Basis Set Independent Calculation of Molecular Properties

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Numerical solutions of the Hartree-Fock equations for molecules are constructed in cartesian coordinates in three dimensions. The method involves

- Finding approximate molecular orbitals as linear combinations of numerically defined optimized atomic orbitals
- Mapping the approximate solutions to the cartesian mesh
- Obtaining corrections to the approximate solutions
- Exploiting the known behavior of the orbitals and densities at the nuclei

The accuracy of the results is then limited by the finite difference approximations. The procedure for obtaining the corrections requires the inversion of the Fock operator. The same procedure can then be applied to the evaluation of the response to single-particle perturbations, in particular static polarizabilities. In this poster, accurate, basis set independent, Hartree-Fock energies and polarizabilities will be given for a number of small molecules.