

Stereochemistry Lab Report

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Introduction

The purpose of this preparatory experiment is to use melting point to determine whether a compound is erythro or threo by adding aqueous hydrogen bromide and hydrogen peroxide to a stirring solution of trans-Stilbene and ethanol while heating under reflux.

Procedure

1. Rinse glassware with ethanol
2. Put 0.002 moles of trans-stilbene and 10 mL of ethanol in a 50 mL round bottom flask
 - a. Add a stir bar and place on stirring hot plate
 - b. Fit flask to reflux condenser
3. Heat flask to a boil. Adjust the hotplate settings so that the vapor condenses halfway up the condenser
 - a. Once the mixture refluxes properly, add 0.8 mL of concentrated hydrobromic acid to the flask using a pasteur pipet (each drop is approximately 0.05 mL, so ~16 drops)
 - b. Then add 0.3 mL (~6 drops) of hydrogen peroxide¹. Initial colorless mixture will change to a dark golden yellow color
 - c. Keep heating at least 20 minutes until yellow color fades and mixture becomes cloudy white
4. Clean NMR tube with acetone and let it dry
5. After 20 minutes, remove the flask from the heating mantle and allow to cool
6. Use pH paper to adjust the pH of the solution 5 to 7 through adding NaHCO₃
7. Continue the cooling of the reaction mixture in an ice bath to crystallize the rest of product out of solution
8. Collect the solid using vacuum filtration
9. Carefully wash with cold ethanol to remove trace impurities
10. Determine melting point and yield of product
11. Submit the sample for NMR

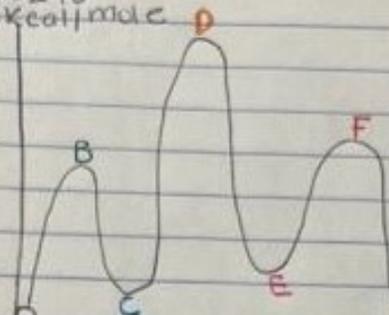
$$\Delta G_{\text{reaction}} = \Delta G_{\text{products}} - \Delta G_{\text{reactants}}$$

$$K_{\text{eq}} = \frac{[\text{Products}]}{[\text{Reactants}]}$$

$$= e^{-\Delta G/RT}$$

Butane

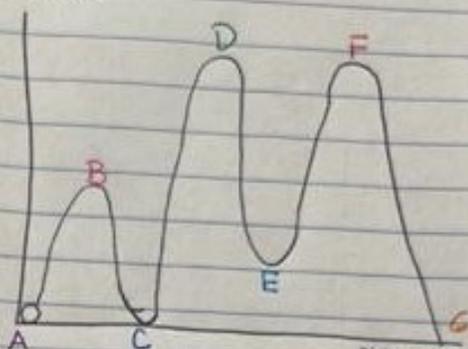
Energy
4.02 to
9.06 kcal/mol



Dihedral Angle 1
-180.02

<p>A</p>	<p>0 interactions</p>	<p>4.019 kcal/mol</p>
<p>B</p>	<p>1 hydrogen-hydrogen eclipsing 2 Methyl-hydrogen eclipsing</p>	<p>4.019 kcal/mol 6.93</p>
<p>C</p>	<p>4.978 kcal/mol</p>	
<p>D</p>	<p>9.062 kcal/mol</p>	
<p>E</p>	<p>5.008 kcal/mol</p>	
<p>F</p>	<p>7.281 kcal/mol</p>	

2-methylbutane Energy
7.27 to 12.11 kcal/mol



Dihedral Angle 1
-180.02 to 180.02

