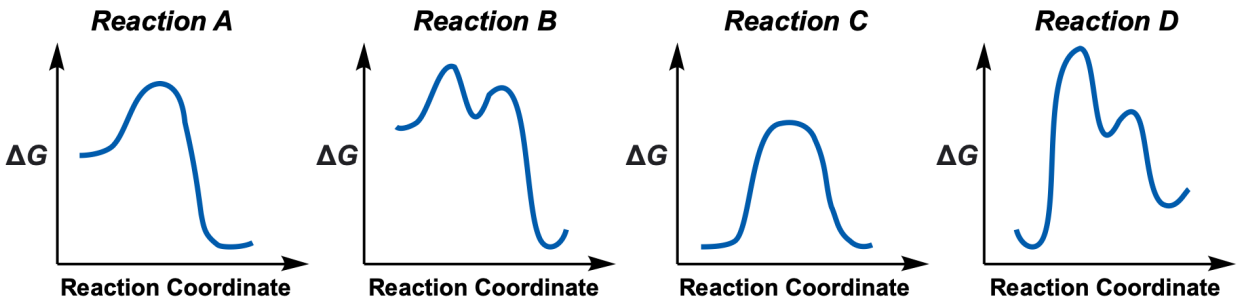
Name: _____
Class: _____

S_N2 Reactions Worksheet

Warm-Up Questions:

Read the Khan Academy article on endothermic vs. exothermic reactions. Then, consider the following four reaction energy diagrams.



1) Which energy diagram(s) correspond with a two-step mechanism?

2) Which energy diagram(s) correspond with a one-step mechanism?

3) Compare energy diagrams A and C. Which has a relatively larger activation energy (E_a) barrier?

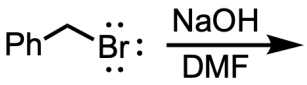
4) Compare energy diagrams A and D. Which has a positive ΔG?

5) Compare energy diagrams A and C. Which has a negative ΔG?

6) Compare all four energy diagrams. Which has the largest activation energy (E_a) barrier?

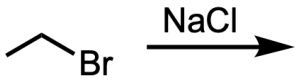
Example #1

Predict the product and arrow-pushing mechanism of the following SN2 reaction



Example #2:

Predict the product and arrow-pushing mechanism of the following SN2 reaction. Include the transition state structure of the reaction.



Example #3:

Using the AutoTS results, let's analyze the S_N2 reaction further. Answer the following questions:

a) Take screenshots of the optimized geometries for the reactants, transition state structure, and products.
b) List the bond distances of each molecule using the Measure button in units of ångstroms.

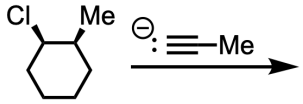
Reactants	Transition State Structure	Products
Screenshot:	Screenshot:	Screenshot:
C–C bond distance: C–Br bond distance:	C–C bond distance: C–Br bond distance: C–Cl bond distance:	C–C bond distance: C–Cl bond distance:

c) Now let's analyze the transition state structure. Look at the animation of its vibration. What is the geometry of the central carbon atom at the transition state? How does this differ from the electrophile's starting geometry as a reactant?

d) Take a screenshot of the reaction energy diagram. Is the reaction exergonic or endergonic? What is the activation energy barrier in units of kcal/mol? Would the reaction speed up or slow down if the nucleophile was iodide instead? Why?

Individual Exercise:

Answer the following questions based on the following S_N2 reaction:



a) Predict the product and arrow-pushing mechanism of the S_N2 reaction. Include the transition state structure of the reaction. Take note of any stereochemical inversions as well.

b) Look at the AutoTS results of this reaction. Go to **Tasks** and type **AutoTS Results**. Then import `SN2_1-Chloro-2-Methylcyclohexane_full_path.mae`. Recall that cyclohexane is not planar but is in a chair conformation. Redraw your S_N2 mechanism in chair conformation and take note of the substituent positions – are they in axial or equatorial positions? (Note: The carbon with chloride is C1 and the carbon with methyl is C2; the numbering of the ring is going clockwise).

c) Take screenshots of the optimized geometries for the reactants, transition state structure, and products. Try your best to capture the chair conformations by rotating the molecule. Also, list the bond distances of each molecule using the Measure button in units of ångstroms.

Reactants	Transition State Structure	Products
Screenshot:	Screenshot:	Screenshot:
C–Cl bond distance:	C(chair)–C(alkyne) bond distance: C–Cl bond distance:	C(chair)–C(alkyne) bond distance:

d) Take a screenshot of the reaction energy diagram. Is the reaction exergonic or endergonic? What is the activation energy barrier in units of kcal/mol?