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Book review

Mezey P. G. (ed) (1991) VCH Publishers, New York 386 pp, DM 265

This book provides a collection of papers concerning the title topic as presented at the December 1989 International Congress of the Pacific Basin Chemical Societies and as originaly published in volume 7 of the Journal of Mathematical Chemistry. As it turns out there is a notable bent toward certain types of modelling: namely as concerns chemical graph theory and geometric-topological shape analyses. There is a lesser focus on standard quantum-chemical and statistical-mechanical modelling. Within the realm of focus this book provides a number of interesting articles which typically indicate a body of literature separate from the other articles in this collection. The 386 pages and 21 articles are divided into four areas: "Stereochemistry and Shape Analysis", "Reactivity and Reaction Modelling", "Chemical Properties and QSAR", and "Algorithmic Approaches and Miscellaneous Topics". For instance, the second of these topical areas consists of four articles: the first by Whittington, Soteros, and Madras concerns temperature-dependent polymer statistics (e.g. free energies and size extensions) of branched polymers in dilute solution; the second by Tachibana concerns a geometric-topological modelling of the reaction-coordinate pathway and the nearby accessible region on a potential hypersurface; the third by Fujita concerns a formal graphic-group-algebraic scheme for enumerating and characterizing all possible reactions of a molecular skeleton with any of a variety of substituents changing to a new skeleton via a particular mode; and the fourth by Klin, Tratch, and Zefirov concerns a graphico-group-theoretic investigation of individual rearrangement graphs for fluxional molecules (such as bullvalene, with over a million equivalent conformational minima). Overall the collection offers an interesting selection of articles which exhibit little overlap and which reasonably cover a selected range of chemical mathematical modelling schemes.

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