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OBITUARY

Stefan Berger: A *Praeceptor* of Magnetic Resonance

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Stefan Berger
09 Sept. 1946—02 April 2023

Longum iter est per praecepta, breve et efficax per exempla.

On April 2, 2023, our community lost one of our great teachers who educated a generation of students and popularized NMR to become a widely used analytical tool in academics, public authorities, and industry.

Stefan Berger was born in 1946 in Heidelberg and grew up in Weinheim an der Bergstraße. He studied Chemistry in Tübingen where he obtained his Ph.D. in organic chemistry with Anton Rieker in 1972. After a postdoc at the Caltech in Pasadena, 1974, he became head of the new NMR department at Marburg University. In 1997, he received a professorship at the University of Leipzig. He retired in 2013. Although he suffered from a heavy disease, he remained productive until his death.

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Around 1974, NMR research was still mainly localized at physics departments and the applicability of chemical shifts and J coupling was still under discussion among chemists. Berger, his time ahead, established in Marburg the prototype of a modern NMR service lab, as we all know it today. In this time, three standard textbooks were written by Kalinowski, Berger, and Braun, which laid the corner stone for practical work for a generation of chemists:

- The first book was dedicated to ^{13}C chemical shifts in organic compounds. For this book, the authors needed to do a large number of own reference experiments as the data were not yet available in literature (with Hans-Otto Kalinowski, Siegmar Braun: 13-C-NMR-Spektroskopie. Thieme, Stuttgart u. a. 1984, ISBN 3-13-632801-9; English Edition: Carbon-13 NMR Spectroscopy. Wiley, Chichester u. a. 1988, ISBN 0-471-91306-5.)
- The generalization to other nuclei followed in a four-volume textbook. Again, a large number of own experimental studies were required to round up the textbook (with Hans-Otto Kalinowski, Siegmar Braun: NMRSpektroskopie von Nichtmetallen. 4 Bände. Thieme, Stuttgart u. a. 1992–1994. English Edition: NMR Spectroscopy of the Non-Metallic Elements. Wiley, Chichester u. a. 1997, ISBN 0-471-96763-7.)
- The third book provided an overview on available NMR pulse sequences and appeared since 1996 in several editions with constantly incorporating the newest technologies (with Hans-Otto Kalinowski, Siegmar Braun: 100 and more basic NMR Experiments. A Practical Course. VCH, Weinheim u. a. 1996, ISBN 3-527-29091-5; with Hans-Otto Kalinowski, Siegmar Braun: 150 and more basic NMR Experiments. A Practical Course. 2. expanded edition. Wiley–VCH, Weinheim u. a. 1998, ISBN 3-527-29512-7; with Siegmar Braun: 200 and more NMR Experiments. A Practical Course. (3., expanded edition). Wiley–VCH, Weinheim 2004, ISBN 3-527-31067-3).

As professor in Leipzig, he was directly involved in designing curricula in chemistry and established comprehensive NMR education in the chemistry studies. In addition to the German language chemistry MSc program, he taught in the postgraduate program (*Aufbaustudium Analytik & Spektroskopie*) to update professionals in companies, in NMR courses offered by the German Chemical Society (GDCh), and in two English language MSc programs he created. Teaching NMR in chemistry was his mission.

His NMR teaching concerned the physical basics, the application to diverse nuclei, and in organic structure analysis using all 1D and 2D NMR methods. Regarding the content of learning, he was keen to move away from "lifeless" basic bodies of homologous series and the like, which he felt inhibited any interest. To this end, he started a collaboration with the organic chemistry department in Leipzig (group around Dieter Sicker) with the aim to write a textbook on isolation and complete spectroscopic analysis of natural products. For this purpose, a program was set up, in which a total of 30 natural substances were to be isolated from different categories: alkaloids, aromatic compounds, dyes, carbohydrates, terpenoids, all rooted in daily life. The aim was to isolate these substances from natural sources using classical means of separation (such

as extraction, distillation, crystallization, chromatography) in an optimized and spectroscopically clean form (which proved to be highly challenging). In the process, students learn how structural features underlie material properties that can be used to distinguish substances in sometimes highly complex matrices, thus enabling their separation. The gain from such work was thus twofold: preparative knowledge and spectroscopic interpretations, both sometimes at the highest level. The resulting textbook "Classics in Spectroscopy—Isolation and Structure Elucidation of Natural Products" (ISBN 978-3-527-32617-4) was published by Wiley–VCH in 2009 and was awarded the 2009 Literature Prize of the *Fonds der Chemischen Industrie*.

Work on this natural product isolation and spectroscopy project continued thereafter. In the following phase, an extensive series of articles on natural products (meaning, isolation, spectroscopy) was first published in the journal *Chemie in unserer Zeit* (2013–2019). From these 29 articles, after translation into English, a second textbook was compiled with an additional 20 natural products. It was published in 2019 under the title "Natural Products—Isolation, Structure Elucidation and History" (ISBN 978-3-527-34194-8). As in the first book, historical backgrounds are presented in detail. In addition, this time quantum chemical calculations were used to determine the molecular structures and chemical shifts for ^{1}H and ^{13}C. The authors of the first textbook (S. Berger, D. Sicker) were joined by Hans-Ullrich Siehl (Ulm) and Klaus-Peter Zeller (Tübingen). These books provide chemical education at its best, something that is unfortunately missing from the "middle of society" today.

Stefan Berger deserves credit for coming up with the quite unusual idea of this interinstitute cooperation. It means not real-world examples for spectroscopy training, but also the reawakening of the unjustly forgotten, often very challenging natural substance isolation in classroom, which imparts enormous preparative knowledge that later will be useful everywhere.

Stefan Berger was not only a great educator but also an excellent scientist with a fine sense able to identify relevant problems. To give an example: one of the most surprising phenomena in magnetic resonance is the Haupt effect [1]: Upon temperature jump, the methyl group of γ-picoline provides nuclear hyperpolarization. Finding more compounds directly by dissolution quantum-rotor induced polarization, as this technique has been coined later [2], is indeed a challenge for "chemical intuition": Stefan Berger successfully proved to have this "magic chemical sense" [3, 4], while his epigones were much less successful and experienced that the effect requires very special conditions of crystal packing [5].

In the NMR community, Stefan Berger will be remembered as one of the great pioneers who established NMR in chemistry education, and who knew how urgently chemical education should be embedded in society if society is to have a future.

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