Solid-State Vibrational Spectroscopic Investigation of Cocrystals and Salt of Indomethacin

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Abstract:

Knowledge and control of the solid forms of active pharmaceutical ingredients are important aspects of drug development in the pharmaceutical industry. In this paper, the process of the molecular self-assembly of saccharin cocrystals and the 2-amino-5-methylpyridine salt of indomethacin, in terms of the hydrogen bonding patterns, has been studied in the solid-state using vibrational spectroscopy (Raman and infrared). Interaction patterns in the respective crystalline states were obtained from the single crystal data. The effects of cocrystal and salt formation on the frequencies of the vibrational modes of motion were explained by vibrational spectroscopy and supported by quantum chemical calculations at the density functional theory level, leading to unambiguous assignment of the vibrational spectra of the starting materials and their respective products. Both Raman and infrared spectroscopies were useful, reliable tools for characterizing and distinguishing the indomethacin cocrystals and salt.

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