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

A. Zunger and E. Huler

Citation: The Journal of Chemical Physics 62, 3010 (1975); doi: 10.1063/1.430888

View online: http://dx.doi.org/10.1063/1.430888

View Table of Contents: http://scitation.aip.org/content/aip/journal/jcp/62/8?ver=pdfcov

Published by the AIP Publishing

Articles you may be interested in

Far infrared spectroscopy and empirical intermolecular potential for ¸ ُ and ¸ ُN2 under pressure
J. Chem. Phys. 74, 2675 (1981); 10.1063/1.441436

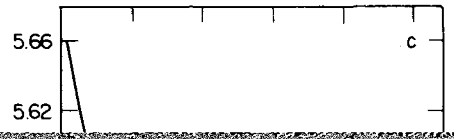
Comment on ῾Vibron and lattice frequency shifts in the Raman spectra of solid ¸ ُN2 and ¸ ُN2 and librational force constants of diatomic molecular crystals῾
J. Chem. Phys. 71, 3893 (1979); 10.1063/1.438802

Vibron and lattice frequency shifts in the Raman spectra of solid ¸ ُN2 and ¸ ُN2 and librational force constants of diatomic molecular crystals
J. Chem. Phys. 67, 3659 (1977); 10.1063/1.435306

Raman spectrum of ¸ ُN2
J. Chem. Phys. 59, 6175 (1973); 10.1063/1.1679989

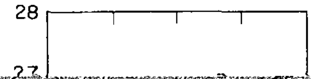
Raman spectra of solid ¸ ُN2 and ¸ ُN2 under high pressure at 4.2 K
J. Chem. Phys. 59, 4559 (1973); 10.1063/1.1680655

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 128.138.65.149 On: Tue, 14 Jul 2015 17:58:23



$$K = 3244.18\ \text{kcal/Å}^2$$

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



VI) in the volume range of 40–55 Å^3/molecule. At this range the graph of $d\ln\omega_i$ vs $d\ln V$ was practically linear

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 128.138.65.149 On: Tue, 14 Jul 2015 17:58:23