475. 标题: Solid-state Raman spectra of non-centrosymmetric crystals - Theoretical vs. experimental study towards an application in THz-regime

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摘要: Experimental and theoretical solid-state Raman spectroscopic study of five model derivatives of amino acids (AAs), crystallizing in the non-centrosymmetric space groups, with the number molecules per unit cell Z = 1-8 were studied. The self-assembly association effects within the frame of crystals with P2(1). Pca2(1), and P2(1)2(1)2(1), space groups and their effect on the Raman frequencies, within 10-0.3 THz were discussed. The assignment of the spectroscopic properties and the hydrogen bond interactions, depending of the crystal packing of the model tyramine hemihydrate was performed. The paper aims to make a bridge between the methods for analysis of the optical phenomena within the THz-region, such as far-IR, Raman and THz-spectroscopy. The observed individual characteristic excitations of materials within THz-region, provided unique opportunity for chemical identification in solid-state. The specific advantages of each of the methods provided unique combination allowing both qualitative and quantitative analysis, especially of macro-components, and achievement of the analytical information at an extremely high degree of certainty towards the individual characteristics of each of the studied chemicals as properties of evidence, and would contributed in varying degrees to the evidence in the field of forensic chemical analysis. (C) 2012 Elsevier B.V. All rights reserved.

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