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5.4 Practical Considerations5.5 Making Use of Experimental Data; 6 Conclusions; Part II: Applications; 7 Structural Aspects; 7.1 Accuracy of Structure Prediction; 7.2 Molecular Visualization; 7.3 Isomer Analysis; 7.4 Analysis of Structural Trends; 7.5 Prediction of Complex Polymerization; 7.6 Unraveling Crystallographic Disorder; 7.7 Enhanced Structure Determination; 7.8 Comparison with Solution Properties; 8 Stereoselectivities; 8.1 Conformational Analysis; 8.2 Enantioselectivities; 8.2.1 Racemate Separation; 8.2.2 Stereoselective Synthesis; 8.2.3 Prediction of Enantioinduction
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13.1 Complexes of Amino Acids and Peptides

Sommario/riassunto

After the second edition introduced first density functional theory aspects, this third edition expands on this topic and offers unique practice in molecular mechanics calculations and DFT. In addition, the tutorial with its interactive exercises has been completely revised and uses the very latest software, a full version of which is enclosed on CD, allowing readers to carry out their own initial experiments with forcefield calculations in organometal and complex chemistry.