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harmonic approximation

The approximation of the full nuclear potential of a molecular system in its equilibrium geometry and in the vicinity of the respective minimum on the potential energy surface by the function

$$V = \frac{1}{2} \sum_{i,j=1}^{3N} \frac{\partial^2 V}{\partial q_i \partial q_j}$$

where q_i are mass-weighted cartesian displacements of nuclei relative to their equilibrium positions. The approximation allows one to describe vibrational motion in terms of independent vibrational modes (normal modes) each of which is governed by a simple one-dimensional harmonic potential.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1941

