

Supporting Information

Mechanochemical Synthesis and Structural Characterisation of a Theophylline-Benzoic acid Cocrystal (1:1)

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1. Raman spectroscopy

Raman spectroscopic investigations were performed with a LabRam single stage spectrograph (Horiba Jobin-Yvon) at an excitation wavelength of 785 nm using a liquid nitrogen cooled CCD detector (256 × 1024 pixels) at a laser power of 6 mW and an acquisition time of 5 s (TP and cocrystal TP:BA) and 1 s (BA).

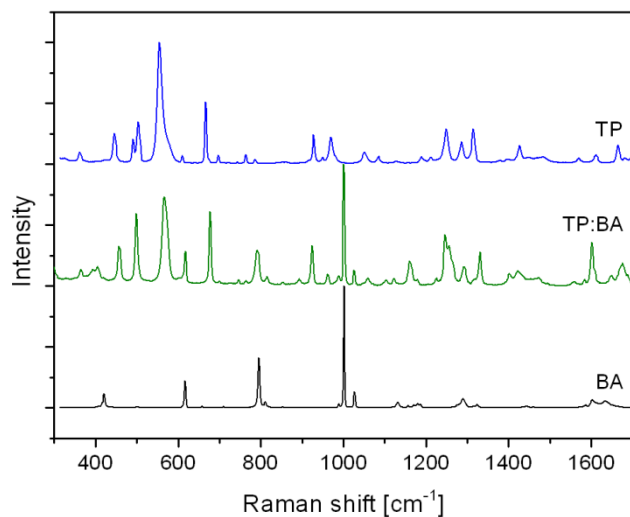


Figure S 1: Raman spectra of the cocrystal TP:BA (green) and the educts TP (blue) and BA (black).

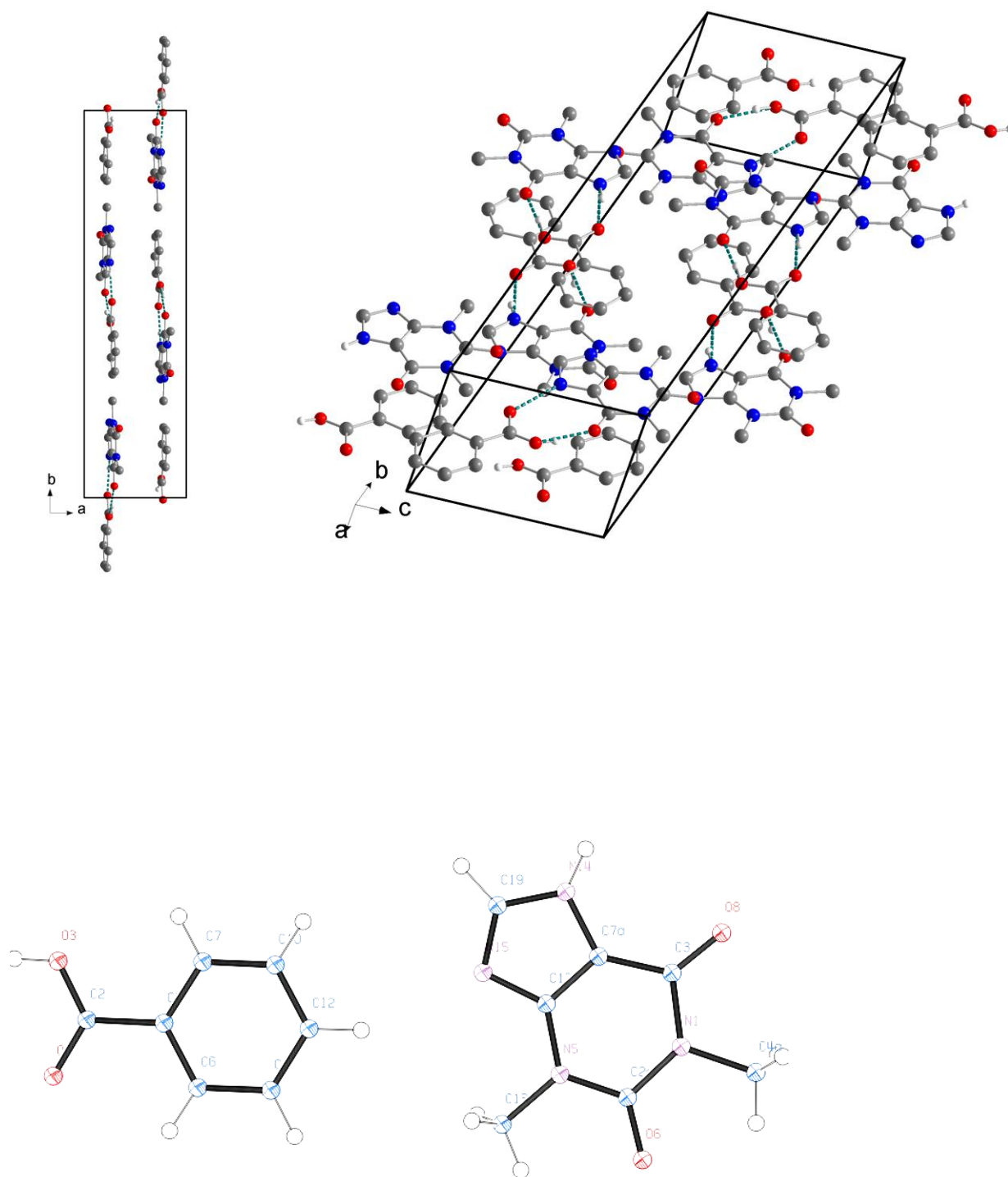


Figure S 2: Packing diagrams (upper row) and ORTEP representation (lower row) of the cocrystal TP:BA..