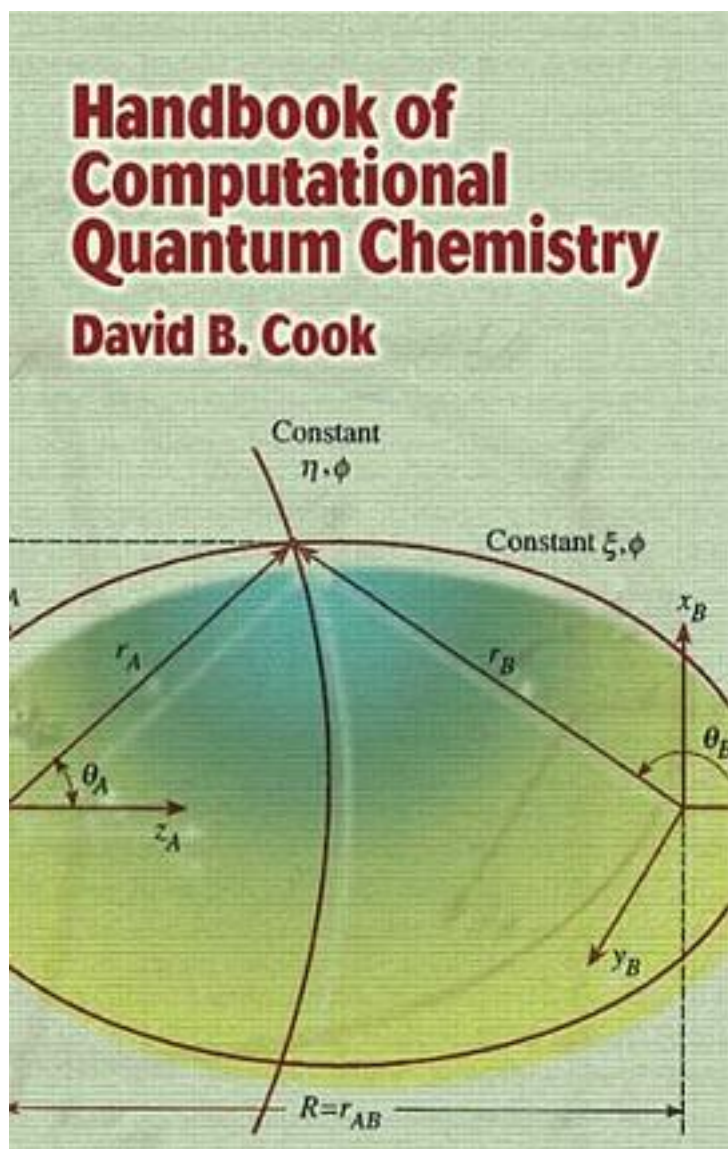


Handbook of Computational Quantum Chemistry



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著者: Cook, David B.

出版者: Dover Pubns

出版时间: 2005-8

装帧: Pap

isbn: 9780486443072

This comprehensive text provides upper-level undergraduates and graduate students with an accessible introduction to the implementation of quantum ideas in molecular modeling, exploring practical applications alongside theoretical explanations. Topics include the Hartree-Fock method; matrix SCF equations; implementation of the closed-shell case; introduction to molecular integrals; and much more. 1998 edition.

作者介绍:

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