

Born–Oppenheimer (BO) approximation

Representation of the complete wavefunction as a product of an electronic and a nuclear part

$$\Psi(r,R) = \Psi_e(r,R) \Psi_N(R)$$

where the two wave-functions may be determined separately by solving two different Schrodinger equations. The validity of the Born–Oppenheimer approximation is founded on the fact that the ratio of electronic to nuclear mass ($\frac{m}{M} \cong 5 \times 10^{-4}$) is sufficiently small and the nuclei, as compared to the rapidly moving electrons, appear to be fixed. The approximation breaks down near a point where two electronic states acquire the same energy (see Jahn–Teller effect). The BO approximation is often considered as being synonymous with the adiabatic approximation. More precisely, the latter term denotes the case when Ψ_e diagonalize the electronic Hamiltonian. Thus, the adiabatic approximation is an application of the BO approximation.

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1929