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QUANTUMCHEMICAL METHODS, Kém/254
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INTRODUCTION

Postulates of the Classical and the Non-Relativistic Quantum Mechanics. Atomic units.

THE HARTREE-FOCK METHOD

Orbital-approximation Separation of the eigenvalue problem in L_2 space. Antisymmetry Postulate, Pauli-principle, exclusion principle. Slater-determinant. Energy expression for spinorbitals. Core integrals. Coulomb integrals. Exchange integrals. Unrestricted Hartree-Fock (UHF) method . Restricted Hartree-Fock (RHF) method. Orbital energies. Numerical solution for atoms. LCAO-approximation. Requirements for the basis set. Types of basis sets. Determination of the LCAO coefficients (Roothaan-Hall). Method of the Lagrange-multipliers. Roothaan-Hall LCAO-SCF equation. Canonical orbitals. Hartree's Self-Consistent Field (SCF) method. Direct (Almlöf) and semi-direct (Ahlrichs) SCF method.

DERIVATIVES

Potential surface. External perturbations. Calculation of derivatives. Variational deduction (without and) with constraints. First derivative of the Hartree-Fock energy. Jahn-Teller principle. Cartesian and internal coordinates. The characters of stationary points. Saddle points, reaction paths. Yeljasevich-Wilson vibrational equation. Natural Internal Coordinates and the INTC program.

POST-HARTREE-FOCK METHODS

Dynamic and non-dynamic correlation. Configurational Interaction (CI). Many Body Perturbation Theory, MP2. Coupled Cluster methods. Truncated CI methods. Size-onsistency, size-extensivity. RHF determinant. VB, MC-SCF, CAS-SCF, GVB, projected UHF methods. First- and second order reduced density matrices. Natural spinorbitals, natural orbitals. UNO-CAS method (Pulay).

DENSITY FUNCTIONAL METHODS

Hohenberg-Kohn theorems. Holographic electron density theorem (Mezey). Kohn-Sham method. HFS method. Basis sets in DFT (Gauss, Slater, Augmented Plane Waves). Exchange-correlational (XC) energy. Non-local functional approximations.

MAGNETIC PROPERTIES – NMR CHEMICAL SHIFTS

Electric field, magnetic induction, vector potential. External fields, homogeneous magnetic field. Nuclei: magnetic dipoles. Implementation into the Hamiltonian. Chemical shift (shielding), isotropic and anisotropic parts. Gauge-invariance, Gauge Invariant Atomic Orbitals (GIAO, London). GIAO-GTO method (Pulay).

APPENDIX

The Born-Oppenheimer approximation.