Vibration spectra of water molecules in the paraelectric phase of K4[Fe(CN)6].3H2O

M. A. Gaffar and Mostafa Ibrahim Abd-Elrahman

Abstract:

Lattice, rotation and intermolecular vibrations of water molecules in the paraelectric phase of potassium ferrocyanide single crystals (KFCT) are calculated using the correlation theorem based on the group theory. The correlation between the site group symmetry C2 of the first type of the water molecules, H2O-I, and the factor group C2h of the crystal yield six fundamental lattice vibrations allowed in the infrared and Raman spectra. The same number for rotations are also expected to be allowed in both spectra. The active number of intermolecular vibrations in Raman and infrared spectra are the same as that for lattice vibrations. For the second type of the water molecules, H2O-II, existing in the C1 site, the total number of vibrations are 18 active modes in each spectrum. The FTIR spectrum of KFCT crystal measured at room temperature (in the paraelectric phase) in the energy range 4000-200 cm-1 gives exactly the same modes of vibrations as those expected theoretically. The effect of irradiating KFCT crystals with a dose of 5 x 105 Gy gamma radiation on the IR spectrum indicates changes in absorption bands.

Keywords:

Potassium compounds ; Iron complexes ; Cyano complex ; Ferrocyanides ; Monocrystals ; Potassium ; Hydrates ; Ferroelectric materials ; Absorption spectra ; Infrared radiation ; Gamma radiation ; Fourier transform spectra ; Raman spectra ; Infrared spectra ; Symmetry groups ; Site symmetry ; Group theory ; Lattice vibrations ; Vibrational modes

Published In:

Physica B (condensed matter) , vol. 304, No1-4 , pp. 423-436