Calculation of structural properties and vibrational frequencies of α- and γ-N2 crystals

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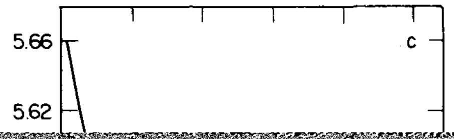

$$K = 3244.18\ \text{kcal/Å}^2$$

for the harmonic intramolecular potential [Eq. (19)]. The molecular bond length b_0 was not treated as a parameter but set at the experimental N–N bond length of

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to construct such potentials.[63-67] However, both the reliability of the potential and the values of its free parameters have been determined only in relation to fluids and condensed gases (viscosity, second virial coefficients, vibrational frequencies of dimers, etc.) where

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