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Large Molecular Systems; 3.1 Introduction; 3.2 Existing Excited-State Methods for Medium-Sized and Large Molecules; 3.2.1 Wavefunction-Based ab initio Methods; 3.2.2 Density-Based Methods; 3.3 Analysis of Electronic Transitions; 3.4 Calculation of Static Absorption and Fluorescence Spectra; 3.5 Dark States; 3.5.1 Excited Electronic States with Large Double Excitation Character
3.5.2 Charge-Transfer Excited States3.6 Summary and Conclusions; References; 4 Assigning and Understanding NMR Shifts of Paramagnetic Metal Complexes; 4.1 The Aim and Scope of the Chapter; 4.2 Basic Theory of Paramagnetic NMR; 4.2.1 The Origin of the Hyper.ne Shift; 4.2.1.1 The Contact Shift; 4.2.1.2 The Pseudocontact Shift; 4.2.2 Relaxation and Line Widths; 4.2.2.1 Electronic Relaxation; 4.2.2.2 Dipolar Relaxation; 4.2.2.3 Contact Relaxation; 4.2.2.4 Curie Relaxation; 4.2.3 Advice for Recording Paramagnetic NMR Spectra; 4.3 Signal Assignments; 4.3.1 Comparison of Similar Compounds
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7.8.2 Force Fields, Docking, and Scoring

Sommario/riassunto

Molecular modeling encompasses applied theoretical approaches and computational techniques to model structures and properties of molecular compounds and materials in order to predict and / or interpret their properties. The modeling covered in this book ranges from methods for small chemical to large biological molecules and materials. With its comprehensive coverage of important research fields in molecular and materials science, this is a must-have for all organic, inorganic and biochemists as well as materials scientists interested in applied theoretical and computational chemistry. The 28