

Ion-Molecule Interactions and Reactions in the Gas Phase

Summary for INSTRUCTORS

Below are links to a series of 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 be 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 second and third animation. 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. [Separate out text for students and text for instructors](#). 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.

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>

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 little 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).

Suggested question on Electronegativity: Which is the most electronegative element in CH_3Br [Br]? What makes give a negative charge to the chlorine atom [one extra electron above the number possessed by neutral chlorine]?

Follow-up questions on Intermolecular Forces: What causes the Cl^- ion to be repelled from the CH_3Br [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]?

Animation #2

<http://octopus.chem.wayne.edu/hase/img/type6-200.gif>

Background Information for INSTRUCTORS: CH_3Br has a dipole. The interaction of an ion with a dipole is very strong; much stronger than the interaction of two dipolar (neutral) molecules, or an ion with a non-polar molecule, or a polar molecule with a non-polar molecule, or two non-polar molecules (the weakest sort of interaction). In many cases, ion-dipole attractions are strong enough to form a (relatively stable) complex that stays together for a significant period of time (hence, the potential energy of the complex drops in relation to the reactants?); however, the energy holding the complex together is

significantly weaker than a covalent bond. If you plot the potential energy due to those forces, it might look like this (note that this is a two-dimensional representation of (or two-dimensional slice through) a function which has many more dimensions in space).

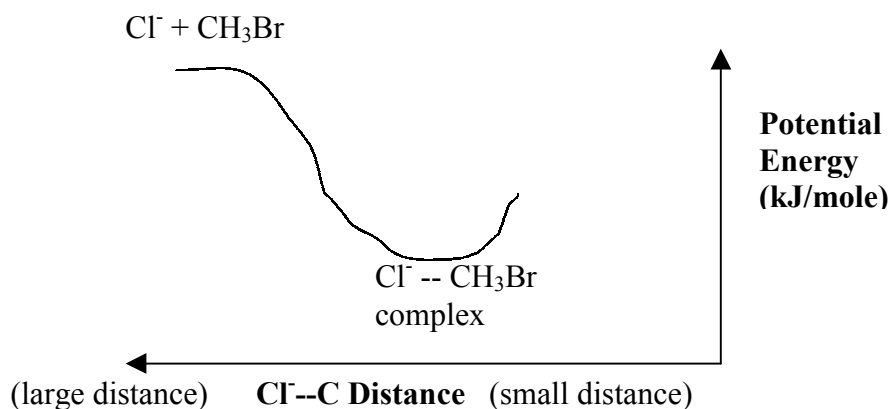


Figure 1. The potential energy decreases as the Cl⁻ approaches the carbon atom of methyl bromide, so there is an attractive force between them. The x-axis is reversed from the usual direction to be consistent with Figure 2; we hope this does not create confusion.

Suggested advanced-level questions: Which atoms of the CH₃Br comes into contact with the Cl⁻ in this simulation [C and H]? When the Cl⁻ approaches the CH₃Br, does its speed stay constant [No, it accelerates]? When the Cl⁻ bounces off the CH₃Br the first four times, does it go away as far as its starting position before heading back to the CH₃Br [No]? What could cause the Cl⁻ to accelerate [There must be a force attracting the Cl⁻ to the CH₃Br. The label for this force is ion-dipole attraction]? If, instead of Cl⁻ ion, an atom of Argon collided with CH₃Br, would the Argon atom be likely to bounce away and keep going away (as Cl⁻ ion does in the first animation), or stay close and collide a few more times, as in this second simulation [keep going away]?

Suggested summary statement: Ions and molecules often form complexes that are held together much less strongly than in a typical chemical bond (so they eventually fall apart), but more strongly than other forces between molecules (so they can stick together instead of just bouncing off). A typical chemical bond might require 400 kJ/mole to break (bond strength). The strengths of ion-dipole attractions are often about ___ kJ/mole. By comparison, the strength of a hydrogen bond is only about 20 kJ/mole.

Animation #3

<http://octopus.chem.wayne.edu/hase/img/type4-200.gif>

Background Information for INSTRUCTORS: (This animation and potential energy diagram is more suitable for college-level instruction and some second year high school chemistry students. However, the follow-up questions could be adapted to an introductory-level syllabus.)

The CH₃Br --Cl⁻ complex reacts to form a CH₃Cl -- Br⁻ complex that exists for some time before falling apart. Let's expand the potential energy plot to include a transition state for the substitution of Cl for Br, and the dissociation of the CH₃Cl -- Br⁻ complex:

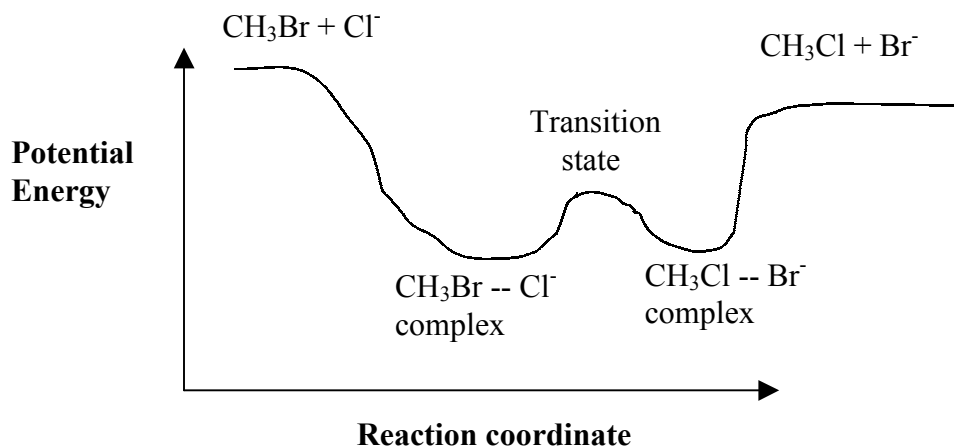


Figure 2. Potential energy profile versus reaction coordinate for the entire reaction.

Suggested questions: Is there a period of time when the sphere of the chlorine atom, but not the bromine atom, overlaps the sphere of the carbon atom [Yes, for roughly the second half of the simulation]? Does this indicate that bonds have been broken and formed [Yes, a chemical reaction has occurred: the C-Br bond has been broken and a C-Cl bond has been formed]?

Follow-up questions on Electronegativity and Bonding: In neutral CH₃Cl and CH₃Br, 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]

Suggested Summary Statement: The strong attractions between the molecules and the atomic anions can cause formation of a complex of the reactants and, after the reactions, of the products.

Legal/ Copyright Issues

This material is copyright 2002 by Theodore S. Dibble and Rebecca A. Jarrell. Educators in public and private schools, colleges and universities are free to use this material in part, with modifications, or as a whole without charge, providing they cite the authors and copyright.

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