

Low-Frequency Vibrations of Tartaric Acid Cocrystals

Margaret P Davis^a and Prof. Timothy M. Korter^a

^a*Syracuse University, Department of Chemistry, 1-014 Center for Science and Technology,
Syracuse, NY - USA*

e-mail: presenting mdavis23@syr.edu

Organic cocrystals are actively researched materials for their promising ability to enhance the solubility and thus bioavailability of various drugs in solid-state formulations. While cocrystallization has long been recognized as a means for tuning the physical properties of organic solids, the intermolecular forces responsible for these modifications are more rarely studied. In the present work, the intermolecular forces within organic cocrystals have been investigated using a combination of experimental and theoretical tools including terahertz time-domain spectroscopy, low-frequency Raman spectroscopy, and solid-state density functional theory. Specifically, the model systems of DL-tartaric acid co-crystallized with either urea or water were selected to compare and contrast the intermolecular forces found within molecular crystals of meaningful complexity. Crystals of all samples were grown and confirmed by powder and single-crystal X-ray diffraction before spectroscopic study. The sub-200 cm⁻¹ Raman and terahertz spectra both show unique spectral fingerprints indicative of the crystal packing and intermolecular forces in each solid. Simulated solid-state structures and vibrational spectra enable a greater understanding to be obtained of the cohesion and conformational energies contained within the cocrystals. For example, the results indicate that the monohydrate cocrystal has greater cohesion energy as compared to the anhydrous DL-tartaric acid solid. This is achieved through the formation of an extended hydrogen bonding network, at the expense of the conformational energy of the tartaric acid molecules. The trends identified in these studies provide new insight for the efficient crystal engineering of new cocrystalline materials.