

IR absorption spectra of molecular crystals: Signature of small-polaron formation?

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The idea that the appearance of the so called anomalous peak at 1650 cm^{-1} in the IR-absorption spectra of crystalline acetanilide (ACN) [1, 2, 3, 4] has been critically assessed on the basis of conventional small-polaron theories [5, 6]. Characteristic temperature variation of small-polaron binding energy is predicted. Anticipated effect should be manifested as a shift of the position of unconventional (temperature dependent) peak in the IR absorption spectrum of ACN towards the position of the normal peak. Experimental observation of such behavior would be the clear evidence of the small-polaron existence in molecular chain and confirmation of the relevance of the self-trapping mechanism as the general theoretical framework for the understanding of charge and energy transfer in molecular chain such as α -helix and ACN.

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