

## COMPARISON OF AB INITIO QUANTUM CHEMISTRY WITH EXPERIMENT FOR SMALL MOLECULES%0A

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1985; Rodney J. Bartlett, ed. Comparison of Ab Initio Quantum Chemistry With Experiment for Small Molecules For the reaction exoergicity the Davidson correction has little effect. There is also a problem with the theoretical description of the kinetics of the addition reaction.

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**Ab initio quantum chemistry methods - Wikipedia**

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 inputs into an ab initio calculation are physical constants.

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