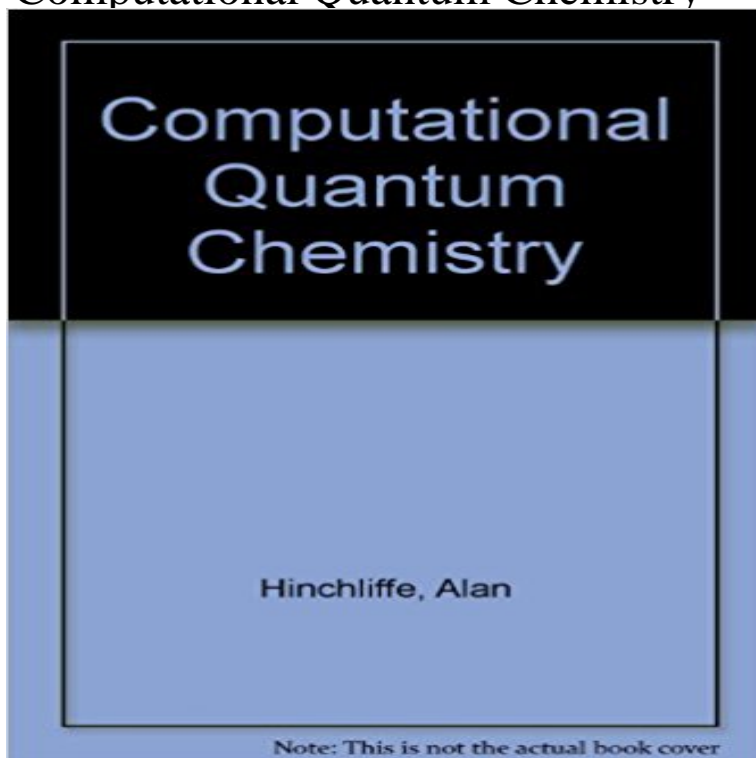


Computational Quantum Chemistry



Ab initio calculations are playing an increasingly important role in all areas of experimental, theoretical and physical chemistry. The aim of this text is to provide a brief, easy to follow introduction to this area, where complex computer driven calculations can often be bewildering for the newcomer. Computational Quantum Chemistry can be used as a text, and should be of great value to those starting research or on specialist courses involving ab initio calculations. It does not deal with the in-depth theory, but with the application of these methods to the validation of experimental work by the use of computer models.

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