The Beilstein Handbook of Organic Chemistry: The First Hundred Years

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The historical development of Beilstein's Handbook of Organic Chemistry is reviewed, and the general value and significance as well as the principal concepts and main goals of this unique work in the field of organic chemistry are briefly discussed.

Exactly a hundred years ago, the first edition of Beilstein's Handbook of Organic Chemistry was published in two volumes containing descriptions of 15 000 organic compounds. Publication of this first edition, preceded by decades of preparation, was the work of a single man, Friedrich Konrad Beilstein, whose name the work bears.

F. K. Beilstein was born of German parents in 1838 in former St. Petersburg, today Leningrad. After studying chemistry in Heidelberg and Munich, he moved to Göttingen to work with Wöhler, where at the age of 27 he became professor of organic chemistry. A year later, in 1866, he was appointed as the successor of Mendeleev at the Imperial Technical Institute in St. Petersburg, where plans for the publication of the handbook on organic chemistry rapidly evolved, a labor to which he was to devote the greater part of his energies up to his death in 1906.

The immense success of the first edition of his handbook, published in 1881, soon compelled Beilstein to produce a second edition, which appeared as three volumes between 1885 and 1889. The third edition, published between 1892 and 1896, included a supplementary series and a complete register for the third edition. This edition, including the supplementary series, ran to eight volumes and contained critically assessed material on all the then known carbon compounds on a total of around 11 000 printed sides.

Even before completion of the third edition, Beilstein realized that the future publication of a handbook of this nature would greatly exceed the working capacity of a single individual. He therefore transferred responsibility for further publication of the "Beilstein" to the German Chemical Society in 1896, which commenced publication of the fourth edition (to which the supplementary series appearing today also belong) in 1918 with P. Jacobson and B. Prager as joint editors in chief. At this point, the close and fruitful collaboration between the Beilstein editorial staff and the scientific publishing house, Springer-Verlag (Berlin–Heidelberg–New York), began—a collaboration which can now look back on 63 years of unbroken tradition.

In 1933, F. Richter took over responsibility for Beilstein, followed by H. G. Boit, handbook publisher and director of the Beilstein Institute in Frankfurt-am-Main, West Germany, between 1961 and 1978. Since April 1, 1978, executive responsibility for the institute has been in the hands of R. Luckenbach. The Beilstein Institute has had the legal status of a foundation since 1951. The founder was the Max Planck Gesellschaft under its former president Otto Hahn.

The organization and methods of using the Beilstein handbook are discussed elsewhere[1-6] as are current and possible future trends and developments.[5,7,8] This article is confined to reviewing the historical development of this unique work in the field of organic chemistry.[9]

First of all, let us review Beilstein's scientific career. At the age of 15 he left Russia to study chemistry. His initial scientific work, carried out in Bunsen's laboratory in Heidelberg in 1856, was largely concerned with the study of inorganic and analytical chemistry problems. However, like many of his contemporaries, he felt himself irresistibly drawn to the sphere of organic chemistry in which interest was steadily growing, stimulated by Liebig's and Wöhler's investigations. In 1857, Beilstein moved to Göttingen, where he carried out his doctorate studies on the subject of murexide under Wöhler's guidance. Having received his doctorate, Beilstein then moved to Wurtz's laboratory in Paris where he became involved in numerous research projects in the field of organic chemistry.

Following his Paris experience and a short spell of a few months in Breslau, where he renewed acquaintance with his old friend and fellow student from Heidelberg days, Lothar Meyer, Beilstein returned to Göttingen in 1860, where he became Wöhler's assistant. The next six years are described by Beilstein as his personally happiest and scientifically most productive years. Five years after his habilitation in 1860, he became a professor. One year later, in 1866, with the appointment in St. Petersburg, physical separation from Germany, up till then his spiritual homeland, became unavoidable. The work started in Germany (on isomeric aspects of the benzene series) was to occupy him for many years. Other interesting studies involved the reduction of aromatic nitro compounds, the homologues of benzene (toluene, xylene), and the relationship between glyceric acid and lactic acid.

In 1880, after about a decade and a half of teaching and research at the Imperial Technological Institute, his interest centered on another project, which was to occupy the greater part of his working life up to his death: production of "his" handbook, which, after publication of the first edition in 1881, was to bring him initially unexpected renown throughout the world.

The historical studies of Liebig and Wöhler and, in particular, the structural theories of Kekulé (whom Beilstein had also met during his studies in Heidelberg), van't Hoff, and Le Bel not only influenced Beilstein's own experimental work but also provided the stimulus for reinterpretation and reclassification of the known facts of organic chemistry in terms of these new ideas. This was thus an ideal moment for the birth of a new handbook of organic chemistry, as Beilstein presumably realized when he accepted this new challenge and started work on the "Handbook of Organic Chemistry", usually simply referred to as "Beilstein" by chemists the world over.

The structural diversity of organic compounds calls for a classification system which allows for their almost limitless variety. This led Beilstein to develop a systematic classification of compounds according to their constitutional features. This system was further expanded by the Beilstein editorial staff prior to publication of the fourth edition, beginning in 1918, into a fully comprehensive system, the "Beilstein System" which has retained its full value as a highly suitable and freely extendable method of classifying organic compounds up to the present day.[1,4-6,8] The significance of the free extendability of Beilstein's system becomes particularly apparent when the staggering increase in the number of chemical compounds described over the last 100 years is considered; in 1883 about

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20 000 compounds had been described, in 1899 about 75 000, in 1910 about 140 000. The further rapid increase is illustrated by the following features: In 1940 about 400 000 compounds had been described, 1960 about 1 200 000, 1980 about 5 000 000 compounds, of which an estimated 90% belong to the realm of organic chemistry. These figures provide impressive evidence of the quantitative increase in research results produced by the scientific discipline of "organic chemistry" over the last decades. Despite all efforts of the Beilstein editorial staff to present the handbook user with a comprehensive "concentrate" of checked, reliable, and reproducible data, by critical appraisal of all published data and facts, the increased volume of primary publications has unavoidably had its impact on Beilstein. Up to the end of 1980, about 220 subvolumes of the fourth edition (main series plus four supplementary series), begun in 1918, have been published. With completion of Supplementary Series IV in 1984/1985 the total will have reached about 280 subvolumes. Supplementary Series V, which will make its appearance in 1984/1985—in English—will deal with the chemical literature between 1960 and 1980, i.e., two decades which belong to the most fruitful of all in organic chemistry. In processing the literature of this period, as other periods, the Beilstein editorial staff have to keep foremost in their minds the objectives defined by Beilstein himself in compiling the first edition, i.e., only to allow data and facts known to be reliable in terms of current scientific knowledge to appear in the handbook and so provide Beilstein users with a comprehensive concentrate of original literature, free of erroneous results and trivial information. Scientists working in the field of organic chemistry throughout the world may rest assured that in its second century, as in its first, "Beilstein" will remain a competent and dependable aid in dealing with day-to-day research problems, able to save many hours of painstaking literature searching through its systematic organization and critical assessment of the known facts.

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Evaluation and Implementation of Topological Codes for Online Compound Search and Registration

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A topological search code has been found to have high discriminatory power within large sets of disparate structures. The technique has been implemented in a pharmaceutical company's computerized chemical information system, for interactive registration and structure search.

INTRODUCTION

Structure search, the matching of a compound against a machine-readable file of chemical structures to see whether it is already present in the file, is one of the most common and essential functions in a computer-based chemical information system.[1] A routine application of this procedure is compound registration in which compounds not found by structure search, and thus identified as being novel, are incorporated into the system. If structure search is not to involve a time-consuming serial search through the whole file, some form of initial file partitioning must be carried out, such as the use of a molecular formula check in the "isomer sort" approach to registration.[2] Structures occurring in the same partition as the query compound are then compared with it by direct comparison of unique structure representations, e.g., canonical connection tables or WLNs, atom-by-atom matching in the case of non-unique representations, or by eye. It is obviously desirable for purposes of efficiency that the numbers of compounds in each partition should be as small as possible: molecular formula groups are not ideal in this respect since their sizes are highly disparate.[3]

An online system for compound registration and full structure search offers many advantages both to the operators and to the users of such systems. One approach to the provision of such facilities involves the calculation of a numeric search key for a structure representation. The search key for the query structure may then be compared with the keys for structures already in the file by using standard search techniques such as hashing or binary search. A detailed comparison is then carried out when the keys match. Howe and Hagadone described a design for such a system which involved the calculation of a hash address from a canonical connection table and subsequent visual inspection of possible matching

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