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1.4.2.2 Calculations and Results Using Different Quantum Methods for the Zaib4 Molecule
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 1.4.9.1 Vesicular Stomatitis Virus Nucleoprotein (2QVJ) Molecule
 1.4.9.2 Hydrogen Bond Calculations; 1.4.9.3 Comments regarding the 2QVJ Calculations; 1.5 Summary and Conclusions; References; 2 Getting the Most out of ONIOM: Guidelines and Pitfalls; 2.1 Introduction; 2.2 QM/MM; 2.3 ONIOM; 2.4 Guidelines for the Application of ONIOM; 2.4.1 Summary; 2.5 The Cancellation Problem; 2.6 Use of Point Charges; 2.7 Conclusions; References; 3 Modeling Enzymatic Reactions in Metalloenzymes and Photobiology by Quantum Mechanics (QM) and Quantum Mechanics/Molecular Mechanics (QM/MM) Calculations
 3.1 Introduction

Sommario/riassunto

Divided into five major parts, the two volumes of this ready reference cover the tailoring of theoretical methods for biochemical computations, as well as the many kinds of biomolecules, reaction and transition state elucidation, conformational flexibility determination, and drug design. Throughout, the chapters gradually build up from introductory level to comprehensive reviews of the latest research, and include all important compound classes, such as DNA, RNA, enzymes, vitamins, and heterocyclic compounds. The result is in-depth and vital knowledge for both readers already working in the
