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1.2 Theories and computation in chemistry

Consider a theory that predicts the appearance of the infrared absorption spectrum of a diatomic molecule in the gas phase from knowledge of its mass, m , and bond length, r , and the shape of the potential energy curve for interaction between the two atoms. This theory can be written in the form of an equation for the vibrational frequency ν :

$$\nu = \frac{1}{2\pi} \sqrt{\frac{V''(r)}{m}}$$

where ν is the reduced mass of the two atoms (and is equal to $m_1 m_2 / (m_1 + m_2)$), and $V''(r)$ is the second derivative of the bond, with the potential energy V for the system assumed to be given by Equation (1.2) for values of the internuclear distance r close to r_0 , the equilibrium bond length.

This theory can be tested and compared with experiments in chemistry, and the results can be used to improve the theory. One possibility is to use a more