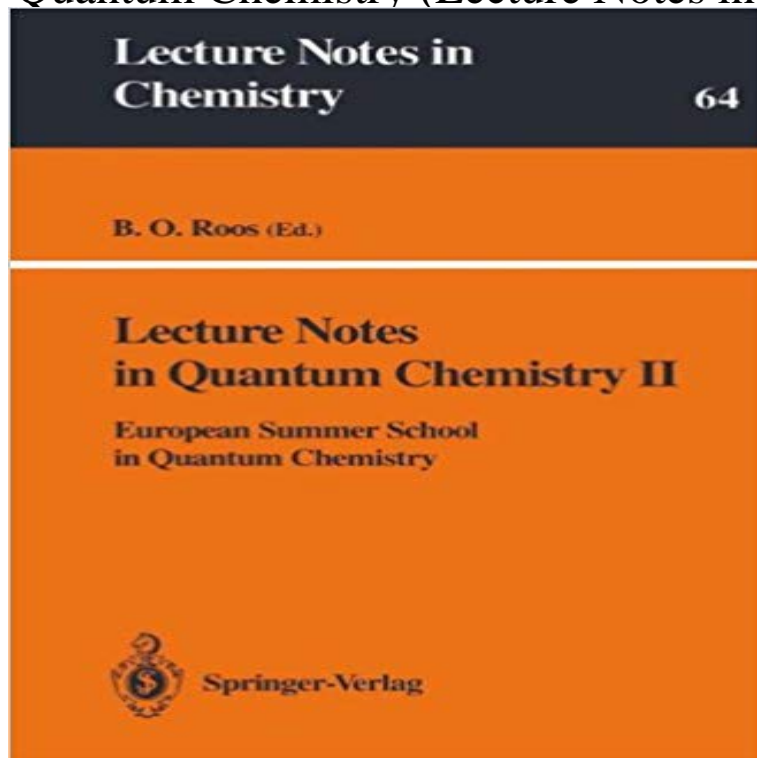


Lecture Notes in Quantum Chemistry II: European Summer School in Quantum Chemistry (Lecture Notes in Chemistry)



The first volume of Lecture Notes in Quantum Chemistry (Lecture Notes in Chemistry 58, Springer Verlag, Berlin 1992) contained a compilation of selected lectures given at the two first European Summer Schools in Quantum Chemistry (ESQC), held in southern Sweden in August 1989 and 1991, respectively. The notes were written by the teachers at the school and covered a large range of topics in ab initio quantum chemistry. After the third summer school (held in 1993) it was decided to put together a second volume with additional material. Important lecture material was excluded in the first volume and has now been added. Such added topics are: integrals and integral derivatives, SCF theory, coupled-cluster theory, relativity in quantum chemistry, and density functional theory. One chapter in the present volume contains the exercise material used at the summer school and in addition solutions to all the exercises. It is the hope of the authors that the two volumes will find good use in the scientific community as textbooks for students, who are interested in learning more about modern methodology in molecular quantum chemistry. The books will be used as teaching material in the European Summer Schools in Quantum Chemistry, which are presently planned. Lund in July 1994 Bjorn Roos NOTES ON HARTREE-FOCK THEORY AND RELATED TOPICS JanAlmlof Department of Chemistry University of Minnesota Minneapolis, MN 55455. USA Contents: 1 Introduction. 2 . The Born-Oppenheimer Approximation. 3. Determinant Wavefunctions and the Pauli Principle. 4. Expectation Values With a Determinant Wavefunction.

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