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Applications of Chemical Dynamics

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Abstract

Chemical dynamics is a field in which scientists study the rates and mechanisms of chemical reactions. It also involves the study of how energy is transferred among molecules as they undergo collisions in gas-phase or condensed-phase environments. Therefore, the experimental and theoretical tools used to probe chemical dynamics must be capable of monitoring the chemical identity and energy content (i.e., electronic, vibrational, and rotational state populations) of the reacting species. Moreover, because the rates of chemical reactions and energy transfer are of utmost importance, these tools must be capable of doing so on time scales over which these processes, which are often very fast, take place.

History

In 1864, Peter Waage and Cato Guldberg pioneered the development of chemical kinetics by formulating the law of mass action, which states that the speed of a chemical reaction is proportional to the quantity of the reacting substances.

Van 't Hoff studied chemical dynamics and published in 1884 his famous "Etudes de dynamique chimique". In 1901 he was awarded by the first Nobel Prize in Chemistry "in recognition of the extraordinary services he has rendered by the discovery of the laws of chemical dynamics and osmotic pressure in solutions".After van 't Hoff, chemical kinetics deals with the experimental determination of reaction rates from which rate laws and rate constants are derived. Relatively simple rate laws exist for zero order reactions (for which reaction rates are independent of concentration), first order reactions, and second order reactions, and can be derived for others. Elementary reactions follow the law of mass action, but the rate law of stepwise reactions has to be derived by combining the rate laws of the various elementary steps, and can become rather complex. In consecutive reactions, the rate-determining step often determines the kinetics. In consecutive first order reactions, a steady state approximation can simplify the rate law. The activation energy for a reaction is experimentally determined through the Arrhenius equation and the Eyring equation. The main factors that influence the reaction rate include: the physical state of the reactants, the

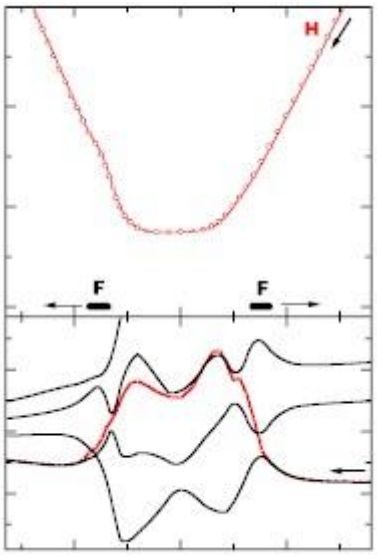
concentrations of the reactants, the temperature at which the reaction occurs, and whether or not any catalysts are present in the reaction.

Gorban and Yablonsky have suggested that the history of chemical dynamics can be divided into three eras.The first is the van 't Hoff wave searching for the general laws of chemical reactions and relating kinetics to thermodynamics. The second may be called the Semenov--Hinshelwood wave with emphasis on reaction mechanisms, especially for chain reactions. The third is associated with Aris and the detailed mathematical description of chemical reaction networks.

> The question ‘what exactly happens when a new molecule is born in a chemical reaction’ surely lies at the heart of chemistry. The experimental and theoretical investigations of this question at the level of single collisions between molecules or molecular species constitute the realm of ‘Chemical Dynamics’. Experiments with crossed molecular beams approach the ideal of a complete state specificity of the reagents and products. Still more adventurous experimental venues include the outer atmosphere and outer space, where nascent molecules can be observed by spectroscopic methods.

The theoretical description of molecular processes from first principles calls for quantum mechanics and quantum electrodynamics, although classical mechanics and electrodynamics are valid approximations under a wide range of conditions. An important contribution of theoretical chemistry is the computer simulation of molecular collisions on the basis of *ab initio* potential energy surfaces (PESs). However, simplistic model PESs can also be valuable tools, which is an important consideration in view of the fact that the calculation of accurate *ab initio* PESs for reactive systems is a notoriously difficult problem. Simulations of collision processes can lead to a detailed understanding of the mechanisms of chemical reaction and of energy transfer. Processes and phenomena which are not (or not well) accessible experimentally may also be investigated in this way. But above all the understanding of these phenomena provides a handle to manipulate molecular processes in a specified manner, and thus to approach the old dream of chemists to completely control the course and outcome of reactions.

Computer Simulations of Elementary Reactions and Energy-Transfer Processes



A stroboscopic view of the dissociation of F2 triggered by a collision with an energetic ("hot") H atom (top panel). The bottom panel illustrates the evolution of the electronic energy during the collision. The black lines represent the four lowest potential energy surfaces. An intermediate transition to an electronically excited state is apparent .

In general, computer simulations of elementary reactions have still some way to go to reach the ideal of an accurate prediction of cross sections, rates or product distributions from first principles. To date this objective has only been approached for the H+H2 and F+H2reactions, whereas various approximations or model assumptions have to be invoked in the treatment of other systems.

For quite a few years, in our group we have been studying the dynamics of atom+diatom exchange reactions like H+F2 and Cl+HCl using model PES. In particular, a long series of investigations has been devoted to the H+F2 reaction and its isotopomeric analogues. A recurring topic of our investigations is the correlation between localized features of the PES and the dynamical observables of molecular collisions. The knowledge of such correlations is essential for the inversion of experimental results in the construction of PESs backwards from experimental data. Recently we have extended our studies to the hyperthermal energy range, where electronic transitions to excited PES have to be considered. These calculations relate to experimental muonium and tritium hot-atom chemistry and address questions of isotope effects and of high-energy mechanisms of reaction, collision-induced dissociation and charge transfer.

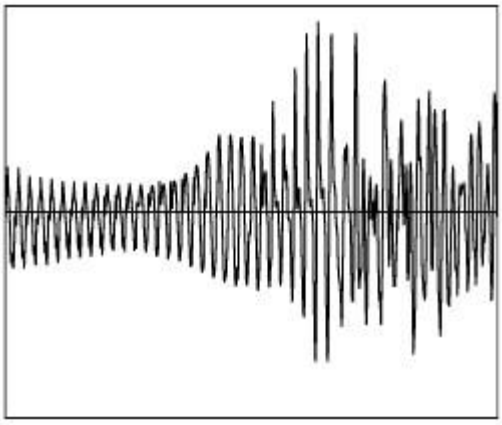
In the field of non-reactive collisions, a line of research in this lab concerns collisional deactivation of vibrationally or rotationally excited molecules. We address questions like the relative importance of the energy-transfer pathways "vibration-to-vibration" or "vibration-to-rotation-and-translation", and the influence of topological features of the PES on the extent and mechanism of vibrational relaxation.

Dynamical Stereochemistry

Dynamical Stereochemistry deals with the effects of molecular orientation in elementary processes. Basically a branch of molecular collision dynamics, Dynamical Stereochemistry has established itself as a research field in its own right, boosted by the rapid development of experimental methods resolving detailed differential cross sections, vector properties and vector correlations of molecular collision processes. The concept of an angle-dependent barrier forms the basis of simplistic models like the angle-dependent line of centres (ADLOC) model, which assist the interpretation and inversion of the wealth of experimental information.

Our investigations in this field focus on the relations of the parameters of the models to the properties of the PES on the one hand and to reaction attributes like differential cross sections and excitation functions on the other.

Laser Control of Chemical and Photochemical Elementary Processes



A shaped laser pulse designed to pump HCN from its ground state to a delocalized state above the isomerisation barrier. The pulse length is 1 ps, the peak field strength is 0.02 atomic units. The quantum nature of molecules can be exploited to manipulate molecular systems in unprecedented ways. By creating and utilising interference patterns in the nuclear wavefunctions, molecular processes can be driven selectively and can be made to follow prescribed pathways. Mode-selective

chemistry is one of the practical goals of this approach, and purpose-designed shaped laser pulses and tailored trains and sequences of pulses are appropriate tools. Concurring intramolecular relaxation processes can be effectively suppressed by employing ultrashort pulses in the femtosecond regime. Altogether, this means not only that the expended energy is used in the most efficient way, but also that processes may become accessible which otherwise would not be observed.

Recent investigations in our group include simulations of the femtosecond multiphoton-excitation of small molecules of specific, highly excited vibrational states (this may also serve as a model for the specific excitation of chromophors in large molecules), and the simulation of state selective HCN ® HNC isomerisation by shaped sub-picosecond pulses obtained from Optimal Control Theory or alternatively by sequences of simple picosecond pulses.

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