

***ab initio* quantum mechanical methods**

(synonymous with non-empirical quantum mechanical methods)

Methods of quantum mechanical calculations independent of any experiment other than the determination of fundamental constants.

The methods are based on the use of the full Schroedinger equation to treat all the electrons of a chemical system. In practice, approximations are necessary to restrict the complexity of the electronic wavefunction and to make its calculation possible.

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N.B. This supersedes an *earlier definition*.