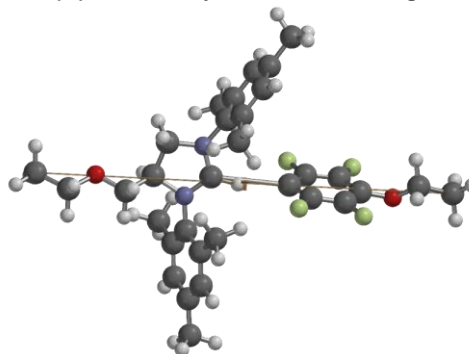
13.275 Å

(ii) Immediately Prior to Bond Cleavage



17.025 Å

(iii) Immediately After Bond Cleavage



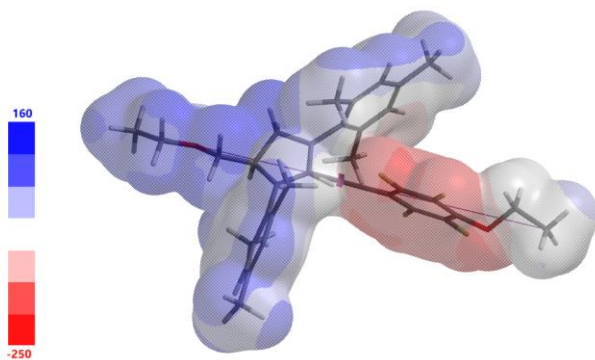
17.075 Å

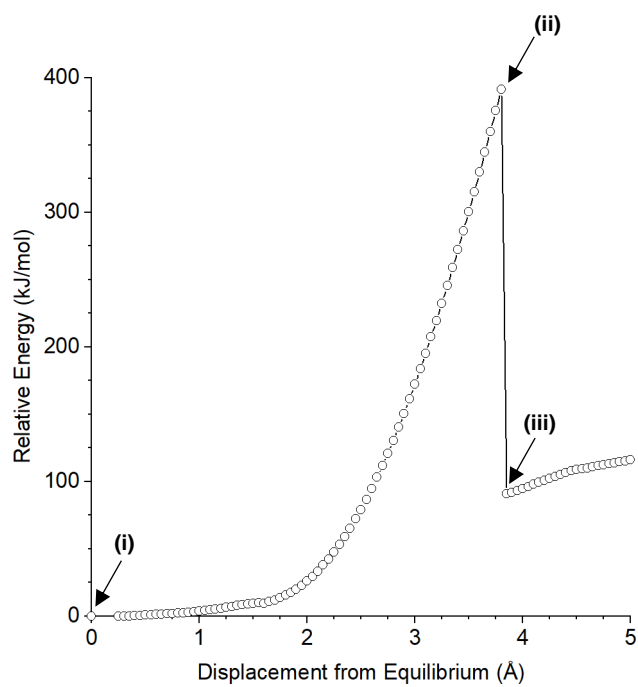
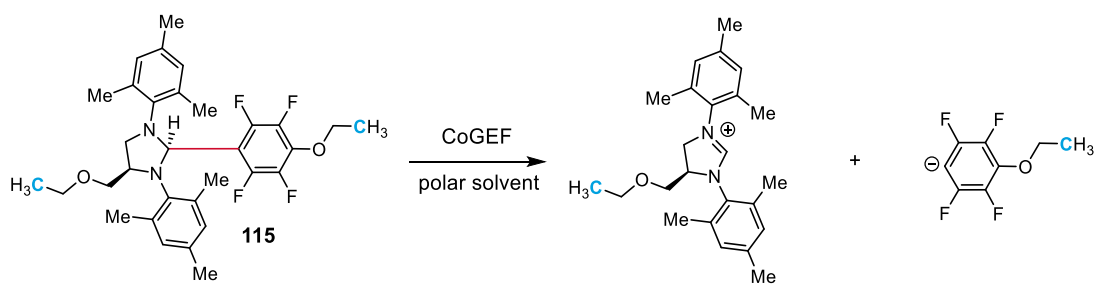
**Summary of CoGEF Results**

$F_{max}$  5.2 nN

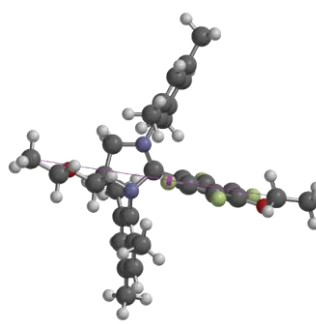
$E_{max}$  388 kJ/mol

Force-Bond Angle 13°



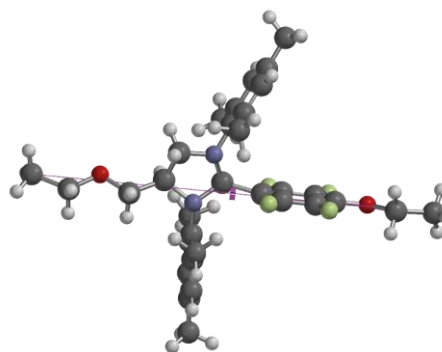


(i) Equilibrium Geometry



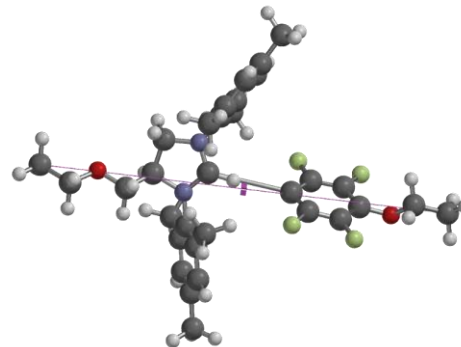
13.275 Å

(ii) Immediately Prior to Bond Cleavage



17.075 Å

(iii) Immediately After Bond Cleavage



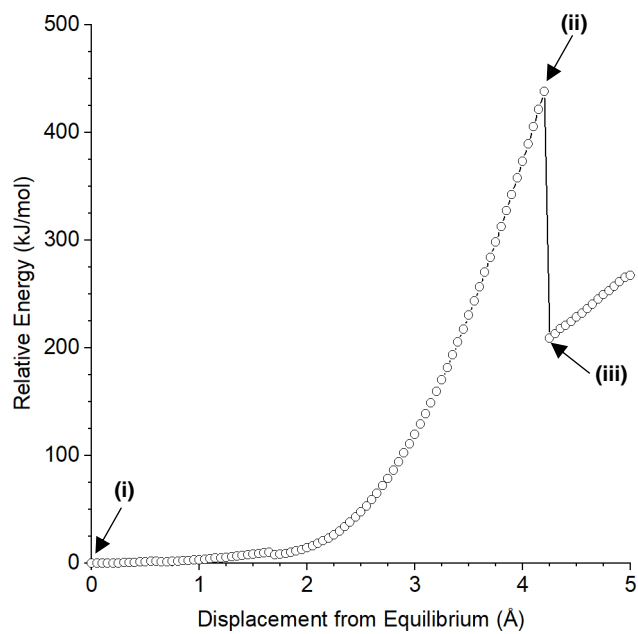
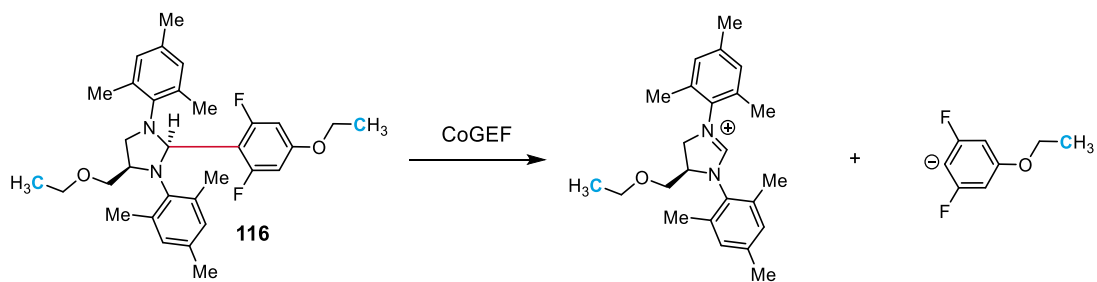
17.125 Å

**Summary of CoGEF Results**

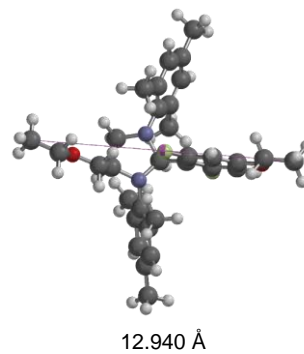
$F_{max}$  5.2 nN

$E_{max}$  391 kJ/mol

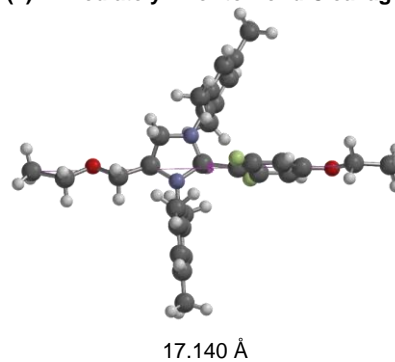
Force-Bond Angle 13°



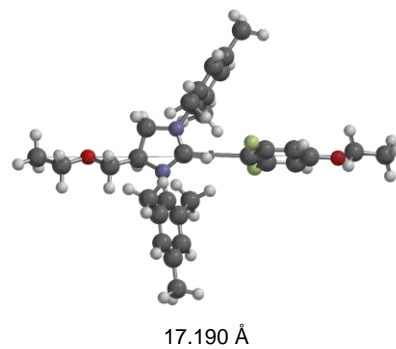
(i) Equilibrium Geometry



(ii) Immediately Prior to Bond Cleavage



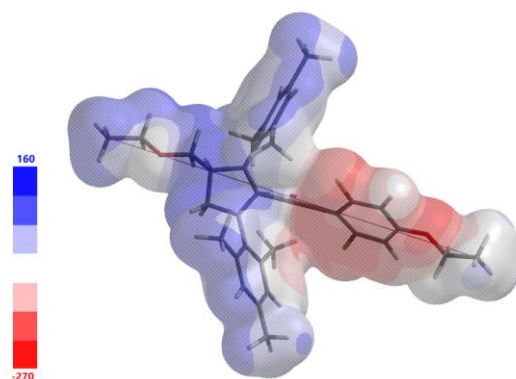
(iii) Immediately After Bond Cleavage

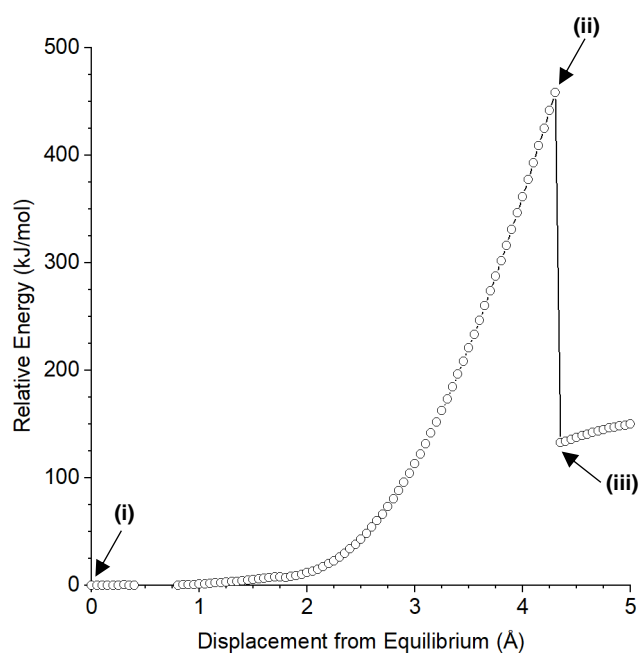
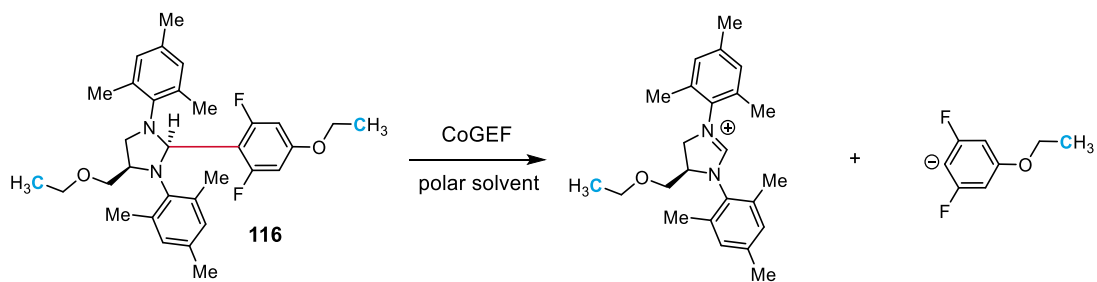


**Summary of CoGEF Results**

$F_{max}$  5.5 nN  
 $E_{max}$  438 kJ/mol

Force-Bond Angle 13°





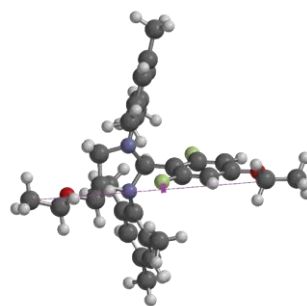
**Summary of CoGEF Results**

$F_{max}$  5.5 nN

$E_{max}$  458 kJ/mol

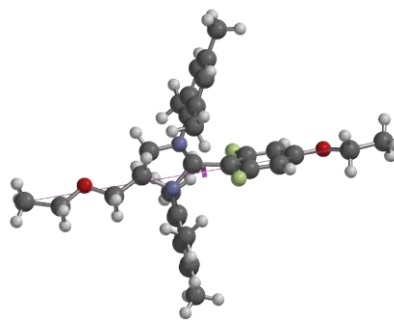
Force-Bond Angle 12°

**(i) Equilibrium Geometry**



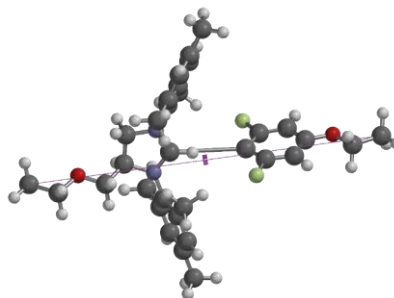
12.940 Å

**(ii) Immediately Prior to Bond Cleavage**

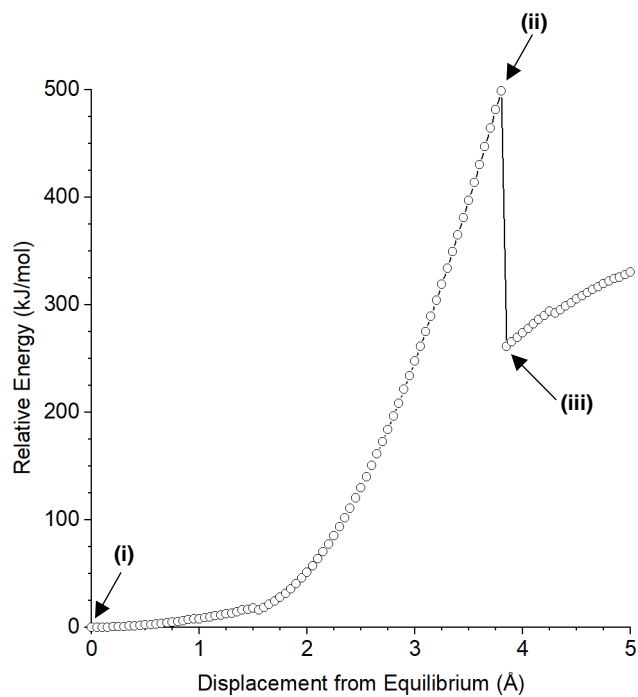
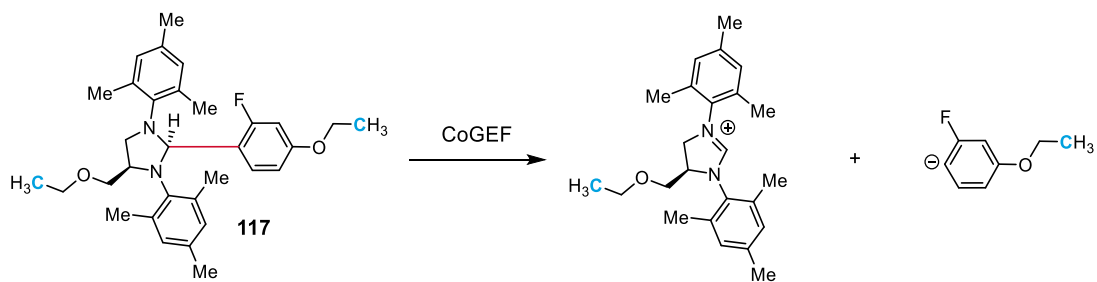


17.240 Å

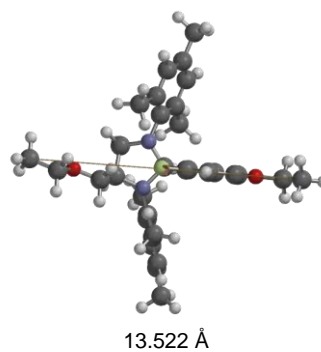
**(iii) Immediately After Bond Cleavage**



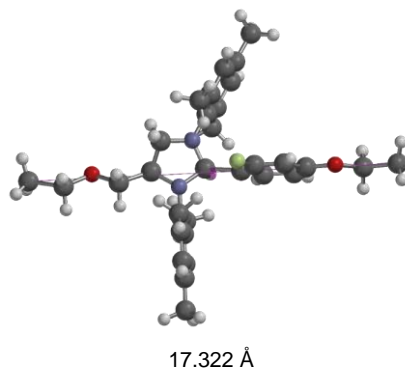
17.290 Å



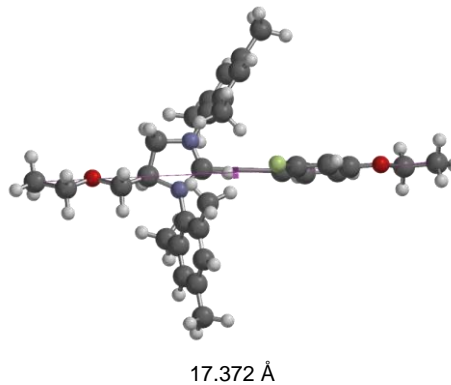
(i) Equilibrium Geometry



(ii) Immediately Prior to Bond Cleavage



(iii) Immediately After Bond Cleavage

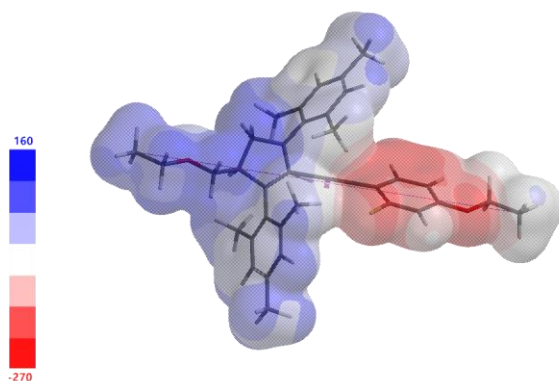


**Summary of CoGEF Results**

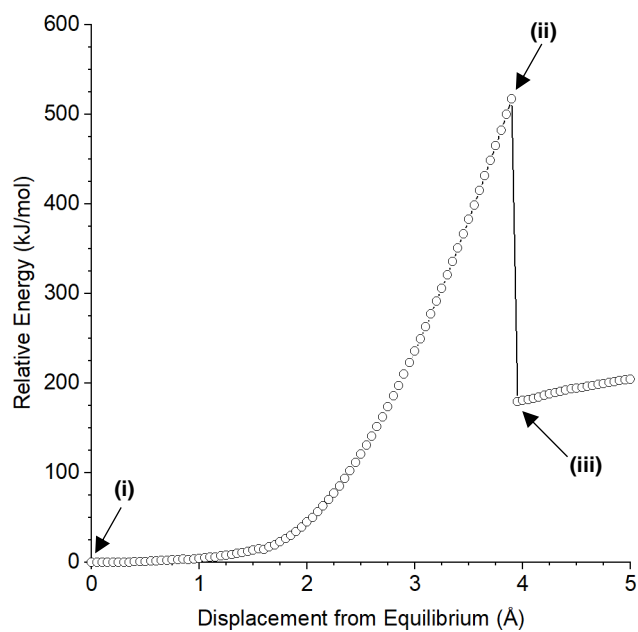
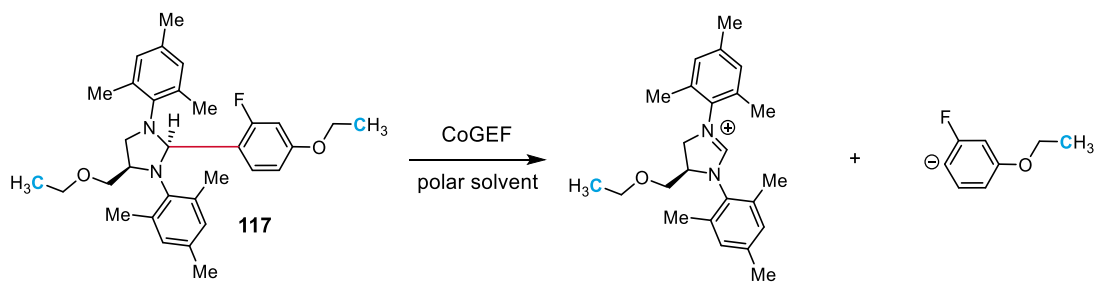
$F_{max}$  5.8 nN

$E_{max}$  499 kJ/mol

Force-Bond Angle 14°







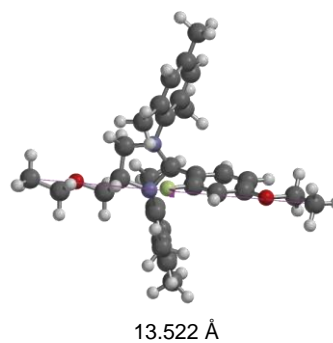
**Summary of CoGEF Results**

$F_{max}$  5.8 nN

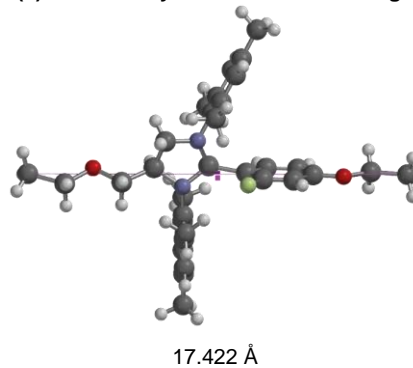
$E_{max}$  517 kJ/mol

Force-Bond Angle 14°

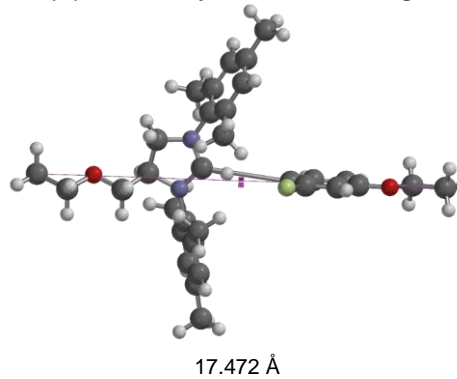
**(i) Equilibrium Geometry**

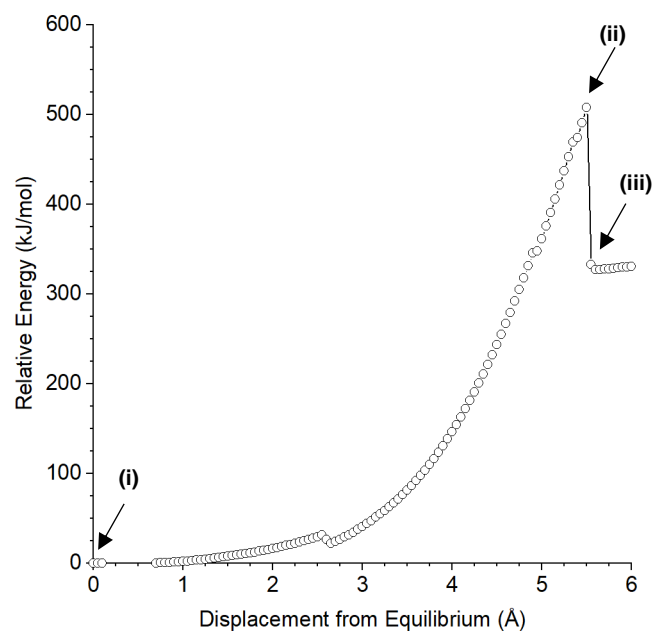
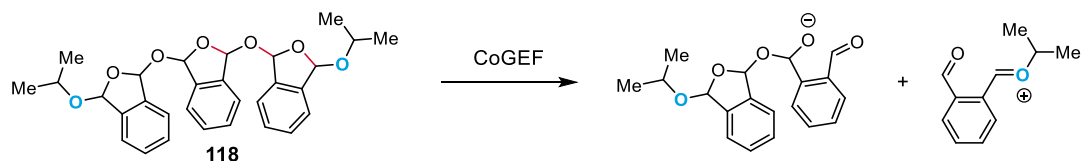


**(ii) Immediately Prior to Bond Cleavage**

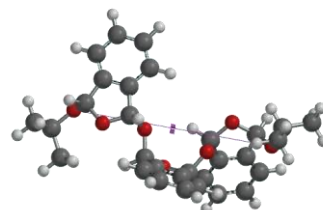


**(iii) Immediately After Bond Cleavage**



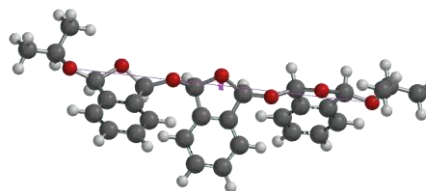


(i) Equilibrium Geometry



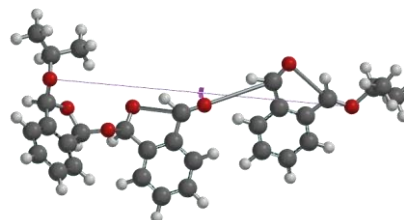
10.099 Å

(ii) Immediately Prior to Bond Cleavage



15.599 Å

(iii) Immediately After Bond Cleavage

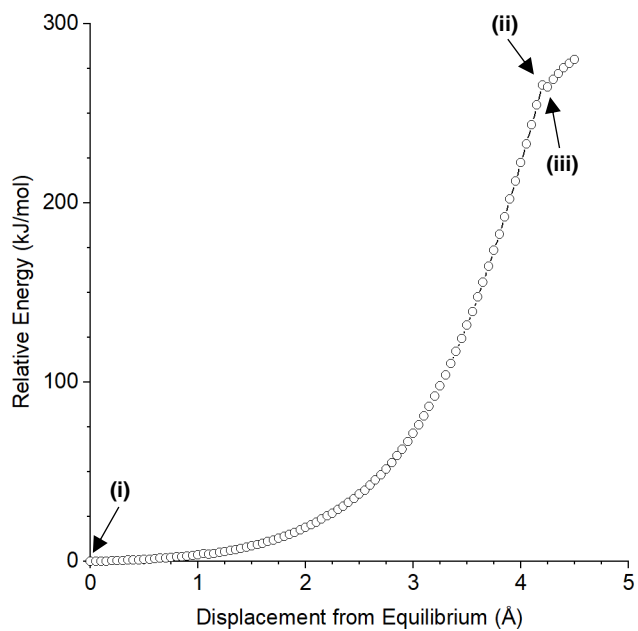
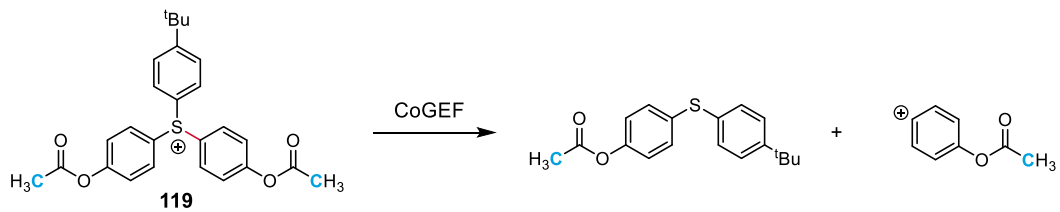


15.649 Å

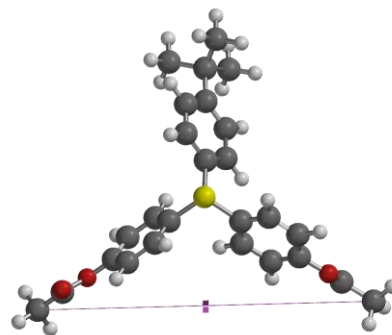
**Summary of CoGEF Results**

$F_{max}$	5.6 nN
$E_{max}$	507 kJ/mol
Force-Bond Angle	32°



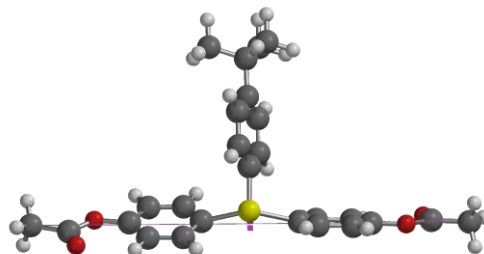


(i) Equilibrium Geometry



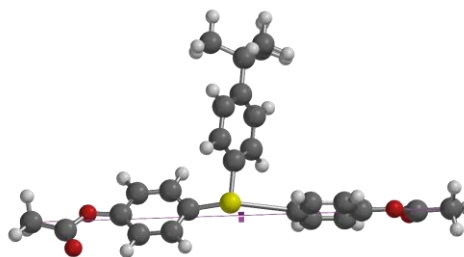
13.405 Å

(ii) Immediately Prior to Bond Cleavage



17.605 Å

(iii) Immediately After Bond Cleavage



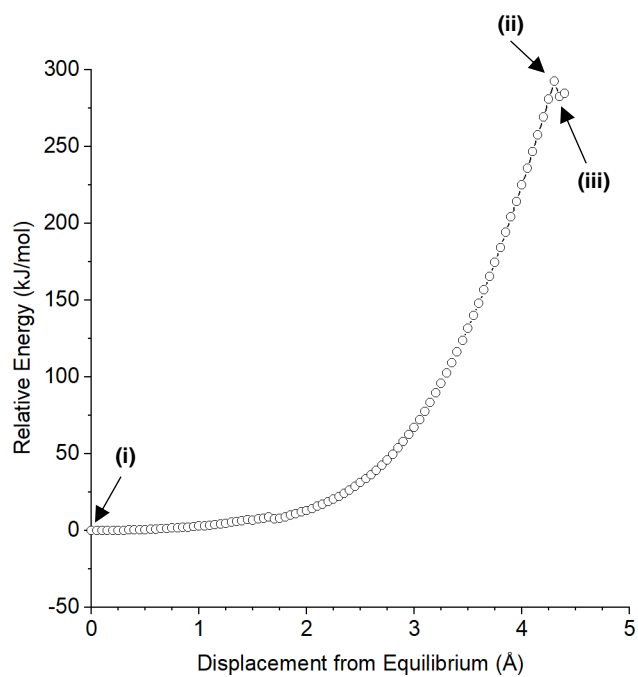
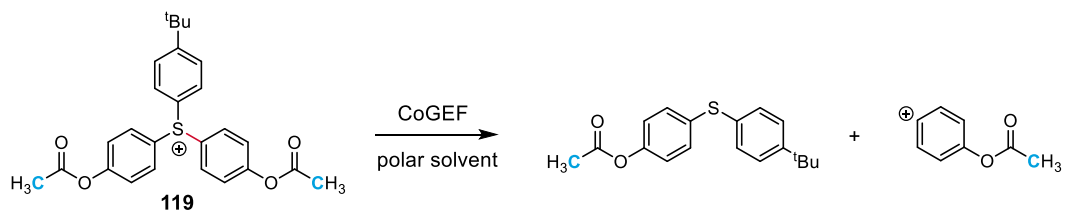
17.655 Å

**Summary of CoGEF Results**

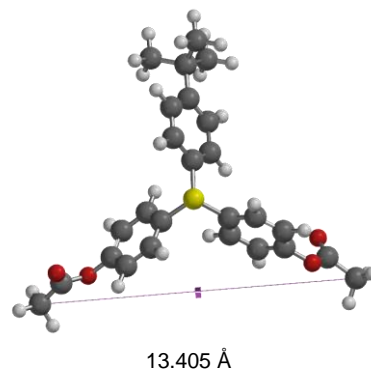
$F_{max}$  3.7 nN

$E_{max}$  266 kJ/mol

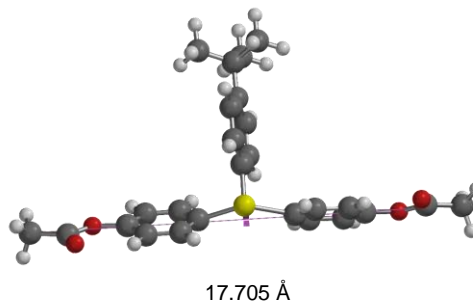
Force-Bond Angle 17°



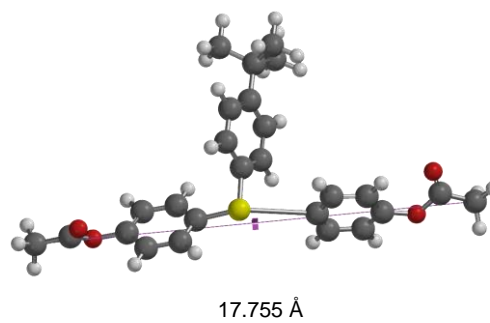
(i) Equilibrium Geometry



(ii) Immediately Prior to Bond Cleavage

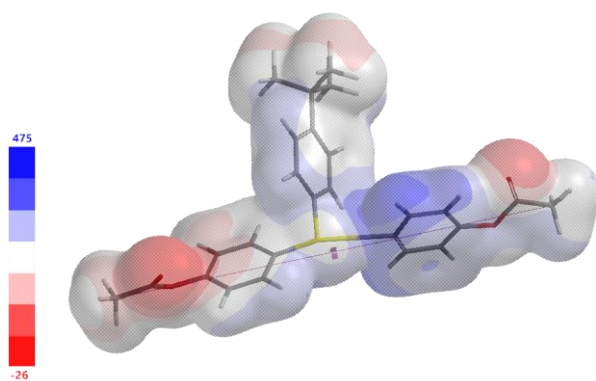


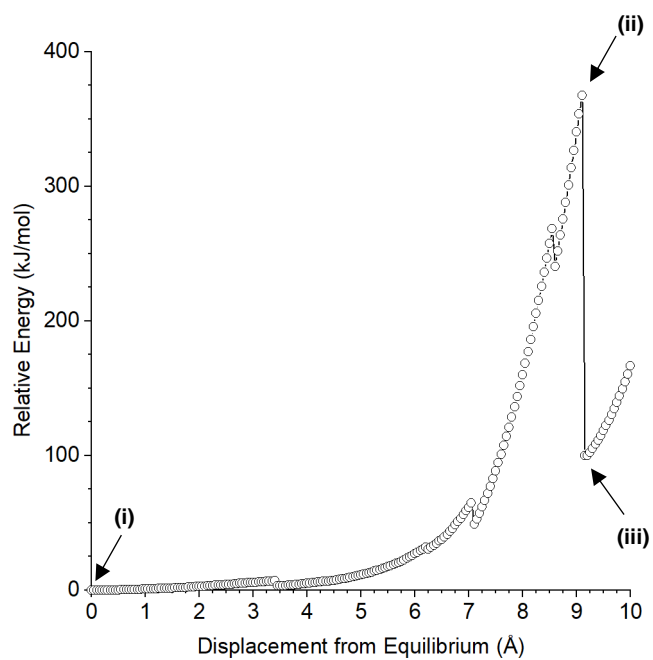
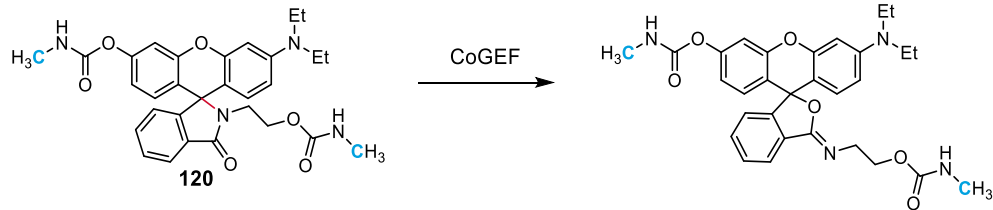
(iii) Immediately After Bond Cleavage



**Summary of CoGEF Results**

$F_{max}$	3.9 nN
$E_{max}$	292 kJ/mol
<b>Force-Bond Angle</b>	18°

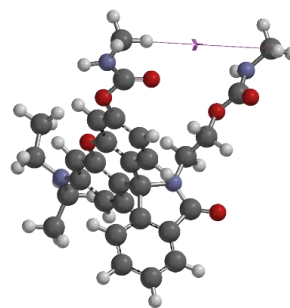




**Summary of CoGEF Results**

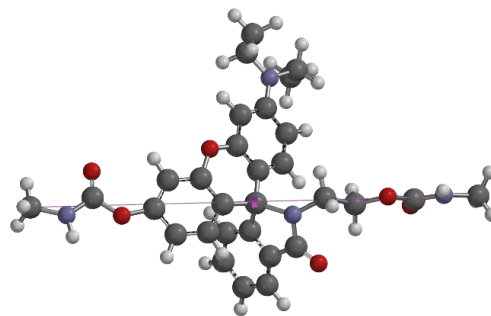
$F_{max}$	4.6 nN
$E_{max}$	368 kJ/mol
<b>Force-Bond Angle</b>	32°

**(i) Equilibrium Geometry**



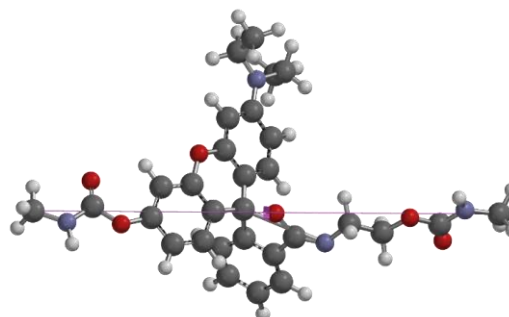
9.989 Å

**(ii) Immediately Prior to Bond Cleavage**

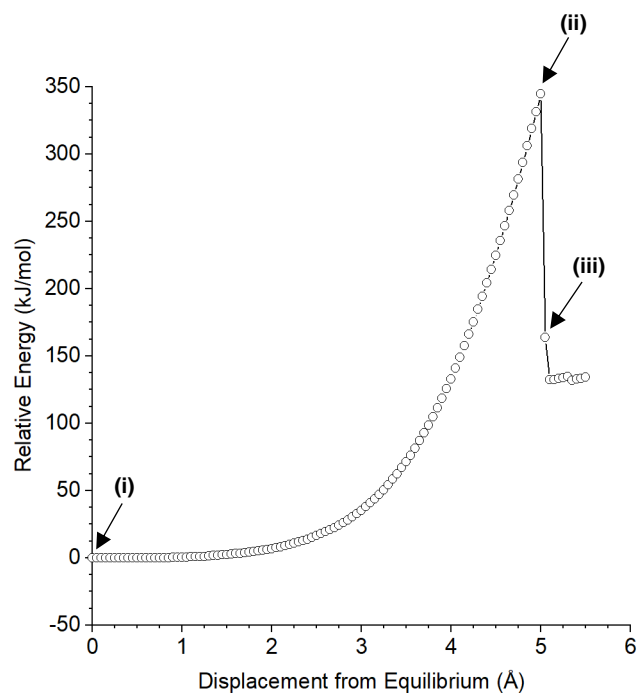
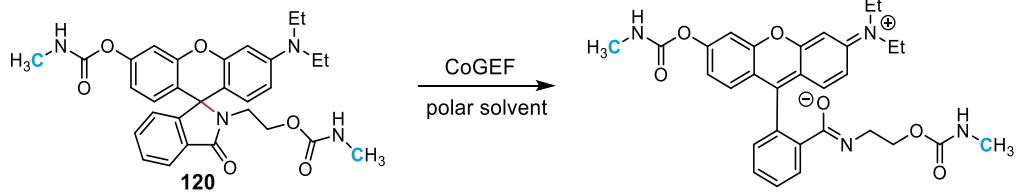


19.089 Å

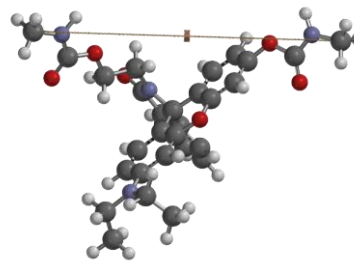
**(iii) Immediately After Bond Cleavage**



19.139 Å

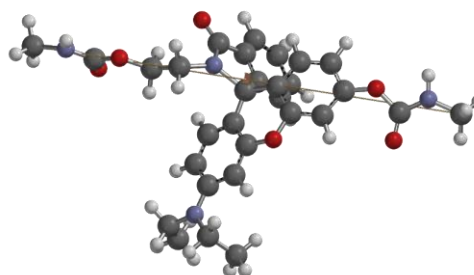


(i) Equilibrium Geometry



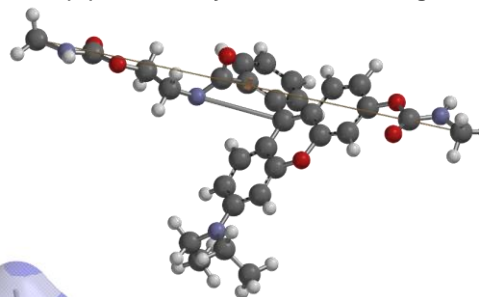
14.019 Å

(ii) Immediately Prior to Bond Cleavage



19.019 Å

(iii) Immediately After Bond Cleavage



19.069 Å

**Summary of CoGEF Results**

$F_{max}$  4.3 nN

$E_{max}$  345 kJ/mol

Force-Bond Angle 32°

