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Concluding Remarks

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Concluding remarks

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It is good that from time to time, a group of leading workers in a field should come together to discuss the current status of their research, and the direction in which it will most probably develop. We should all be grateful to the Royal Society in acting as hosts to this conference and to Professor Johnson and Professor Beynon for organizing it. I think that all will agree that the high quality of the papers presented have made this occasion a very memorable and valuable one. I should also like to thank the organizers for the relaxed atmosphere of the Conference, which made it so enjoyable.

The last decade has seen a tremendous growth in both the instrumentation and techniques of mass spectrometry and the applications of mass spectrometry to organic and biological chemistry. On the instrumentation side, the modification of a double focusing mass spectrometer to yield ion kinetic energy spectra, giving information about the progenitors of a given ion, and the reversed geometry instrument, yielding information as to the daughter ions of a given parent, have both considerably contributed to our knowledge of the fragmentation of organic molecules. Again the development of special sources, field ionization and field desorption, the linking of a gas or high pressure liquid chromatograph to a mass spectrometer, and the introduction of high pressure sources for chemical ionization, have all made important contributions to organic and biological chemistry. The study of negative ions has also shed considerable light on the structure of organic molecules. Finally, the linking of computers with mass spectrometers has enabled results to be obtained very much more rapidly than in the past, and also made possible library searches to identify the substances present.

Mr Craig discussed recent modifications in the source, analysis systems and detector systems of commercial mass spectrometers. Of particular importance was the increased sensitivity obtained by more effective ion collection. Among the newer techniques described during the meeting were g.c.–m.s. (Professor Jellum, Professor Jackson, Dr Morris, Professor Brooks and Professor Eglinton), collisional activation (Professor McLafferty and Dr Morris), negative ion mass spectrometry (Professor Jennings) and reversed geometry mass spectrometry (Professor Beynon).

Professor Jellum showed how the g.c.–m.s. technique could be applied to body fluids to determine metabolite profiles with the object of diagnosing and studying metabolic disorders. It is interesting to note that some 25 new metabolic disorders have been discovered in this way. This technique will undoubtedly become of increasing importance in the biomedical field. The determination of the structure of organic molecules still remains a central theme of organic mass spectrometry. Professor Nakanishi discussed the application of mass spectrometric principles to the study of certain biologically active compounds. Of interest were two new techniques: droplet counter-current separation, and plasma desorption mass spectrometry. In the latter method, dimer molecules are thought to be desorbed and then dissociated to give $(M+H)^+$ and $(M-H)^-$. It was of interest to learn that his magical powers were not confined

to organic chemistry. Professor Jackson (porphyrins), Dr Morris (peptides and glycopeptides) and Professor Brooks (steroids) also demonstrated the use of various mass spectrometric methods in structure determination.

Professor Eglinton dealt with the identification of various geolipids: waxes, sterols and porphyrins in sediments ancient and modern. Various mass spectroscopic techniques were used: low resolution electron impact, chemical ionization and high resolution electron impact. Routine search procedures have been developed, and classification routines which can give a guide to unknown structures.

Professor Beynon showed how the use of a 'reversed geometry' mass spectrometer can be used to build up fragmentation routes of a given compound which lead to its structure. He illustrated the approach by the masterly analysis of a mass spectrum. A particular use of this technique is to the determination of the side chain of a steroid, by selecting only the side chain for study.

Professor McLafferty dealt with the technique of chemical activation and its application of a determination of the mass spectra of ions. This is achieved by mass-selecting a given ion, energizing it by collision and mass-analysing the fragments. Such spectra are highly characteristic of the species. He invented the term m.s.–m.s. for this method. Of great interest was his report of the determination of chirality by mass spectrometry.

Mechanistic studies were reported by Dr Nibbering and Dr Williams. The former discussed the application of ion cyclotron resonance spectroscopy to investigate ions formed as collision complexes by chemical ionization. Field ionization kinetics and isotope labelling studies were also used in the investigation of ion structures. The use of isotopic labelling experiments and kinetic energy release studies in providing a detailed mechanistic picture of the ionic decomposition process was discussed by Dr Williams. Thanks to the excellent work of Dr F. P. Lossing over the years, heats of formation of certain ions are now known to a high degree of accuracy. This can enable fragmentation pathways to be predicted. Dr Williams concerned himself with the determination of potential energy profiles for the reactions of simple ions, using evidence from kinetic energy release and deuterium kinetic isotope effects in conjunction with the known thermochemistry of the process. As a result of these studies a great deal is now known about the topology of ions.

The study of negative ions was reported by Professor Jennings. Just as negative ion mass spectra show rather less fragmentation than their positive ion equivalents, so do negative chemical ionization mass spectra. The use of fluorinated derivatives often increases the probability of electron attachment and thus increases sensitivity to the compound. With selected ion monitoring, sub-picogram samples may be detected in certain cases.

The meeting has, I think, touched on most of the growing points in organic mass spectrometry and thus is likely to be a pointer to the development of the subject over the next decade. One gap in the subjects discussed, although the subject was touched upon in part by Dr Nibbering, concerns the kinetics of ion fragmentation, both at times of the order of 1 μs as revealed by a conventional electron impact source and also by the study of very fast processes (10 ps to 1 ns) with the use of the technique of field ionization kinetics. Such studies can reveal structural details of organic ions that are not accessible to other techniques. However, a great deal of ground has been covered in the last two days and I am sure that much of the work described will generate further investigations, and this seems to me to be a primary purpose of a meeting such as this. Finally, I should like to thank the speakers for their contributions.

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