

Abstract Submitted
for the APR10 Meeting of
The American Physical Society

Raman Spectroscopy of Cocrystals FRANK ROONEY, PAUL REARDON, ROMULO OCHOA, HEBA ABOURAHMA, MARCUS MARTI, RACHEL DIMEO, The College of New Jersey — Cocrystals are a class of compounds that consist of two or more molecules that are held together by hydrogen bonding. Pharmaceutical cocrystals are those that contain an active pharmaceutical ingredient (API) as one of the components. Pharmaceutical cocrystals are of particular interest and have gained a lot of attention in recent years because they offer the ability to modify the physical properties of the API, like solubility and bioavailability, without altering the chemical structure of the API. The APIs that we targeted for our studies are theophylline (Tp) and indomethacin (Ind). These compounds have been mixed with complementary coformers (cocrystal former) that include acetamide (AcONH₂), melamine (MLM), nicotinic acid (Nic-COOH), 4-cyanopyridine (4-CNPY) and 4-aminopyridine (4-NH₂Py). Raman spectroscopy has been used to characterize these cocrystals. Spectra of the cocrystals were compared to those of the coformers to analyze for peak shifts, specifically those corresponding to hydrogen bonding. A 0.5 m CCD Spex spectrometer was used, in a micro-Raman setup, for spectral analysis. An Argon ion Coherent laser at 514.5 nm was used as the excitation source.

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Date submitted: 22 Oct 2009

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