Molecular Crystals and Liquid Crystals

ISSN: 1542-1406 (Print) 1563-5287 (Online) Journal homepage: http://www.tandfonline.com/loi/gmcl20

A Review of "Aromaticity and Other Conjugation Effects"

Daniel J. Sandman

To cite this article: Daniel J. Sandman (2014) A Review of "Aromaticity and Other Conjugation Effects", Molecular Crystals and Liquid Crystals, 605:1, 261-261, DOI: 10.1080/15421406.2014.925720

To link to this article: http://dx.doi.org/10.1080/15421406.2014.925720

Mol. Cryst. Liq. Cryst., Vol. 605: pp. 261, 2014

ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421406.2014.925720

BOOK REVIEW

Aromaticity and Other Conjugation Effects by Rolf Gleiter and Gebhard Haberhauer, Wiley VCH: Weinheim, 2012; ISBN 978-3-527-32934-2 (softcover); xiv + 452 pages; $80.00 (paperback).

The authors based this book on graduate courses in physical organic chemistry taught in their universities. It was written for advanced undergraduate and graduate level students. In the book, the authors present various concepts of bonding by presenting the experimental results followed by simple molecular orbital arguments based on perturbation theory within a one-electron model. The model is refined by ab initio treatments. The reader is expected to have a good knowledge of first year organic and theoretical chemistry. The authors touch a number of topics of interest in the area of modern materials chemistry as they take students on this journey. There is a significant emphasis on photoelectron spectroscopy and its quantum chemical interpretation. There is a two page forward by Roald Hoffmann who touts the authors' approach as leading to a good understanding of the subject matter.

There are a number of topics in the text that would benefit from additional detail or a somewhat different emphasis. The discussion of polyacetylene on pp. 15–17 ignores the pi-amphoteric character of $(CH)_x$ by ignoring *n*-doping. It also ignores the possible role of solitons in the properties of $(CH)_x$. The discussion of donor–acceptor complexes in Section 3.1 does not distinguish between systems that do not involve electron transfer and those that do. The discussion of organic metals and superconductors is quite incomplete. The discussion of interactions in cyclic *bis*-acetylenes would be more valuable if it included the attempted correlation of the acetylenic angle with ^{13}C NMR chemical shifts. (See Gleiter, R., & Merger R. (1995). In: *Modern Acetylene Chemistry*, Stang, P. J. & Diederich, F. (Eds.), pp. 285–319, VCH: Weinheim). Since resonance structures typically do not involve contributors with different numbers of unpaired electrons, the structures in Figure 5.20 should probably be renamed. On p. 316, the suggestion that hyperconjugation plays an important role in the barrier of ethane is contradicted by other theoretical work supporting the traditional ideas about repulsion. (See Mo, Y., & Gao, J. (2007). *Acc. Chem. Res.*, 40, 113–119). In Chapter 6, the discussion of the theory of UV-VIS spectra should note that it should be in the framework of time-dependent perturbation theory. Fluorescence is not discussed.

As an amusing aside, the two German authors lapse into their native language on p. 200 with the use of "und" for "and."

Overall the authors have given us a useful book not only for students but also for more experienced scientists as they cover much material in depth.

Daniel J. Sandman
Center for Advanced Materials
Department of Chemistry
University of Massachusetts Lowell
Lowell, MA 01854-5046