

Modeling Marvels

Errol G. Lewars

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Computational Anticipation
of Novel Molecules

 Springer

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A survey of a variety of novel compounds which have been studied theoretically but have not yet been made. Some of these molecules defy conventional concepts of chemical bonding; all should exhibit novel properties.

To Anne and John

Preface

The aim of this book is to survey a number of chemical compounds that some chemists, theoretical and experimental, find fascinating. Some of these compounds, like planar carbon species or oxirene, offer no obvious practical applications; nitrogen oligomers and polymers, in contrast, have been touted as possible high-energy-density materials. What unites this otherwise eclectic collection is that these substances are unknown and offer a challenge to theory and to synthesis. That such a challenge exists is in some cases almost obvious to most chemists: the instability of nitrogen polymers, for example, might be taken nearly as an axiom, to be quantified but not refuted by computations and to be subjected to an almost superfluous (but rather challenging) validation by synthesis. On the other hand, oxirene, the unsaturated relative of the prosaic oxirane, presents no immediately obvious oddity, yet this molecule has defied all attempts at synthesis and remains a theoretical conundrum, in that it is not certain if it can even exist! I hope that this collection of quirky molecules will appeal to chemists who find the study of chemical oddities interesting and, on occasion, even rewarding.

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