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Federal Support for Chemistry

During the past 2 years a substantial fraction of leading chemists has been associated with George Pimentel of Berkeley in the preparation of a National Research Council report detailing some of the progress, triumphs, and needs of their discipline. Much has happened in the two decades since the last NRC chemistry report. Chemistry retains a historic role as a crossroads of the sciences and a tremendous source of practical applications, but new capabilities and new tools have been added. A host of powerful analytical instruments has become available. Theoretical chemistry, in part based on the Schrödinger wave equation, is increasingly productive. Computer-produced three-dimensional displays of molecules are providing chemists with sharper insights into the geometries and interactions of molecules. Many of the approaches of physics are now being applied to obtain data on excited states of molecules and reaction mechanisms.

Last summer, before the choice of the new editor and the selection of John Brauman as Deputy Editor for Physical Sciences, the decision was made to mark the occasion of the issuance of the Pimentel Report with the publication of a number of articles in *Science*. They are being published in this issue, which anticipates slightly the appearance of the report. The articles sample some of the research activities that are now making chemistry a less empirical and far more powerful discipline than most of our readers encountered during their undergraduate and graduate days. A few examples from these articles are cited.

Molecular interactions (supramolecular chemistry) are the basis of the highly specific processes occurring in biology, such as substrate binding to an enzyme. Recognition of a substrate to a receptor requires both a geometrical fit and binding between the interacting species. In this issue a large number of different synthetic molecules are described that have cave-like structures which are capable of selective binding and hence separation of similar cations and anions. Other synthetic receptors may bind a substrate, effect a reaction on it, and release the products.

Three articles describe relatively new work on the dynamics of chemical reactions. Experimental tools include ion beams, mass spectroscopy, ion cyclotron resonance, and lasers. Use of tunable lasers permits selective excitation of particular states with photons ranging from infrared to deep ultraviolet. One laser may be used to excite a molecule to participate in a reaction; a second may be used to probe the reaction products. Since very short laser pulses can be used, the time between excitation and interrogation can be less than 10^{-8} seconds. A fundamental question to be investigated by short pulse lasers is the time required for the redistribution of intramolecular vibrational energy. That is, one excites a particular bond and then observes fluorescence from other vibrational states. For the C–H stretching motion the time required to transfer energy to other vibrational motions is of the order of 100 femtoseconds.

Heterogeneous catalysis plays a crucial role in the production of most industrial chemicals. Articles in this issue touch on efforts to achieve a better basic understanding of the mechanisms involved. Three factors that control surface catalysis are the atomic surface structure, an active overlayer on the surface, and the oxidation states of surface atoms. For example, the (111) crystal face of iron produces ammonia from N_2 and H_2 at 500 times the rate of the (110) face at 20 atmospheres and 450°C. In the hydrogenation of CO over rhodium the yields are predominantly CH_4. However, when Rh_2O_3 was used, oxygenated C_2 and C_3 compounds were produced, including ethanol, acetaldehyde, and propionaldehyde.

Important progess is being made in chemistry. In proportion to its contribution to the advancement of other sciences and its contributions to the economy, chemistry is the most underfunded of all the natural sciences. It is to be hoped that the efforts of Pimentel and his collaborators will be rewarded by a generosity that is merited.—PHILIP H. ABELSON