

Budzikiewicz H, Djerassi C & Williams D H. *Mass spectrometry of organic compounds*. San Francisco: Holden-Day, 1967. 690 p.
[Technische Hochschule, Braunschweig, Federal Republic of Germany; Dept. Chem., Stanford Univ., Stanford, CA; and Univ. Chem. Lab., Univ. Cambridge, Cambridge, England]

The approach to rationalize the fragmentation behaviour of organic molecules ionized by electron impact by formulating bond fission and rearrangement processes triggered by a localized charge allowed systemization of the vast experimental material and thus enabled the organic chemist to use mass spectrometry efficiently in his work. [The SC® indicates that this book has been cited in over 2,700 publications since 1967.]

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"Though mass spectrometry had been used for many years —especially in the petrol industry —to characterize and identify organic substances, only vague ideas had been developed regarding the fate of a molecule after ionization. The early observation that mass spectra may show ions which do not correspond to structural sub-units present in the original molecule had led to ideas of a complete ('sudden death') or partial ('hydrogen soup') breakdown of the molecular structure upon ionization with subsequent recombination of atoms to give stable ions which then were responsible for the fragmentation pattern. At best, some wiggly lines were drawn across a molecule to indicate where fragmentation might have occurred. A theoretical approach to explain and predict fragmentation patterns —the so-called quasi-equilibrium theory based on kinetic considerations —was not of much help *in praxi* either because molecules larger than small hydrocarbons were beyond

scope. For these reasons standardized mass spectra were indeed employed as

'fingerprints' for the identification of a compound, but their use for structure elucidation of an unknown (except for the determination of the molecular weight) was rather limited. Thus, it was a rather revolutionary idea when F.W. McLafferty¹ and, in particular, K. Biemann² pointed out that especially compounds containing heteroatoms did not decompose in an unpredictable manner and that their fragmentation could be described by specific reaction mechanisms.

"In the group of C. Djerassi, the idea to rationalize fragmentations wherever possible by formulating bond fissions triggered by a localized charge was applied consequently. In this way it was possible to derive generalizations which allowed us to predict the behaviour of related compounds. These results were the basis for our first book,³ where the characteristics of the various functional groups were described in terms familiar to organic chemists. Although the 'mechanistic approach' to the interpretation of mass spectra was not accepted generally for theoretical reasons (a referee of a renowned journal even in 1963 called it 'a hoax to the scientific community'), it was extremely useful for practical purposes. The following three years were filled with lively research into the behaviour of organic compounds under electron impact. Virtually all common and even most esoteric functional groups were examined and the increasing use of exact mass measurements and iso-topic labelling helped to strengthen or to revise earlier conclusions. Thus, in 1967 so much material had accumulated that a new compilation became necessary. In *Mass Spectrometry of Organic Compounds* the tried principle of presentation of the material was retained.

"This book (which has been translated into Russian and Japanese) has been highly cited because it became the standard reference work for practical electron impact mass spectrometry of organic compounds — even the nomenclature laid down in it has been used as a basis for the IUPAC recommendations—and in a way still is. At least, no publication with similar intentions has appeared in the meantime. For progress reports in the field of organic spectrometry see *Mass Spectrometry*.⁴

1. McLafferty F.W. *Mass spectrometry of organic ions*. New York: Academic Press, 1963. 730 p.
2. Biemann K. *Mass spectrometry, organic chemical applications*. New York: McGraw-Hill, 1962. 370 p.
3. Budzikiewicz H, Djerassi C & Williams D H. *Interpretation of mass spectra of organic compounds*. San Francisco: Holden-Day, 1964. 271 p.
4. *Mass spectrometry*. London: Chemical Society, 1971-1982. Vols. 1-6.