



Computer-Based Structure Elucidation from Spectral Data: The Art of Solving Problems (Lecture Notes in Chemistry)

Mikhail E. Elyashberg, Antony J. Williams

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Computer-Based Structure Elucidation from Spectral Data: The Art of Solving Problems (Lecture Notes in Chemistry) Mikhail E. Elyashberg, Antony J. Williams

Here, the authors introduce readers to solving molecular structure elucidation problems using the expert system ACD/Structure Elucidator. They explain in detail the concepts of the Computer-Assisted Structure Elucidation (CASE) approach and point out the crucial role of understanding the axiomatic nature of the data used to deduce the structure. Aspects covered include the main blocks of the expert system and essential features of the mathematical algorithms used. Graduate and PhD students as well as practicing chemists are provided with a detailed explanation of the various practical approaches depending on available spectral data peculiarities and the complexity of the unknown structure. This is supported by a large number of real-world completed examples, most of which are related to the structure elucidation of natural product molecules containing unusual skeletons. Dedicated software and further supplementary material are available at www.acdlabs.com/TeachingSE.

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