

advances in quantum chemistry pdf

Ab initio quantum chemistry methods are computational chemistry methods based on quantum chemistry. The term ab initio was first used in quantum chemistry by Robert Parr and coworkers, including David Craig in a semiempirical study on the excited states of benzene. The background is described by Parr. Ab initio means "from first principles" or "from the beginning", implying that the only ...

Ab initio quantum chemistry methods - Wikipedia

Semi-empirical quantum chemistry methods are based on the Hartree–Fock method formalism, but make many approximations and obtain some parameters from empirical data. They were very important in computational chemistry from the 60s to the 90s, especially for treating large molecules where the full Hartree–Fock method without the approximations were too costly.

Computational chemistry - Wikipedia

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