

Names: _____
Chem 226/ Fall 2005

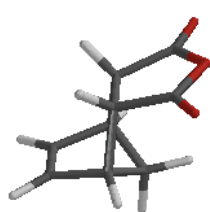
Section _____
Dr. Rusay

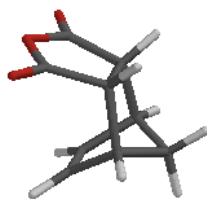
Molecular Modeling: Diels Alder Reactions (II)

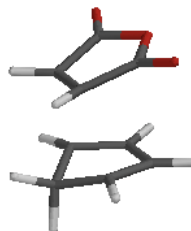
Working with a partner obtain a *Molecular Modeling Workbook* CD; using either a PC or Mac open Spartan View and folder 15-11A. Complete the following table for cyclopentadiene and maleic anhydride (use four decimal places for *au* values). Answer the questions that follow. Complete the work up of your reaction and identify your reaction product from the Diels Alder reaction of maleic anhydride and furan as exo- or endo- from its melting point, *Lehman*, Minilab #27, pp. 504-505 or the University of Saskatchewan publication (handout). Answer all of the accompanying questions.

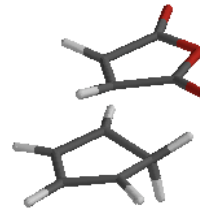
	Energy (<i>au</i>)	E _(Normalized) (<i>au</i>)	E _(Normalized) (kJ)
Reactants	-566.8205	0	
A) endo- T.S.			
B) exo- T.S.			
C) endo-product			
D) exo-product			

1. Match the following structures from the CD with the correct letter from the table above.









2. Normalize the values in column #1 of the table, i.e. subtract -566.8205 from each value and record in column #2. (The reactants will be equal to zero.) Then convert to kJ (1 *au* = 2625.5 kJ/mol); record in the third column and plot a Reaction Coordinate-Energy Diagram below that includes the two transition states and the two products.

ΔG
(kJ)



Which T.S. leads to the kinetic product?

Exo- or Endo

Which product is the thermodynamic product?

Exo- or Endo-

3. A DVC student transferred to the University of Saskatchewan and conducted the actual experiment that was in the handout. She obtained a solid product and when she took the melting point it strangely looked like the solid quickly went to a liquid and then vaporized at 162-163 °C. Search the NIST database for the physical properties of the products: exo-5-norbornene-2,3-dicarboxylic anhydride or use its CAS # [2746-19-2] and also search endo-5-norbornene-2,3-dicarboxylic anhydride [129-64-6]. Which product is obtained from this reaction based on the melting point data, the kinetic or thermodynamic product?
- _____

4. Recrystallize your reaction product and record its melting point. (m.p. _____ °C)
5. Which product did you obtain the exo- or endo-? _____ (It should be opposite of the cyclopentadiene product.)
6. Is your product the thermodynamic or kinetic product? _____
7. Your diene includes an oxygen and cyclopentadiene does not. Draw a resonance structure for furan. Furan has electron delocalization similar to benzene. Use this phenomena to explain why the product formed in your experiment does not form when oxygen is absent in the diene.