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Pressure induced transformations in sorbic acid

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Abstract

This research reports a pressure dependent Raman study of the sorbic acid between 0.0 and 10.0 GPa. The unpolarized Raman spectra were measured in the spectral range of 30-3000 cm⁻¹. The high-pressure Raman scattering study of the sorbic acid showed that it underwent a gradual, disordering process. At the room temperature and at the ambient pressure conditions, the crystal structure of the sorbic acid belongs to the monoclinic system with a $C2/c$ (C_{2h}^6) space group. The pressure increase induced a higher disorder in the monoclinic unit cell, since a single bending mode, and only very broad stretching Raman modes are present at pressure of ~10 GPa. Upon pressure release the high-pressure phase transforms directly into the ambient-pressure phase. The presence of the internal vibrational modes is a guarantee that the molecular structure is maintained. Beyond this, the presence of external modes shows that the crystal has a memory to reverse the process and suggest that the crystal, which was in high disorder (broad Raman bands), does not suffer decomposition in the crystalline structure. The DFT calculations for

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