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semi-empirical quantum mechanical methods

Methods which use parameters derived from experimental data to simplify computations. The simplification may occur at various levels: simplification of the Hamiltonian (*e.g.*, as in the Extended Huckel method), approximate evaluation of certain molecular integrals (see, for example, Zero differential overlap approximation), simplification of the wavefunction (for example, use of a Pi (π) electron approximation as in Pariser–Parr–Pople method), *etc*.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1962

