

Supporting Information

Structure Determination of Theophylline-Nicotinamide Cocrystal: A Combined Powder XRD, 1D Solid-State NMR, and Theoretical Calculation Study

Ping Li,^{1,2,†} Yueying Chu,^{3,†} Lin Wang,¹ Robert M. Wenslow Jr.,⁴ Kaichao Yu,² Hailu Zhang,^{1,*}

Zongwu Deng¹

1 Laboratory of Magnetic Resonance Spectroscopy and Imaging, Suzhou Institute of Nano-tech and nano-bionics, Chinese Academy of Sciences, Suzhou 215123, P.R. China

2 School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology, Wuhan 430074, P.R. China

3 State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, P.R. China

4 Crystal Pharmatech, Suzhou Industrial Park, Suzhou 215123, P.R. China

[†] These two authors made equal contributions.

* corresponding author:

Tel.: +86-512-62872713, Fax: +86-512-62603079, E-mail: hlzhang2008@sinano.ac.cn (HLZ).

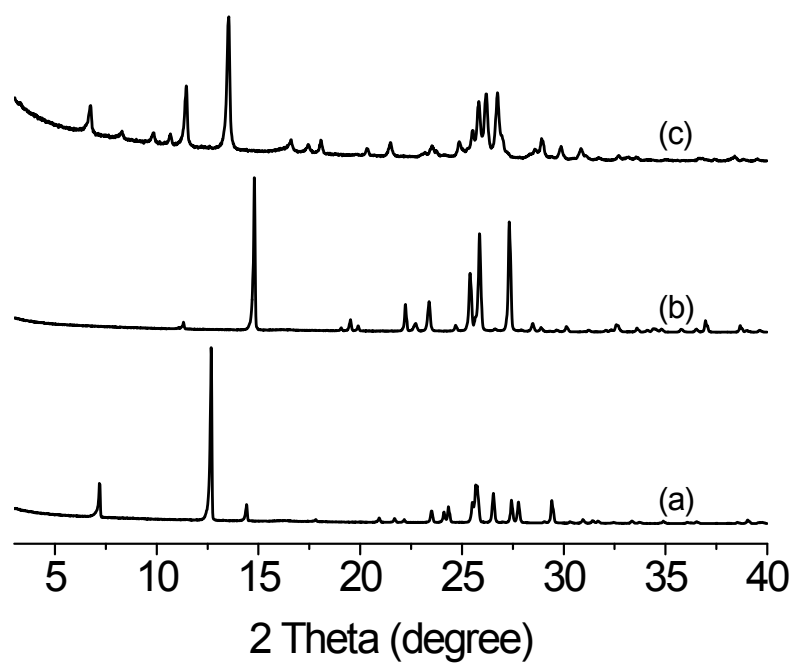


Figure S1 XRPD patterns of TP (a), NCT (b) and TP-NCT cocrystal (c).

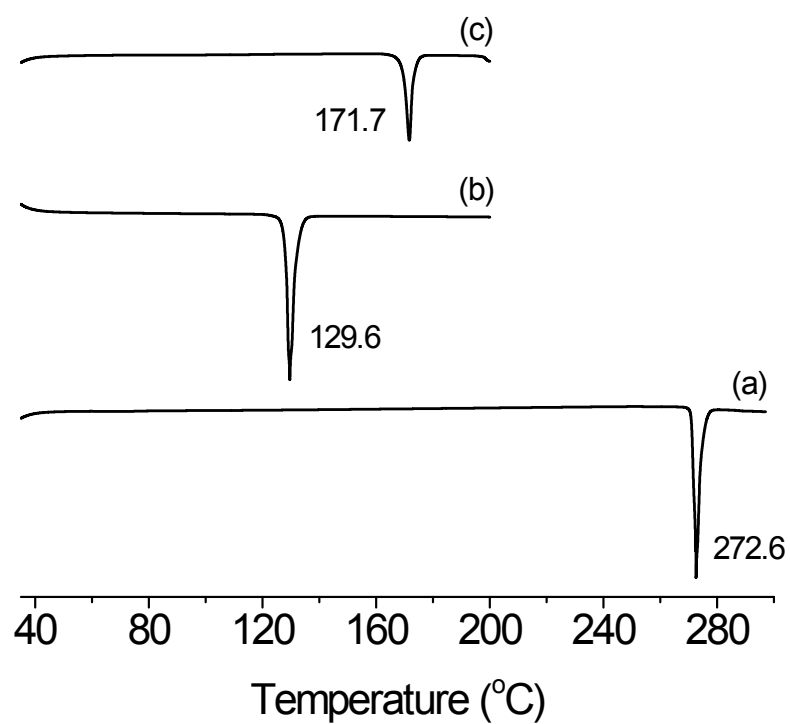


Figure S2 DSC curves of TP (a), NCT (b) and TP-NCT cocrystal (c).

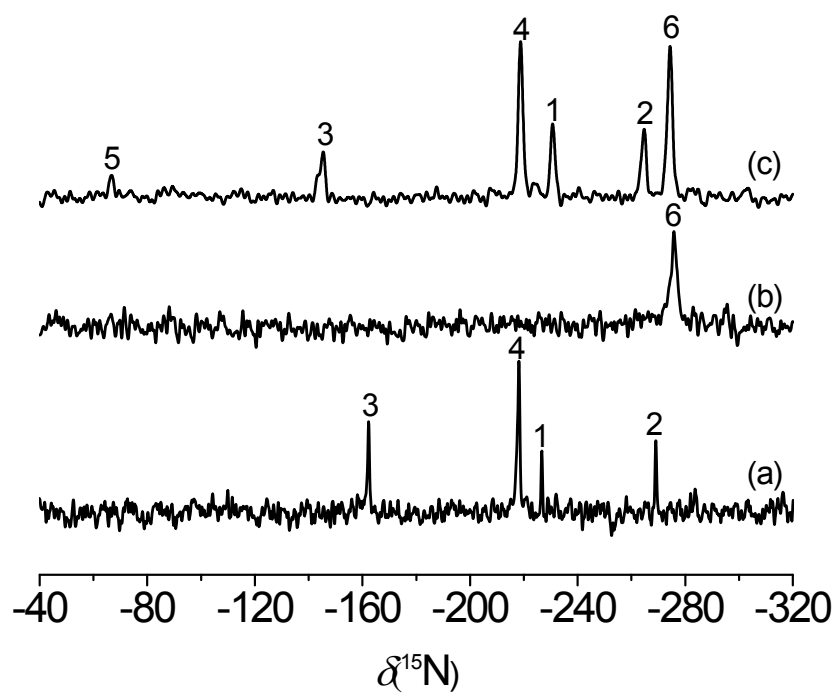


Figure S3 ^{15}N CP/MAS NMR spectra of TP (a), NCT (b) and TP-NCT cocrystal (c).