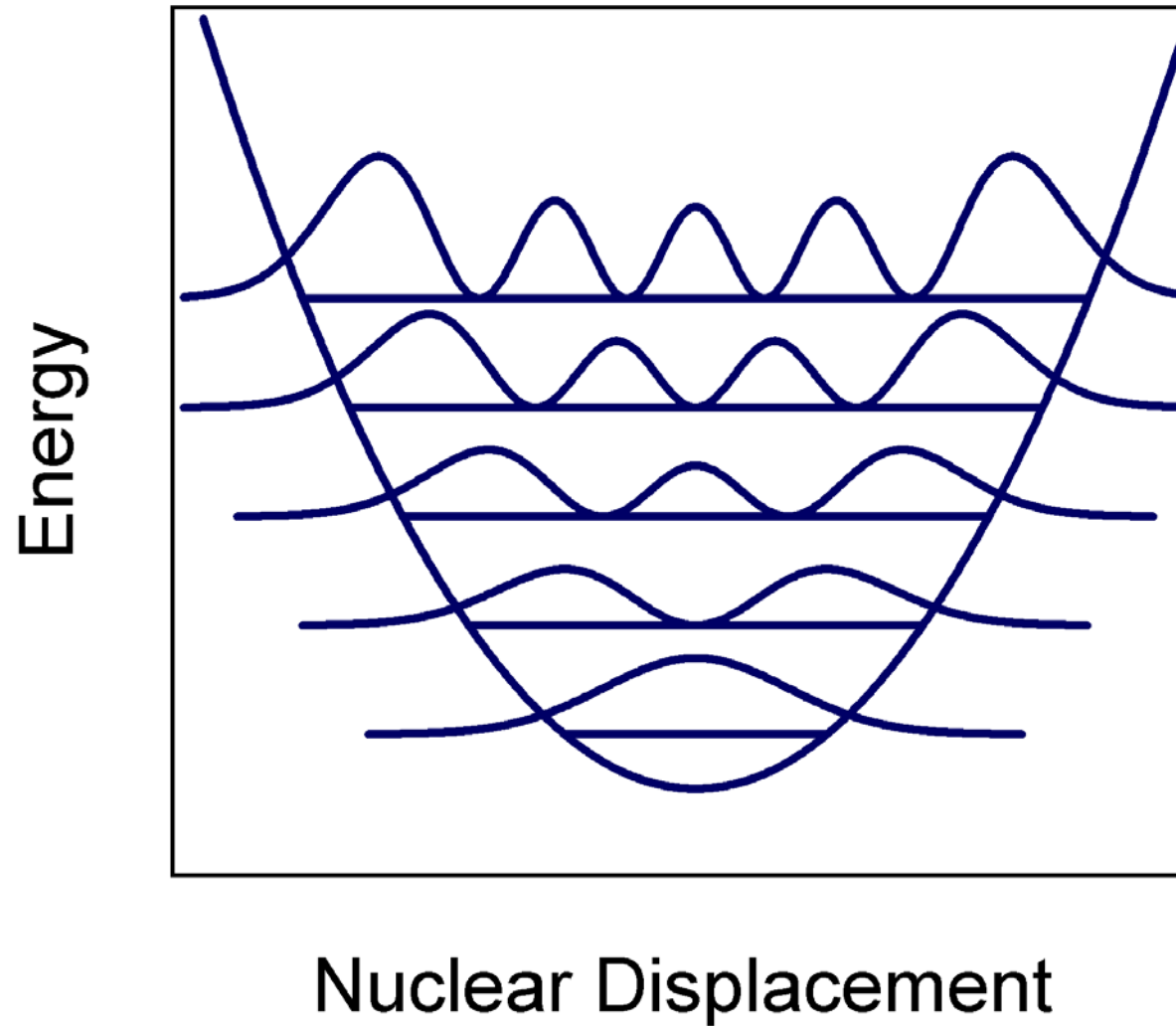


Root-mean-square displacement problem



Root-mean-square displacement problem

Calculate and compare the root-mean-square displacement of H₂ and O₂ in the lowest vibrational eigenstate. The definition of the root-mean-square displacement is:

$$\sqrt{\langle Q^2 \rangle} = \sqrt{\int_{-\infty}^{\infty} \chi_0 Q^2 \chi_0 dQ}$$

The vibrational wavenumbers of H₂ and O₂ are 4,400 and 1,580 cm⁻¹, respectively.