

Teacher's Guide to "Visualizing the Transition State and Reaction Coordinate"

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CHEMICAL CONCEPTS

This demonstration can be used when teaching chemical kinetics in a General Chemistry course or in a Physical Chemistry course.

Chemical Kinetics

- Activation energy
- Modeling chemical reactions, particularly isomerization reactions
- Lindemann mechanism for unimolecular reactions
- Dependence of reaction yield on particular partition of energy into internal modes of motion (vibrational, rotational)

Transition State Theory (Activated Complex Theory)

- Structure of the transition state
- Inherent instability of the transition state
- Observation of the reaction coordinate (reaction progress)

HOW THE DEMONSTRATION ADDRESSES THE CHEMICAL CONCEPTS

Transition state theory (TST), also called activated complex theory, is often introduced in general chemistry courses when discussing kinetics. A reaction energy diagram is used to follow the progress of the reaction from reactants through a transition state to products (see figure 1). The reaction energy diagram plots the system's potential energy versus reaction coordinate (or reaction progress) and shows that reactant molecules must overcome an activation energy barrier to pass through the transition state (activated complex) to form products. This demonstration takes the very abstract concepts of transition state, activation energy, and reaction coordinate and makes them more concrete and accessible. The demonstration uses a child's toy (Hoberman Switch Pitch) to model a chemical reaction that follows a reactant through a transition state before making a product. The reaction coordinate, activation energy, and specific geometry of the transition state are discussed as part of a question and answer dialogue. The complex, multi-dimensionality of a reaction coordinate and the inherent instability of a transition state become evident. The demonstration also shows that certain reactions may "go" more readily if the energy of a reactant is in a particular type of internal mode (vibrations or rotations). Often, the preferential partition of a given total energy into internal modes of motion (vibrational, rotational) versus translational collision energy allows the system to access the transition state more easily.

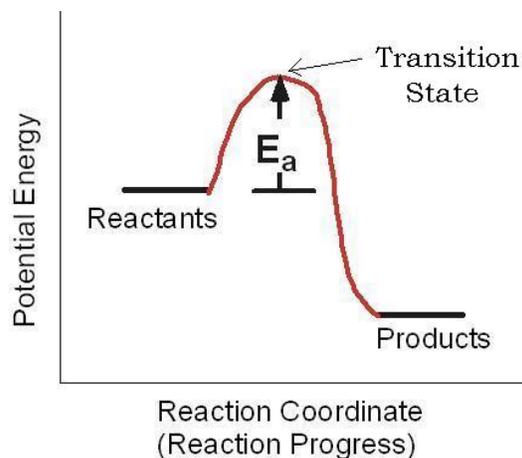


Figure 1: Reaction Energy Diagram

PREPARING THE DEMONSTRATION

Safety

- This demonstration only uses children's toys. No safety measures need to be taken.

Equipment and Materials

- 2 Switch Pitch balls by Hoberman Toys
(<http://hoberman.com/fold/Switchpitch/switchpitch.htm>)
- alternative toy: Switch kick by Hoberman Toys

DEMONSTRATION USE IN THE CLASSROOM

Material Presented before the Demonstration:

In the class leading up to the demonstration, the Arrhenius equation ($k = Ae^{-E_a/RT}$) and collision theory have been covered. Therefore, the students know that only a collision with energy greater than the activation energy, E_a , and the correct molecular orientation will lead to products. Before the demonstration is performed, background into transition state theory is given. A reaction energy diagram (Figure 1) is presented on the chalk board (complete with axes labeled: potential energy vs. reaction coordinate (or reaction progress)). The activation energy, E_a , (the change in energy from reactants to the top of the "hill") is labeled. The students are taught that the species at the top of the activation energy barrier is the **transition state** or **activated complex**. They are also taught that this species is highly unstable (picture a ball precariously positioned on top of a horse's saddle). Once the reaction has proceeded through the transition state, products are quickly formed as the reaction advances steeply downhill. The necessity of reactants to overcome an activation energy barrier to proceed to products has already been introduced in the discussion of the Arrhenius equation. Transition state theory, however, explains *why* the activation energy is needed: bonds in the reactant molecules must stretch and deform in order to reach the transition state. [The reaction of $2\text{BrNO} \rightarrow 2\text{NO} + \text{Br}_2$ is one example that I have used (see figure 2).]

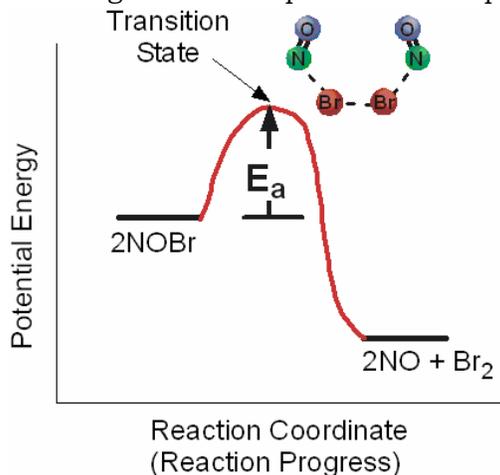


Figure 2: Reaction Energy Diagram for $2\text{NOBr} \rightarrow 2\text{NO} + \text{Br}_2$

Using the demonstration:

The demonstration is performed in a question and answer format.

I begin the demo with some (rhetorical) questions: "OK, now the concepts we just covered are pretty complicated! What does a transition state look like? Why is it unstable? What the heck does the term "reaction coordinate" or "reaction progress" really mean???" Well—you're in luck! I have a toy that will help to clarify these questions!"

I then bring out the Switch Pitch toy. I ask them to note the color of the ball. Then I lightly toss the ball in the air (just a little bit and as straight as possible—try to NOT spin it!). [NOTE: You do NOT want the ball to change colors immediately.] The students will see that the ball is not rigid—its parts move.

Next, toss the ball up a little harder so that it inverts and therefore changes color! Note: this may take a couple of tosses. I usually say “Wow!” or “Cool” or “Did you see that?!!” To preview the action of a Hoberman Switch Pitch, please see the following URL: <http://hoberman.com/fold/Switchpitch/switchpitch.htm>

I then ask the students “How can you relate the demonstration to a reaction energy diagram that shows an actual chemical reaction?” I guide the students as needed to the answers given here:

- The initial color of the ball represents a reactant molecule (R).
- The final color of the ball represents a product molecule (P).
- The activation energy for the reaction is related to how high the ball must be thrown in order to convert from $R \rightarrow P$.
- The configuration of the transition state is when the Switch Pitch is fully extended. You will have to pull the Switch Pitch apart to show the geometry of the transition state.
- The transition state is unstable. Here is one way to show this: after pulling the Switch Pitch apart to be fully extended, place it on the desk—it will collapse back to R or P. If the reaction has proceeded “through” the transition state, products will form.
- The reaction coordinate involves the *entire* “molecule” moving. The reaction coordinate is complicated and multi-dimensional (for the Switch Pitch or *any* (even simple!) chemical reaction). The term “reaction progress” is more descriptive and intuitive. When toggling on the action of the Switch Pitch at <http://hoberman.com/fold/Switchpitch/switchpitch.htm>, the axis that you are controlling is the “reaction progress” or “reaction coordinate.”

After discussing these aspects of the demo, I pose the question, “Does the Switch Pitch model a (bimolecular) reaction between dissimilar molecules (such as the $2\text{BrNO} \rightarrow 2\text{NO} + \text{Br}_2$ example)?” [Answer: NO!] “What type of reaction does this toy model?” [If the students struggle with this, I get them to tell me that it models only a *rearrangement* of a molecule.] “What do we call two molecules that have the same molecular formula but different arrangement of atoms?” [Answer: ISOMERS!!!] “Therefore, the Switch Pitch actually models an *isomerization reaction*.” If desired, at this point more information can be given about a specific isomerization reaction, such as cyclopropane \rightarrow propene.^{1,2} Please see the references for more information about this particular reaction.

Next, I pose the question, “Does the molecule isomerize all by itself?” [Answer: NO!] “What is necessary for this reaction to “go”?” [Answer: energy!] “From where does the energy come to surmount the activation barrier?” If the students were paying attention to the discussion of collision theory, they would immediately shout “from molecular collisions!”

At this point in the demonstration, I have two students participate in colliding two Switch Pitches together. I have the rest of the class predict under what conditions reactants will most efficiently convert to products. Possible variables include:

- total energy of collision
- impact parameter (do the balls collide head-on or off-center)
- angular momentum (amount of rotation of one or both balls)

One aspect that becomes evident is that if one or both “molecules” has extra rotational energy, products form more readily. This conclusion can easily be shown by throwing one Switch Pitch into the air—a very small amount of rotational energy changes the color of the ball, compared to a larger amount of translational energy needed to change the color of the ball (thrown straight up with no spinning). This conclusion mimics many chemical reactions that “go” more readily if, for a given total amount of energy, it is partitioned into internal modes of motion (vibrations and rotations) versus translational energy.^{3,4}

A “glancing blow” (larger impact parameter) also leads more readily to products. If the impact parameter changes, the entire reaction energy diagram changes: the reaction proceeds along a *different* reaction coordinate with different activation energy. For a larger impact parameter, the activation energy barrier is smaller, i.e., less energy is needed to surmount the activation barrier to make products.

Please note that the level of discussion of this demonstration can be further raised to the detail potentially presented in a Physical Chemistry course. The demo can be related to reaction mechanisms (specifically the Lindemann mechanism for unimolecular reactions⁵), potential energy surfaces, and molecular reaction dynamics.

Alternative Presentation Styles:

If desired, the demonstration may be used as a guided-inquiry group activity. A group of students would each be given a Switch Pitch. In much the same manner as described above, the students could be guided to determine:

- how the ball mimics a chemical reaction
- the type of chemical reaction it mimics (isomerization)
- the geometry of the transition state
- the instability of the transition state
- the reaction coordinate
- effect of preferential rotational energy vs. translational energy

Note: The demonstration may also be performed with a Hoberman Switch Kick. The Switch Kick is more durable and foamy but also more expensive.

REFERENCES

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⁴ Atkins, P. and de Paula, J., *Physical Chemistry*, 8th Ed., W. H. Freeman and Company: New York, 2006; pp. 887-890.

⁵ McQuarrie, D. A. and Simon, J. D., *Physical Chemistry: A Molecular Approach*, University Science Books, 1997, pp. 1198-1202.