

## ***ab initio* quantum mechanical methods**

**Synonym:** 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.

**Source:**

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1921

This definition supersedes an earlier definition of *ab initio* calculations.