



A New Dimension to Quantum Chemistry: Analytic Derivative Methods in Ab Initio Molecular Electronic Structure Theory (International Series of Monographs on Chemistry)

By Yukio Yamaguchi, John D. Goddard, Yoshihiro Osamura, Henry Schaefer

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In modern theoretical chemistry, the importance of the analytic evaluation of energy derivatives from reliable wave functions can hardly be overestimated. This monograph presents the formulation and implementation of analytical energy derivative methods in *ab initio* quantum chemistry. It includes a systematic presentation of the necessary algebraic formulae for all of the derivations. The coverage is limited to derivative methods for wave functions based on the variational principle, namely restricted Hartree-Fock (RHF), configuration interaction (CI) and multi-configuration self-consistent-field (MCSCF) wave functions. The monograph is intended to facilitate the work of quantum chemists, and will serve as a useful resource for graduate-level students of the field.

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