Chemical Sciences

Chemical Sciences research cuts across a broad front of basic studies in chemistry and atomic physics. The knowledge gained is essential to understanding key processes which form the basis for future energy technologies.

DYNAMICS OF CHEMICAL REACTIONS

The benefits of modern chemistry so profoundly affect our daily lives that it is difficult to imagine a world without them. Yet, despite all this progress, man's basic understanding of the most fundamental aspects of chemical reactions is just beginning to yield to the scientists' probes.

In 1986, the Nobel Prize in Chemistry was shared by three physical chemists. Two, Dudley R. Herschbach and Yuan T. Lee, were supported in their research by Basic Energy Sciences. The Prize was awarded for discoveries that helped to explain the physical dynamics of chemical reactions.

Specifically, Basic Energy Sciences research revealed how two molecules undergoing a chemical reaction collide, combine and transform themselves, step by step, into very different resultant products. Although the reactions studied were comparatively simple and straightforward, the insights gained revolutionized prevailing thought.

From the point of view of chemical reaction dynamics, the 19th century way of writing down chemical reactions, using arrows and symbols, is misleading. The equations obscure which aspects of chemical reactions are important and which ones are not. If one looks at the reactions in a different light, as did Herschbach and Lee, focusing instead on particular structures of certain atomic electrons and orbitals, the pieces of the puzzle begin to fall into place.

Striking similarities stand out among their experimental data. These form a relatively small number of "rules" which govern chemical reactions and their dynamics. These, in turn, can be generalized to other molecules and other reactions. With this knowledge, it may be possible ultimately to manipulate, using a variety of control mechanisms, the timing, speed, sequence, extent, and very nature of chemical reactions, attended by virtually unlimited variations and possibilities.

The specifics of the Basic Energy Sciences contribution may be appreciated by visualizing a chemical reaction. Imagine, for a moment, an immensely enlarged, slow motion picture of one atom, potassium (K), and one molecule, methyl iodide (CH_3I), hurtling toward each other through the vacuum of a laboratory chamber on a collision course set by the scientists to result in a glancing blow.

In some cases, the expected chemical reaction takes place with the explosive formation of two byproducts, potassium iodide (KI) and an incomplete methyl group (CH_3), flying off in opposite directions. In other cases, the collision results in no chemical reaction, with the original constituents, called reactants, simply bouncing off each other in a physically expected distribution of random directions.

By varying the velocities and angles of the incoming reactants, and by measuring and determining the distributions of the resulting products, Basic Energy Sciences researchers were able to infer the necessary and sufficient conditions under which the reaction would take place. In the case studied, the incoming potassium atom had to strike the opposing methyl iodide molecule on the iodide end, and then bounce backward.

Over the years, the experimental devices used to analyze the reactions became more sophisticated and the kinds of reactants and reactions studied became more complex. Gradually, the data began to reveal patterns and similarities, even though the molecular structures of the varying reactants appeared to be quite different.