

Aromatizität: Geschichte und mathematische Analyse eines fundamentalen chemischen Begriffs (*Aromaticity: Historical and Mathematical Analysis of a Fundamental Chemical Concept*)

by Julia Neus

size: iv + 179pp., 928 kB, publication date: October 2002, ISSN: 1610-6067 (internet), 1610-6075 (cd-rom)

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About the Author

Julia Neus was born in Lennestadt, Germany, in 1973. She studied mathematics, chemistry, and theology at the University of Siegen where she graduated in 1999 with a most remarkable thesis on the history and mathematical analysis of aromaticity, published now as HYLE Study No. 2. After graduation, she worked as a trainee in the chemical industry (LSG Elab Siegen, and Bayer AG Leverkusen). In 2000 she moved to Stuttgart to become a High School teacher. Upon qualifying as an Assessor in 2002, she acts as a teacher at the secondary school in Murrhardt, Southern Germany. (Contact: julia.neus@gmx.de)

About the book

Aromaticity is one of the most important concepts not only in organic chemistry. This book first outlines the historical development of the concept since the discovery of benzene in 1825 and then analyses its meaning in mathematical terms. The author

distinguishes between many different aspects of the notion of aromaticity and discusses a large variety of numerical parameters (energetic, geometric, magnetic, spectroscopic and reactivity parameters). The central issue is whether all these parameters essentially refer to the same basic property of aromaticity, or whether there are several independent factors behind the received notion that allow to distinguish between different types of aromaticity.

Julia Neus discusses in great detail the different opinions and arguments put forward by numerous research groups since 1989. Many chemists have argued for the existence of at least two orthogonal and independent types of aromaticity, based on the mathematical-statistical approach of factor analysis. Others have supported the idea that aromaticity is a single, one-dimensional concept, because of the high correlation coefficients they obtained. By carefully assessing all the arguments and by referring to statistical analyses and to the physical and chemical background, the author concludes that the common set of different aspects of aromaticity comprises more than a single chemical notion. However, a lot of research work has still to be done to identify the quantum chemical basis of these types of aromaticity.

"Quite different opinions have been put forward about the usefulness and about the conceptual contents of aromaticity during the past one and a half centuries. Julia Neus here presents a comprehensive history, and a thorough statistical-mathematical analysis of the physical parameters of this very notion. She convincingly arrives at the conclusion that this basic chemical concept cannot be reduced to physics, but it can be well related to a two- or three-dimensional physical parameter space." **Prof. Dr. W. H. Eugen Schwarz, University of Siegen**