N. D. Epiotis

Unified Valence Bond Theory of Electronic Structure

With collaboration of J. R. Larson, H. L. Eaton

1982. VIII, 305 pages
(Lecture Notes in Chemistry, Volume 29)
ISBN 3-540-11491-2

Contents: Qualitative Valence Bond Theory of Model Systems. - Qualitative Molecular Orbital-Valence Bond Theory.

Qualitative monodeterminantal MO theory, though undeniably stimulating, suffers from lack of conceptual clarity. After some years of preoccupation with this theory, the authors abandoned it. In its place, they have sought to develop a new way of thinking about molecular electronic structure which exploits the positive aspects of MO and VB theories and which eliminates conceptual interdisciplinary barriers. The new approach is described in this work, starting with elementary VB notions and culminating with the presentation of the compact MOVB method a "back of the envelope" theory which operates near the same level as "state of the art" quantum chemical computations. Though much of the space is devoted to the presentation of the theory, a number of chemically significant illustrative applications are provided with the aim of making the reader fully qualified to use and extend the approach in any field of personal interest. The ultimate goal is to establish a new language of chemistry which can eventually lead to a higher level of understanding of why and how molecules exist and react and pave the way to predictions which lie outside the intuitive range of chemists and physicists.

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N. D. Epiotis

Theory of Organic Reactions

1978. 69 figures, 47 tables. XIV, 290 pages
(Reactivity and Structure, Volume 5)
ISBN 3-540-08551-3

Contents: One-determinental theory of chemical reactivity. - Configuration interaction overview of chemical reactivity. - The dynamic linear combination of fragment configurations method. - Even-even intermolecular multicentric reactions. - The problem of correlation imposed barriers. - Reactivity trends of thermal cycloadditions. - Reactivity trends of singlet photochemical cycloadditions. - Miscellaneous intermolecular multicentric reactions. - $\pi + \sigma$ addition reactions. - Even-odd multicentric intermolecular reactions. - Potential energy surfaces for odd-odd multicentric intermolecular reactions. - Even-even intermolecular bicentric reactions. - Even-odd intermolecular bicentric reactions. - Odd-Odd intermolecular bicentric reactions. Potential energy surfaces for geometric isomerization and radical combination. - Odd-odd intramolecular multicentric reactions. - Even-even intramolecular multicentric reactions. - Mechanisms of electrocyclic reactions. - Triplet reactivity. - Photophysical processes. - The importance of low lying nonvalence orbitals. - Divertissements. - A contrast of "accepted" concepts of organic reactivity and the present work.

Structural Theory of Organic Chemistry

By **N. D. Epiotis, W. R. Cherry, S. Shaik, R. L. Yates, F. Bernardi**

1977. 60 figures, 58 tables. VIII, 250 pages
(Topics in Current Chemistry, Volume 70)
ISBN 3-540-08099-6

Contents: Theory. - Nonbonded Interactions. - Geminal Interactions. - Conjugative Interactions. - Bond Ionicity Effects.

This work constitutes the first attempt to develop a new overview of structural chemistry based on quantum theory. A combination of qualitative molecular orbital theory and explicit quantum mechanical computations leads to the identification of the key factors controlling the shape of a molecule. On this basis, the experimentalist can anticipate structural trends for simple as well as complex molecules. In all cases, the theoretical principles are illustrated by reference to available experimental data. (420 references)

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Lecture Notes in Chemistry

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