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Author
Cole JM. Burgi H-B. McIntyre GJ.
Author/Editor Affiliation
Cole JM. : Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, UK
Burgi H-B. : Laboratorium fur Kristallographie, Universitat Bern, Freiestrasse 3, Bern CH-3012, Switzerland
McIntyre GJ. : Institut Laue-Langevin, B. P. 156, Grenoble F-38042, France
Title
Distinction of disorder, classical and quantum vibrational contributions to atomic mean-square amplitudes in dielectric pentachloronitrobenzene
Source
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Abstract
The solid-state molecular disorder of pentachloronitrobenzene (PCNB) and its role in causing anomalous dielectric properties are investigated. Normal coordinate analysis (NCA) of atomic mean-square displacement parameters (ADPs) is employed to distinguish disorder contributions from classical and quantum-mechanical vibrational contributions. The analysis relies on multitemperature (5-295 K) single-crystal neutron-diffraction data. Vibrational frequencies extracted from the temperature dependence of the ADPs are in good agreement with THz spectroscopic data. Aspects of the static disorder revealed by this work, primarily tilting and displacement of the molecules, are compared with corresponding results from previous, much more in-depth and time-consuming Monte Carlo simulations; their salient findings are reproduced by this work, demonstrating that the faster NCA approach provides reliable constraints for the interpretation of diffuse scattering. The dielectric properties of PCNB can thus be rationalized by an interpretation of the temperature-dependent ADPs in terms of thermal motion and molecular disorder. The use of atomic displacement parameters in the NCA approach is nonetheless hostage to reliable neutron data. The success of this study demonstrates that state-of-the-art single-crystal Laue neutron diffraction affords sufficiently fast the accurate data for this type of study. In general terms, the validation of this work opens up the field for numerous studies of solid-state molecular disorder in organic materials. (56 References).