Chemical Reactions and Molecular Interactions in the Gas Phase.

Summary for INSTRUCTORS

Below are links to two simulations carried out by the research group of W. L. Hase at Wayne State University. He has put them on the World Wide Web to accompany a technical manuscript (reference to be added). We are using these simulations to illustrate a number of chemical principles for high school and introductory college chemistry. This document is intended for free use by educators, but please look at the end of this document for information on legal/copyright issues.

This text is set up to used as an interactive learning experience for the students, rather than as a presentation by instructors. An *Initial Statement* gives students some background on how to interpret the animations. *Background Information* for instructors is presented immediately following the animations, together with Figures. These figures are not intended for the use of high school students. Of course, instructors may wish to present part, all, or none of this information to their students in place of, before, or after interactive work by the students. Following the information for instructors there are one or more series of related questions. The questions on electronegativity and on electron affinities should probably not be given to students on the same day as the other questions. Following each set of questions there is a *Suggested Summary Statement* to help students integrate what the animations and the answers to the questions.

Finally, we note that these explanations ignore the much more complicated reality of this system. See "Ion-Molecule Interactions and Reactions in the Gas Phase" for the full story.

Initial Statement on the simulations: The animations you are about to see represent simulations of some of the ways a molecule of methyl bromide (CH_3Br) might interact with a chloride anion (Cl^-). Although the simulations were carried out as part of an advanced research project, we use these animations to illustrate principles of chemistry at the introductory level.

The colored spheres show the electron clouds (van der Waals radii) of the atoms. Where spheres overlap, atoms are closer together than their van der Waals radius. When two spheres are overlapped significantly, it usually indicates the presence of a bond between the corresponding atoms. The simulations take place over about _____ seconds (___). The CH_3Br and Cl^- start out about ___ meters (____) apart.

Animation #1

http://octopus.chem.wayne.edu/hase/img/type5-50.gif

Background Information for INSTRUCTORS: When two inert molecules collide, they bounce off each other. When two reactive molecules collide, there may be no reaction of the reactive parts of the two molecules do not come into contact. In the first simulation, the Cl^- collides with the bromine atom of CH_3Br, not the reactive part of the CH_3Br (the carbon atom). Therefore, there is no reaction.

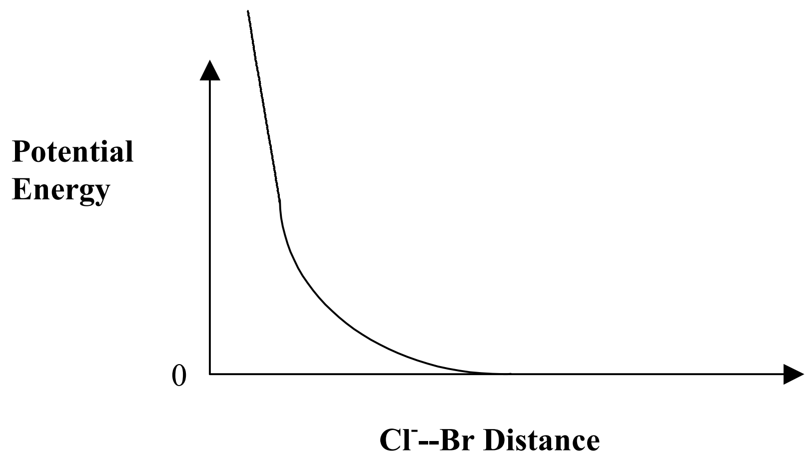

Figure 1 shows (schematically) the repulsive interaction between the bromine atom of CH_3Br and the Cl^-. The closer they come, the higher the potential energy, and the stronger the repulsive force. The simulation starts the CH_3Br molecule and the Cl- ion with high kinetic energy, so they come close together before they bounce apart.

Figure 1. Repulsive Interaction between Cl^- and Br. At long distances, they do not interact, so the potential energy due to their interaction is (defined to be) zero. The exact shape of this curve depends on the C-Br-Cl angle. This figure assumes that angle to be close to 180 degrees (the Cl^- does not interact much with the carbon atom). Figure 2 shows what happens if that angle is close to zero.

Suggested Questions on Collisions: Which atom of the CH_3Br comes into contact with the Cl- in this simulation [Br]? Does the sphere of the Cl^- ever overlap the spheres of the other atoms very much, or does it mostly just come into contact [There appears to be <u>little</u> overlap, and that only briefly]? Have any bonds been broken [No]? Have any bonds been formed [No]? Has there been a chemical reaction [No]?

Suggested Summary statement: Most of the time that two molecules (or a molecule and an atom) collide, they do not react. In this case, the Cl- (blue) collides with the Br (green) and bounces away. For the reaction to occur, the Cl- needs to collide with the carbon atom (light blue).

Animation #2

http://octopus.chem.wayne.edu/hase/img/yfwang4.gif

Background Information for INSTRUCTORS: The maximum in the reaction coordinate is sometimes called the "activated state," but is more properly called the transition state. It is unstable with respect to both reactants and products; the potential energy decreases when either the C-Cl or C-Br distance gets a little larger (and the other gets little smaller). Therefore, the molecule does not stay near the transition state geometry for any length of time.

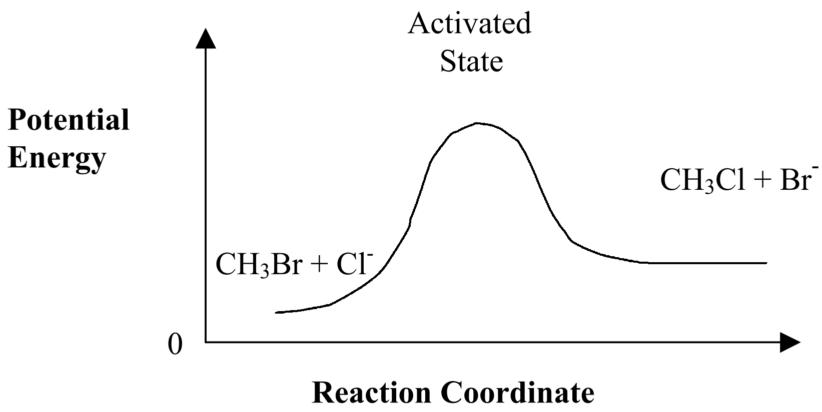

Figure 2. Potential energy profile versus reaction coordinate.

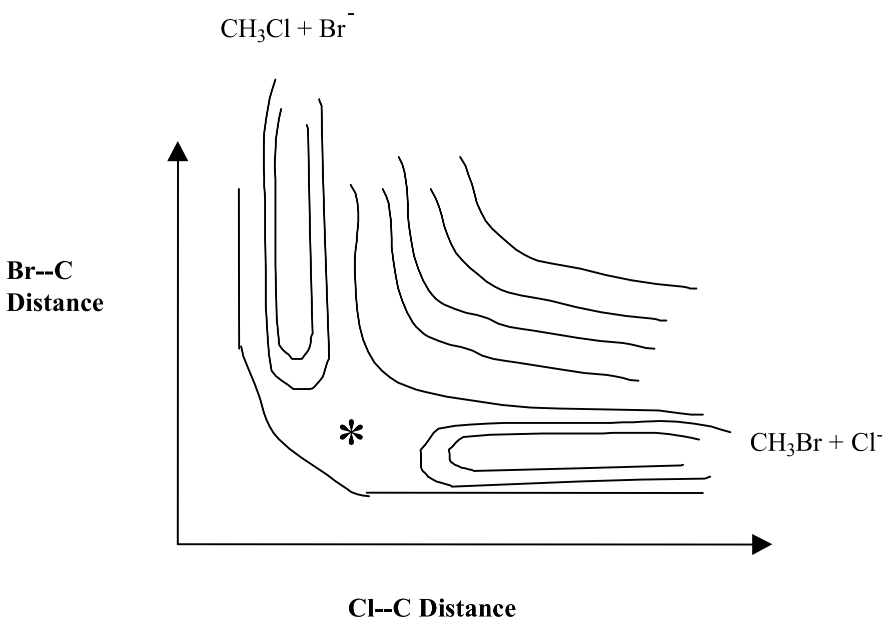

Figure 3. Contour plot showing energy for a range of C-Cl and C-Br distances. The point marked with the asterisk corresponds to the transition state, where the C-Br bond is jut beginning to break and the C-Cl bond is forming. The curve plotted in Figure 2 corresponds to a line which, starting in the "reactant valley" at the bottom right, initially heads straight to the left. It then curves *up* to pass through the transition state, and completes a 90 degree turn to head straight up, finally passing through the "product valley" at the top left.

Suggested Questions on Collisions: Which atom of the CH_3Br comes into contact with the Cl- in this simulation [C]? Is there a time when the spheres for both the Cl atom and the Br atom overlap the sphere of the C atom [Yes] Does this occur for merely one point in time or does this condition last for a significant period of time [Only a point in time]? When a carbon atom is bonded to five other atoms at the same time, is it a stable situation or a very high energy situation, [High energy. Carbon can (usually) be bonded to only four atoms at a time]? On the diagram below, put an X at the place where which corresponds to the point in time when the spheres for both the Cl atom and the Br atom overlap the sphere of the C atom [At the maximum in Figure 2: the transition state or "activated state"] In this reaction, one halogen replaces another. What type of reaction is that? [Substitution.]

Follow-up questions on Electronegativity and Bonding: In neutral CH_3Cl and CH_3Br, are the C-Cl and C-Br bonds covalent or ionic? [covalent, since the electronegativity difference is 0.3 and 0.2 respectively, much less than the 1.7 value used to differentiate between covalent and ionic]

Follow-up questions on Intermolecular Forces: What causes the Cl- ion to be repelled from the CH_3Br in the first simulations [repulsive forces between the electron clouds of the Cl anion and the partial negative charge on the Br; but even two neutral atoms repel each other if they get too close]?

Legal/ Copyright Issues

Theodore S. Dibble
Associate Professor
SUNY-ESF
1 Forestry Drive
Syracuse, NY 13210
(315) 470-6596
(315) 470-6856 (fax)
tsdibble@syr.edu
http://www.esf.edu/chemistry/faculty/dibble.htm

Rebecca A Jarrell
MAT, Secondary Science Education
Liverpool High School
4338 Wetzel Road
Liverpool, NY 13090
(315) 453-1500
rajarrel@syr.edu