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

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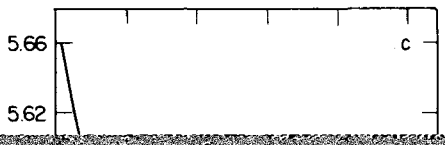
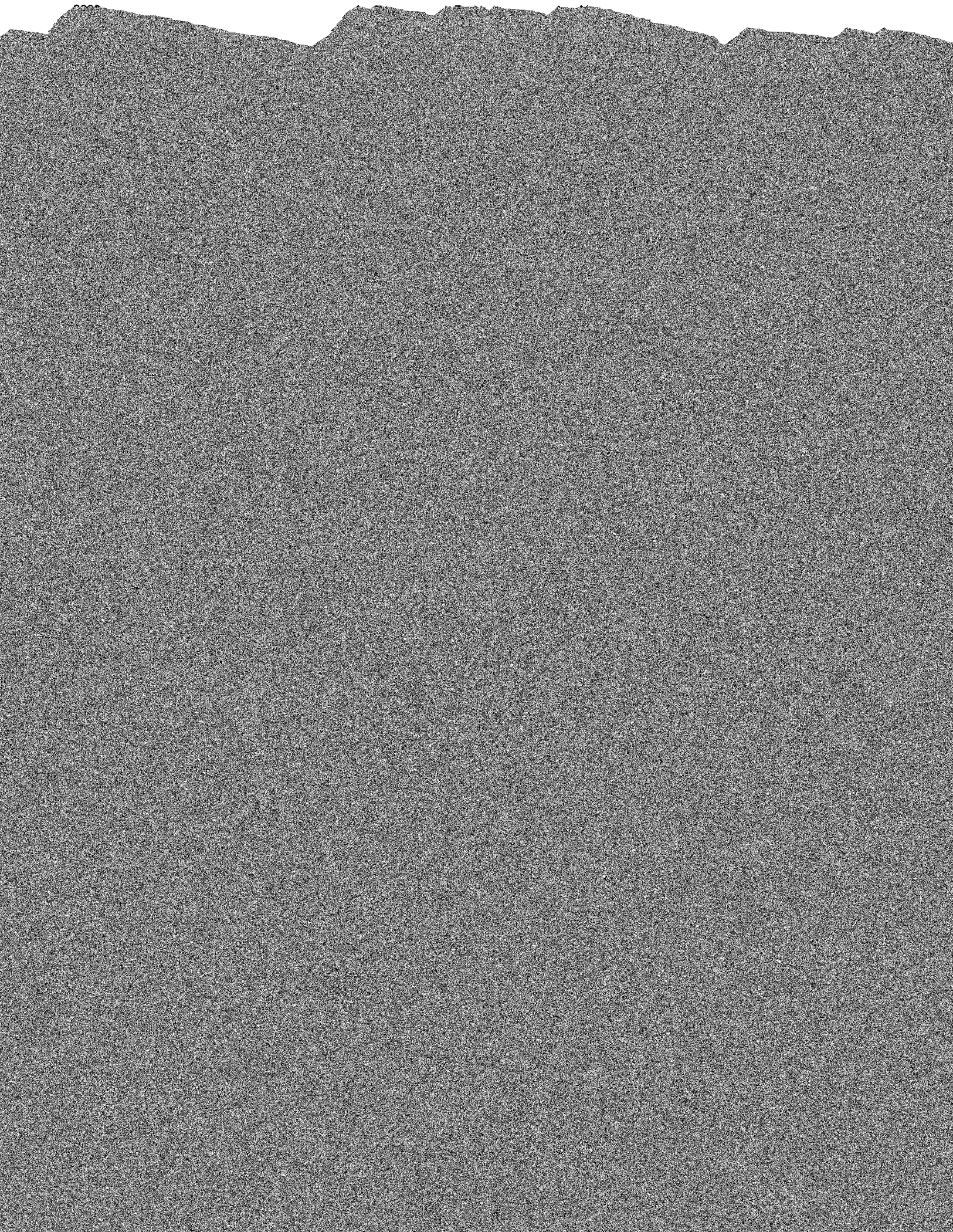


$$K = 3244.18 \text{ kcal/Å}^2$$

for the harmonic intramolecular potential [Eq. (19)]. The molecular bond length b_0 was not treated as a pa-



The Davydov splitting between $\mathbf{q} = 0$ internal modes in γ-N_2 is larger than the corresponding splitting in α-N_2. Experimentally[22] only one Davydov component was ob-

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