

zero-point vibrational energy (ZPVE)

The energy of vibration of a molecule at absolute zero (0 K). It is given by

$$E_{\text{vib}}(0) = (1/2)h \sum_i \nu_i$$

where ν_i is a normal-mode vibrational frequency. Even for a small molecule, the total ZPE can amount to several tens of kcal/mol. ZPE is a quantum mechanical effect which is a consequence of the uncertainty principle.

1999, 71, 1970