Meetings

Chemical Accelerators

The phrase "chemical accelerators" is scarcely older than the conference bearing that name held at the University of Colorado, Boulder, 28–29 March 1968. However, interest in the subject was so great that what was originally intended to be an unpublicized workshop for one or two dozen people grew to include nearly a hundred.

Chemical accelerators is a name suggested by one of us for devices that produce beams of chemically interesting species at relative kinetic energies of a few electron volts. Most studies of chemical kinetics made by traditional thermochemical methods are limited by the properties of container materials to reactions occurring near the classical Arrhenius activation energies. In the past decade or so, however, it has become evident that there is a wealth of important chemistry occurring only at higher energies (of the order of the strength of chemical bonds, 2 to 10 ev). The methods that have revealed this richness and order of medium- and high-energy chemistry have been hot-atom techniques, largely nuclear and also photochemical, and in the case of ions, mass spectrometry.

While hot-atom studies overcome the energy limitations of thermochemical methods, they also share some of the limitations of these classical techniques. Energies of reactive collisions are usually not well defined, and products are generally identified only after undergoing further collisions which modify their original properties. The molecular-beam method can, to a large extent, avoid these ambiguities and also provide valuable information on angular and velocity distributions. It therefore now seems clear that it is desirable to study this new hot chemistry using molecular beams in the electron-volt region. Thus chemical accelerators can provide the same type of information for elementary chemical kinetics that nuclear accelerators have yielded so successfully for nuclear reactions.

Although the conference revealed a surprising number of different concepts for building chemical accelerators, relatively few have been made operational. These methods have been largely confined, because of technical limitations, to a somewhat special class of reaction studies. As a result, the potential power of these methods applied in a concerted way to the broad problem of chemical dynamics has not been given sufficient attention. Accordingly, the conference focused on methods, rather than on results, in order to explore the extent to which technical limitations can be removed, thus permitting the large-scale exploitation of chemical accelerators.

After some brief welcoming remarks, John Willard (University of Wisconsin) conducted the first session. This was a review of what is already known about hot chemistry and provided a background to the problems remaining for chemical accelerators to solve. F. S. Rowland (University of California, Irvine) presented a critical discussion of achievements of hot-atom chemistry using the nuclear and photochemical methods. V. L. Talroze (Institute of Chemical Physics, Moscow) discussed mass spectrometric studies of ion-molecule reactions. John Polanyi (University of Toronto) and Martin Karplus (Harvard University) presented some results of their trajectory calculations of hot-atom reactions. It is obvious that while some methods of theoretical chemical kinetics (for instance, "absolute" rate theory) are based on assumptions which limit them to thermal-equilibrium systems, the more fundamental trajectory–potential-energy–surface approach is as applicable to "hot" as it is to "threshold" reactions. Indeed, studies of hot reactions are essential to gain information on potential energy surfaces over the whole region and not just near the saddle point.

In a discussion of ion accelerators, chaired by Wade Fite (University of Pittsburgh), Arnim Henglein (Hahn-Meirner-Institut, Berlin) gave the introductory talk. His research group has built a device in which a beam of ions strikes a gas target and products recoiling in the forward direction are velocity analyzed. Work with this device has led to Henglein's postulate of the spectator stripping model of ion-molecule reactions. Subsequently, a number of other ion accelerators have been built. In the relatively high-energy region, B. Mahan (University of California, Berkeley) and T. Bailey (University of Florida) have added angular discrimination, thus providing more detail on the validity of the spectator stripping approximation. R. Wolfgang reported on an accelerator, named EVAtron, which he built with Z. Herman and other collaborators. The EVAtron covers the low as well as the higher energy range. By employing a crossed-beam rather than a gas chamber target and using angular as well as velocity discrimination, it has been shown that formation of an intermediate complex does not always occur even at lowest energies. A new and general model for direct reactions occurring at low energies was reported.

Another approach to the somewhat difficult problem of studying ion-molecule reactions in the relatively low-energy (1 to 2 ev) region was discussed by R. Neynaber (General Dynamics/Convair, San Diego) in a session chaired by R. S. Berry (University of Chicago). This is the "merging beam" technique, whereby two beams—ionic, or neutralized—are superimposed so that reaction occurs at energies corresponding to the difference in their velocities. This method provides excellent fine-energy control and allows beam methods to be extended down to the milli-electron-volt region. While it should be useful for measuring cross sections, the method appears to hold less promise for detailed mechanistic studies. This is caused by the large center-of-mass motion which makes it difficult to measure angular distributions. Two other merging beam machines currently in operation were described by E. Entemann (General Dynamics/Convair, San Diego) and W. Aberth (Stanford Research Institute, Menlo Park). The discussion at this session left the feeling that "partial merging" (making beams cross at a small angle) may be a promising adjunctive technique.

Chemical accelerators for neutral species are far more difficult to operate than those for ions, not only because neutrals are harder to accelerate, but also because they are harder to detect. Perhaps the most successful method so far devised for producing

neutral beams is that of neutralizing the charge from ionic beams without disturbing the momentum of the traveling species. N. Utterback (Defense Research Laboratory, General Motors Corp., Santa Barbara) reviewed this topic in a session chaired by E. Greene (Brown University). Using charge transfer, Utterback and his collaborators have produced neutral beams from the high-energy range down to a few electron volts. They have successfully studied several reactions, avoiding the problem of detecting neutrals by choosing processes yielding ionic products. If resonant charge transfer is used, it appears that the internal energy state of the resulting neutral beam can be reasonably well controlled. (Talroze's talk had already made it clear that resonant transfer processes were common and occurred with large cross sections.) L. M. Branscomb (Joint Institute for Laboratory Astrophysics) discussed possibilities of producing neutral beams by photoelectron detachment from negative ions. This technique should become useful when more intense lasers and negative ion beams are developed. In competition with positive-ion-neutralization methods this technique has potential advantages at low energies, at high angular resolution and when excited-state control in the initial beam is needed.

A partial solution to the detection problem is inherent in experiments being performed by J. Paulus (Centre de Recherches Nucléaire, Strasbourg), S. Wexler (Argonne National Laboratory), and M. Menzinger and R. Wolfgang (University of Colorado). They have used beams labeled with radioisotopes to detect labeled products by radioactivity counting. The Colorado group reported experiments in which a tritium ion beam was charge exchanged and reacted with a solid target. By this means they found it possible to make the first determinations of the thresholds of hot-atom displacement reactions. Given the availability of radioisotopes of useful half-life, this detection method could have wide applicability. An even more general, indeed universal, method of detection is reionization of neutrals by electrons or protons. So far, however, such reionizers only operate with low efficiency.

J. Ross (MIT) was chairman of a session in which nozzle expansion techniques were discussed. This method, growing out of a suggestion by Kantrowitz and Grey, has been more intensively investigated than any other

for the production of neutral beams. J. Fenn (Yale University) reviewed the topic, emphasizing "seeding" methods in which a heavy species is swept along by lighter "driver" molecules, thus increasing its translational energy. E. Knuth (UCLA) discussed means of reaching higher energies by plasma heating the gas before expansion. In general, nozzle expansion seems an excellent approach to the low- and medium-energy range (1 to 10 ev). It should provide intense beams and excellent energy control. However, the seeding technique is limited to heavier species, and high-temperature heating before expansion leaves some question as to the internal state of the beam molecules. At the time of the conference, no hot reaction appears to have been identified by using nozzle techniques. However, J. Deckers (University of Toronto) and J. Anderson (Princeton University) discussed some interesting negative results.

In a session conducted by E. Ferguson (ESSA, Boulder), L. Wharton (University of Chicago) first reviewed the historic device of Bull and Moon (University of Birmingham) which can claim the distinction of being the first chemical accelerator. Regretfully, this charming method of acceleration by slapping molecules with a spinning rotor seems limited to the low energies achieved by these pioneers. Wharton then reviewed the building of his accelerator for neutral species having permanent dipole moments or which are highly polarizable. Though expensive and time consuming in its construction, this is a most interesting machine. Cost considerations tend to limit the device to the acceleration of permanent dipolar molecules at low energies. However, it should have excellent energy control. Moreover it was the only concept discussed which inherently yields a polarized beam.

C. Schlier (University of Freiburg) and J. Los (FOM Institute, Amsterdam) discussed sputtering methods in which atoms are dislodged from surfaces by impact of high-energy ions. The atoms in the resulting spray have electron-volt energies, but their velocity distribution is so wide that a high-speed chopper is required to select a reasonably homogeneous beam. To date, sputtering has been used largely to study nonreactive scattering, but its future as a means of studying chemical reactions appears bright.

This does not exhaust the catalog of methods discussed at the meeting. For

instance, D. Hansen (Thompson-Ramo-Woolridge) mentioned experiments aimed at producing bursts of fast atoms by volatilizing electrostatically accelerated dust particles with a laser pulse. And it seems certain that additional techniques will be developed in the future.

The meeting closed with a panel discussion led by I. Amdur (MIT). The panelists, R. Bernstein (University of Wisconsin), S. Datz (Oak Ridge National Laboratories), M. Karplus, A. Kupperman (California Institute of Technology), B. Mahan, and the undersigned organizing committee, discussed the problems and the prospects of the field. Much of the critical appraisal of the comparative merits of chemical accelerators, which has already been mentioned in this report, resulted from this session. Quite obviously the field is in its early infancy and the direction of its development is still far from evident. However, it was generally agreed that in the more distant future the production of beams having not only a high kinetic energy, but also in selected states of internal excitation, would be important. Just what combination of techniques will prove to be most useful in the next 10 years is something about which few participants were willing to speculate. One general conclusion seems quite clear; the field will grow rapidly now that its fundamental importance to elementary chemical kinetics has been recognized.

This conference was supported through a grant from the Advanced Research Projects Agency (Project DEFENDER), monitored by the U.S. Army Research Office, Durham, North Carolina, under contract DA-31-124-ARO-D-139.

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Calendar of Events

National Meetings

December

1. **Medical Aspects of Sports,** 10th, Miami Beach, Fla. (F. Hein, American Medical Assoc., Dept. of Health Education, 535 N. Dearborn St., Chicago, Ill.)

1. American Acad. of **Oral Medicine,** New York, N.Y. (S. Conrad, 133-28 228th St., Laurelton, N.Y. 11413)

1–4. American **Medical** Assoc., Miami Beach, Fla. (F. J. L. Blasingame, 535 N. Dearborn St., Chicago, Ill. 60610)

1–4. **Reticuloendothelial** Soc., 5th, New York, N.Y. (F. J. DiCarlo, Warner-Lambert Research Inst., Morris Plains, N.J. 07950)

1–5. American Inst. of **Chemical Engineers,** 61st, Los Angeles, Calif. (Secretary, 345 E. 47 St., New York 10017)

1–6. **Radiological** Soc. of North America, Chicago, Ill. (M. D. Frazer, 1744 S. 58 St., Lincoln, Neb. 68506)

2. **Quantum Chemistry,** 9th winter inst., Gainesville, Fla. (Winter Institute, 525 Nuclear Sciences Bldg., Univ. of Florida, Gainesville 32601)

2–3. **Applications of Simulation,** 2nd conf., New York, N.Y. (A. Ockene, IBM Corporation, 112 E. Post Road, White Plains, N.Y. 10601)

2–4. New England Conf. on **Air Pollution,** Waterville, Maine. (Director, Colby News Bureau, Colby College, Waterville 04901)

2–4. Western National **Geophysical** Union, San Francisco, Calif. (J. C. Harrison, Dept. of Geophysical Sciences, Univ. of Colorado, Boulder 80302)

2–6. Greater New York **Dental** Mtg., 44th, New York, N.Y. (M. Purdy, Room 106A, Statler-Hilton, New York 10001)

3. American Soc. of **Therapeutic Radiologists,** Chicago, Ill. (J. A. del Regato, Penrose Cancer Hospital, 2215 N. Cascade, Colorado Springs, Colo. 80907)

3–4. **Vehicular Technology** Conf., San Francisco, Calif. (W. G. Chaney, Lenkurt Electric, 1105 Country Rd., San Carlos, Calif. 94070)

3–5. **Entry Vehicle Systems and Technology** Conf., Williamsburg, Va. (M. H. Bloom, Polytechnic Inst. of Brooklyn, Graduate Center, Route 110, Farmingdale, N.Y. 11735)

4–6. **Optical Character Recognition in Computerized Management of Information** in the Next Decade, Hollywood, Fla. (International Business Forms Industries, 20 Chevy Chase Circle, NW, Washington, D.C. 20015)

4–6. Academy of **Psychosomatic Medicine,** Miami Beach, Fla. (E. Dunlop, 150 Emory St., Attleboro, Mass. 02703)

4–7. American Assoc. of **Physicists in Medicine,** Chicago, Ill. (R. O. Gorsop, Stein Research Center, Jefferson Medical College, 920 Chancellor St., Philadelphia, Pa. 19107)

5–6. American **Rheumatism** Assoc., Tucson, Ariz. (M. M. Walsh, 1212 Avenue of the Americas, New York 10036)

6–7. American Federation for **Clinical Research,** Boston, Mass. (H. J. Levine, New England Medical Center Hospitals, 171 Harrison Ave., Boston 02111)

7–12. American Acad. of **Dermatology and Syphilology,** 27th, Chicago, Ill. (S. E. Huff, 1636 Church St., Evanston, Ill.)

8–13. American Soc. of **Agricultural Engineers,** Chicago, Ill. (P. L. Bellinger, Technical Coordinator, 420 Main St., St. Joseph, Mich. 49085)

8–15. Symposium of **Analogue and Digital Computers in Hydrology,** Tucson, Ariz. (American Federation of Information Processing Societies, 211 E. 43 St., New York 10017)

9–11. **Computer** Conf., San Francisco,