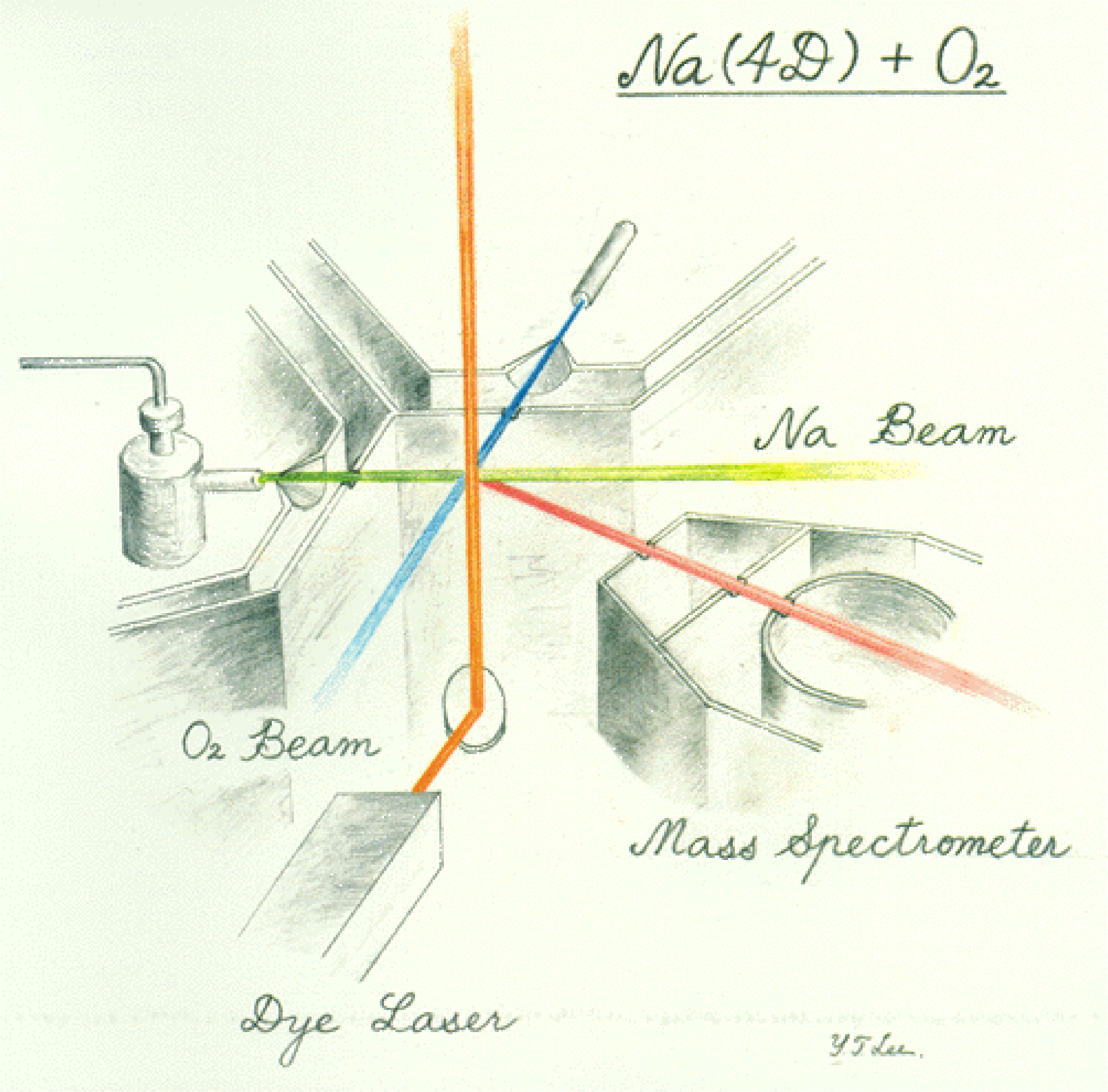
Yuan T. Lee's Crossed Molecular Beam Experiment



The above illustration was drawn by Professor Yuan T. Lee, who shared the 1986 Nobel Prize in Chemistry. It shows the design for his crossed molecular beam experiment described in the story beginning on page 27 of "Basic Energy Sciences: Summary of Accomplishments" (DOE/ER-0455P, May 1990); the story is also copied below. The purpose of this experiment was to study the chemical reaction of sodium atoms with oxygen molecules. In the experiment, a beam of sodium atoms (green, chemical symbol Na) and a beam of oxygen molecules (blue, chemical symbol 0_2) intersect in a vacuum. The products of the sodium-oxygen reaction (red) are ionized by laser radiation (orange) aimed at the point of intersection of the two beams so that the products can be detected and measured by the mass spectrometer.

By tuning the wavelength of the laser, specific products of the chemical reaction can be identified and measured. By moving the position of the mass spectrometer, the spatial distribution of the reaction products can be determined. Through control of the sources of the atoms and molecules, reactants in specific can be selected for study, as in the case of the 4D state of the sodium indicated in the figure.

Shown in black and white is the variety of devices needed to form and shape the beams. Using instruments such as these, chemists have been able at last to study chemical reactions in great quantitative detail. From these studies is emerging a fuller understanding of chemical reactions and an improved ability to control them for the benefit of society. To see Professor Lee in front of the actual apparatus, click here.

DYNAMICS OF CHEMICAL REACTIONS

From "Basic Energy Sciences: Summary of Accomplishments" (DOE/ER-0455P, May 1990), pages 27-28

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 (CHJ), 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 by-products, potassium iodide (KI) and an incomplete methyl group (CH,), 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.

This led to what Herschbach called the "harpoon" model of reaction dynamics. One molecule sneaks up on the other, uses a very specific valence electron orbital as its harpoon, spears its target in one selective and vulnerable spot, and hauls it in. Once these mechanisms are known, many of the other potentially obscuring complexities of molecular shapes, bonds, and electron potentials, fall away as being irrelevant.

The experimental technique used in these studies, developed by Herschbach and Lee, is today known as "crossed-molecular beam" research. The facility recently constructed at Lawrence Berkeley Laboratory, under Lee’s direction and with continued support from Basic Energy Sciences, is widely acclaimed as the best molecular beam instrumentation facility in the world.

In recent years, this facility enabled Lee to study more complex molecules, such as those having long hydrocarbon chains. Pioneering exploration was begun in two key areas of pressing national interest-hydrocarbon (oil and natural gas) combustion and atmospheric chemistry.

With these advances, understanding chemistry from first principles is now a practical goal. Its applicability extends beyond fuel burning and ozone depletion. Insights gained using crossed-molecular beam research may yield new models of how catalysts operate in specific chemical reactions. Because the velocities of molecular collisions, which determine reaction potentials, are related to temperature, the nature of reaction rates is now a subject of detailed and quantifiable research.

Perhaps more importantly, crossed-molecular beam research permits a better understanding of reaction intermediates, the short-lived arrangements of atoms and molecules that are the first results of a molecular collision, but which soon decay to some other or more stable forms. Manipulating the reaction intermediates offers one of the best hopes for precisely controlling chemical reactions and, thus, determining the nature of the final reaction products.

For Herschbach and Lee, more than two decades of fundamental research culminated in the Nobel Prize. They envisioned and devised a productive experimental approach, built and perfected the necessary hardware and instruments, gathered data with sufficient variety and scope to yield robust conclusions, and presented the scientific community with a wholly new view of chemistry and the dynamics of reactions.

Crossed-molecular beam research is now firmly established as a fundamental research tool. With continued support from Basic Energy Sciences, it is being used in a growing number of inquiries. With expanding knowledge, focused more on applications, improved understanding of reaction dynamics and, perhaps, the ability to control the reactions themselves, move closer to reality.

Despite all the wondrous advances of modern chemistry, new frontiers remain to be explored. Crossed-molecular beam research lies at the forefront of this endeavor, with great potential for continuing contributions to industry, health, and environment.

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