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**Analyzing the Proposed Reaction Profile in “Changing the Charge: Electrostatic Effects in Pd-Catalyzed Cross-Coupling”**

Preparing for this Activity:

Read [*Organometallics*, **2016**, *35*, 3257-3260](https://doi.org/10.1021/acs.organomet.6b00622) with a focus on Figure 4

1FLO: Electron Counting and Electrostatic Effects in Palladium Carborane Complexes Activity

Activity Description:

In this activity, you will be working in groups of 3-4 to analyze *Organometallics*, **2016**, *35*, 3257-3260 by analyzing the proposed reaction profile in Figure 4. Please designate roles within your group as such: (1) Scribe: This person is in charge of writing down the group’s answers, (2) Facilitator: Keeps the team on task and on schedule, (3) Reference Manager: Identifies specific location of information within the paper to reference in the group’s answers, (4) Presenter (optional): Presents answers to the class.

**Insert figure 4 from:** [**https://doi.org/10.1021/acs.organomet.6b00622**](https://doi.org/10.1021/acs.organomet.6b00622)

Using the figure provided above to answer the following questions. Where appropriate, provide references to the place in the article where you located this information in the following format:

(Page #, Column #, Paragraph #, Line # when applicable) = (Pg.#:C#:P#:L#)

1. Which states are labeled as intermediates?
2. Which states are labeled as transition states?
3. What is the difference between a transition state and an intermediate?
4. Why does complex 2 have an enthalpy of 0.0 kcal/mol?
5. Identify the substrate of the reaction and in which complex it is included in the reaction profile.
6. Which state is the most stable?
7. What is the relative enthalpy of the most stable state?
8. Why are some states labeled as black and some as blue?
9. What are the major and minor products of this reaction?
10. Is the major or minor product more energetically stable? Why or why not?
11. If you heated the reaction, would you expect the ratio of the products to change? Why or why not?
12. Compare the relative enthalpies of complex 2 and complex II: (1) What effect do the authors attribute to driving the reaction from complex 2 to complex II, (2) What structural differences between these complexes would result in the observed energy difference?
13. Considering the relative strengths of C-Br vs C-Cl bonds, would you expect the catalyst to work better or worse with bromobenzene as a substrate?
14. In the article, the authors describe a number of control experiments that were used to help determine the mechanism of the reaction. Please identify and explain two of these experiments and what the authors concluded about the catalytic mechanism.