Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary information

Discrimination and Quantification of Sulfathiazole Polytypes Using Low-frequency Raman Spectroscopy

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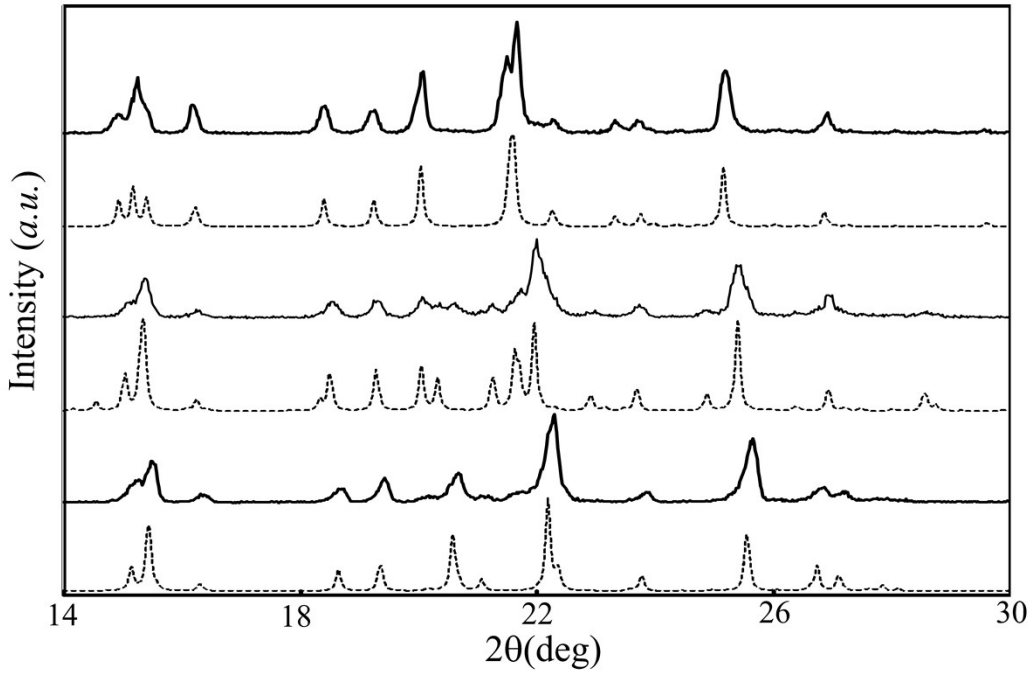
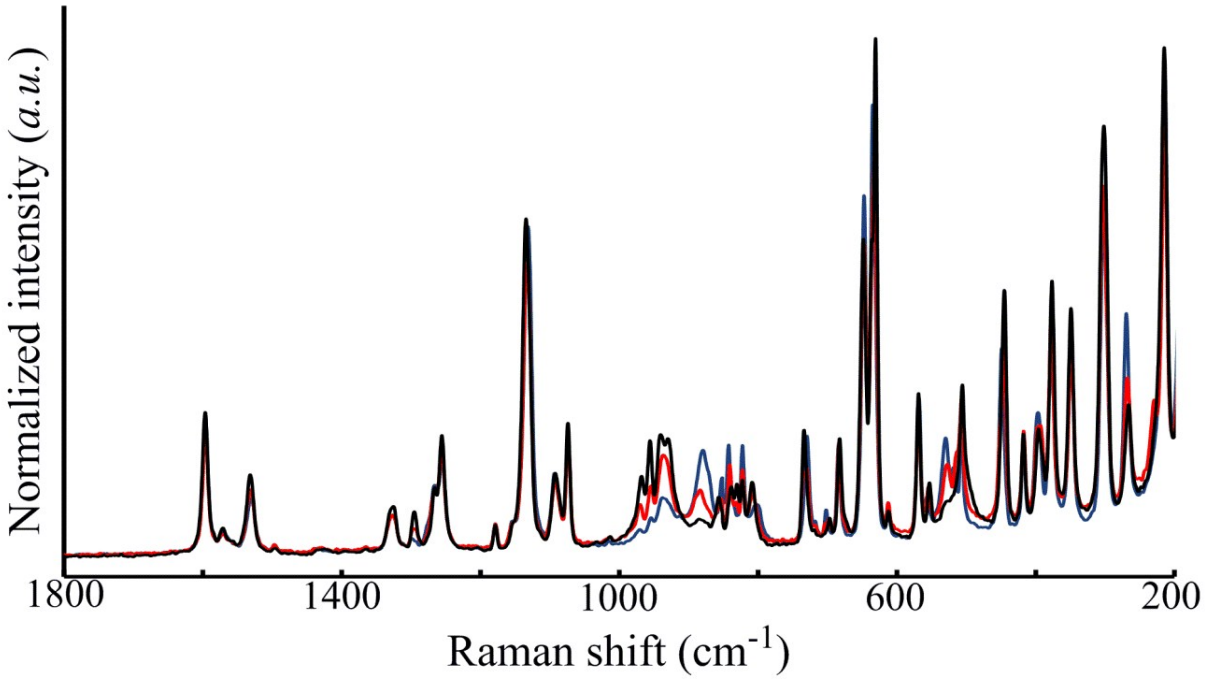
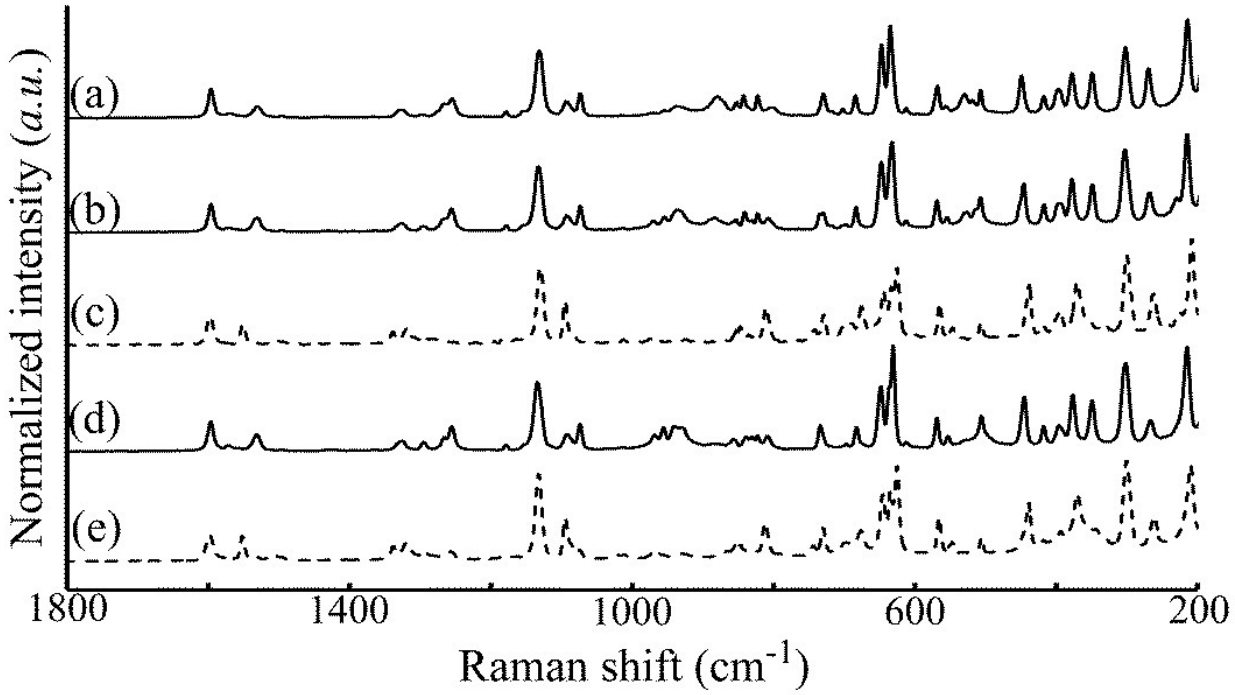


Supplementary Information 1. Expanded overlay of experimental (solid) and calculated (dash) PXRD patterns of Sulfathiazole Forms II, III and IV.

(a) and (b): Form II, (c) and (d): Form III, and (e) and (f): Form IV.

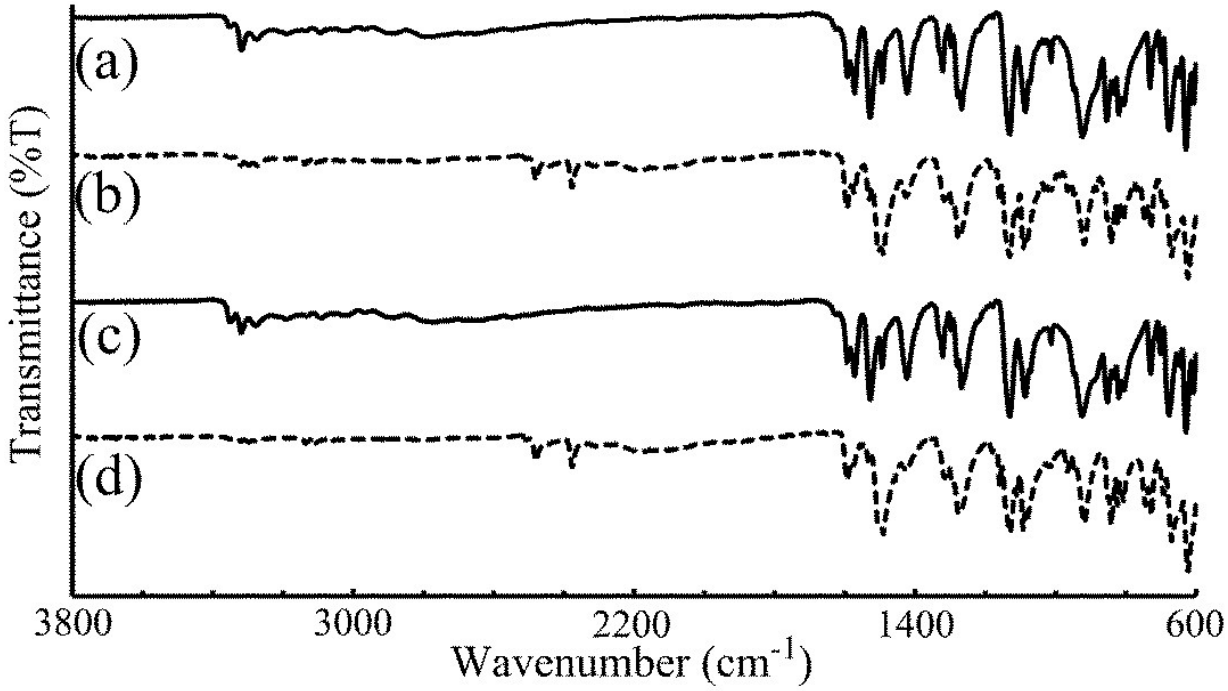


Supplementary Information 2. Overlaid Raman spectra of Forms II (blue), III (red) and IV (black) in the MF region.

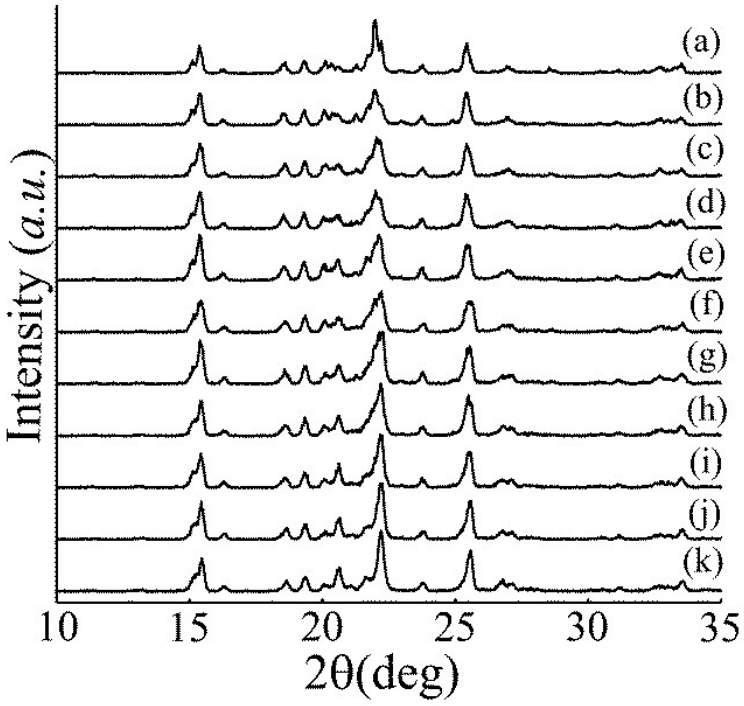


Supplementary Information 3. Raman spectra of Forms II, III and IV crystals (solid) and their H/D exchanged crystals (dash) in the MF region.

(a) Form II, (b) Form III, (c) H/D exchanged Form III, (d) Form IV and (e) H/D exchanged Form IV. The vertical scale is *ca.* 10 times smaller than that in the LF region.

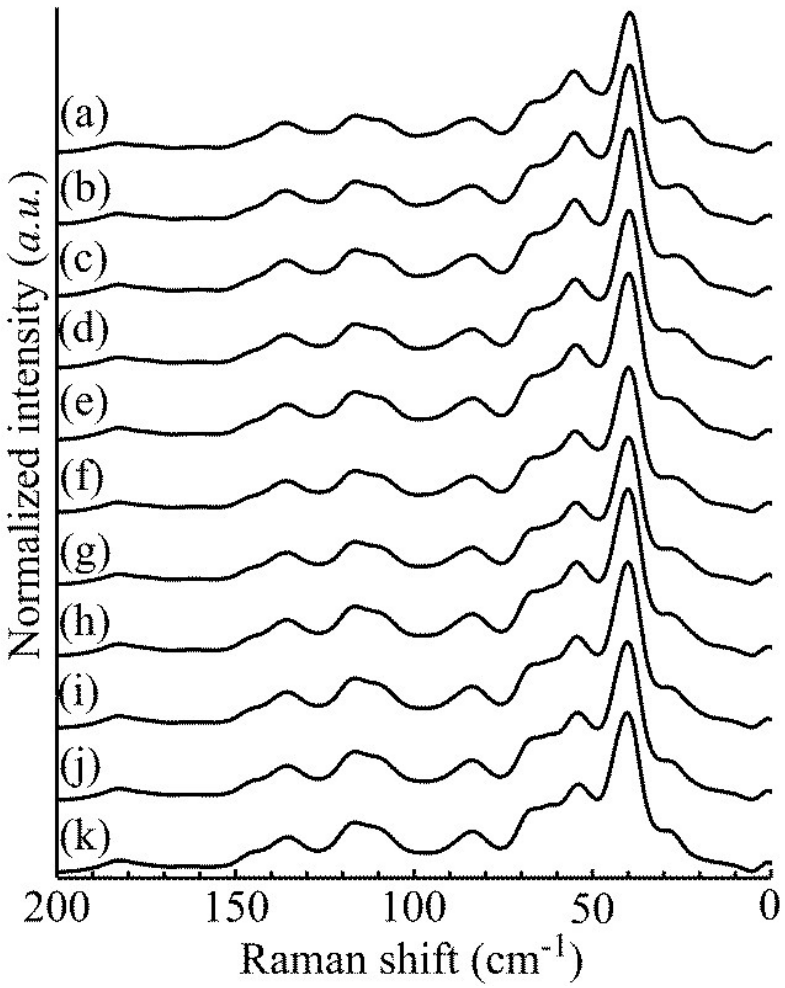


Supplementary Information 4. ATR FT-IR spectra of Forms III and IV crystals (solid) and their H/D exchanged crystals (dash). (a) Form III, (b) H/D exchanged Form III, (c) Form IV and (d) H/D exchanged Form IV.



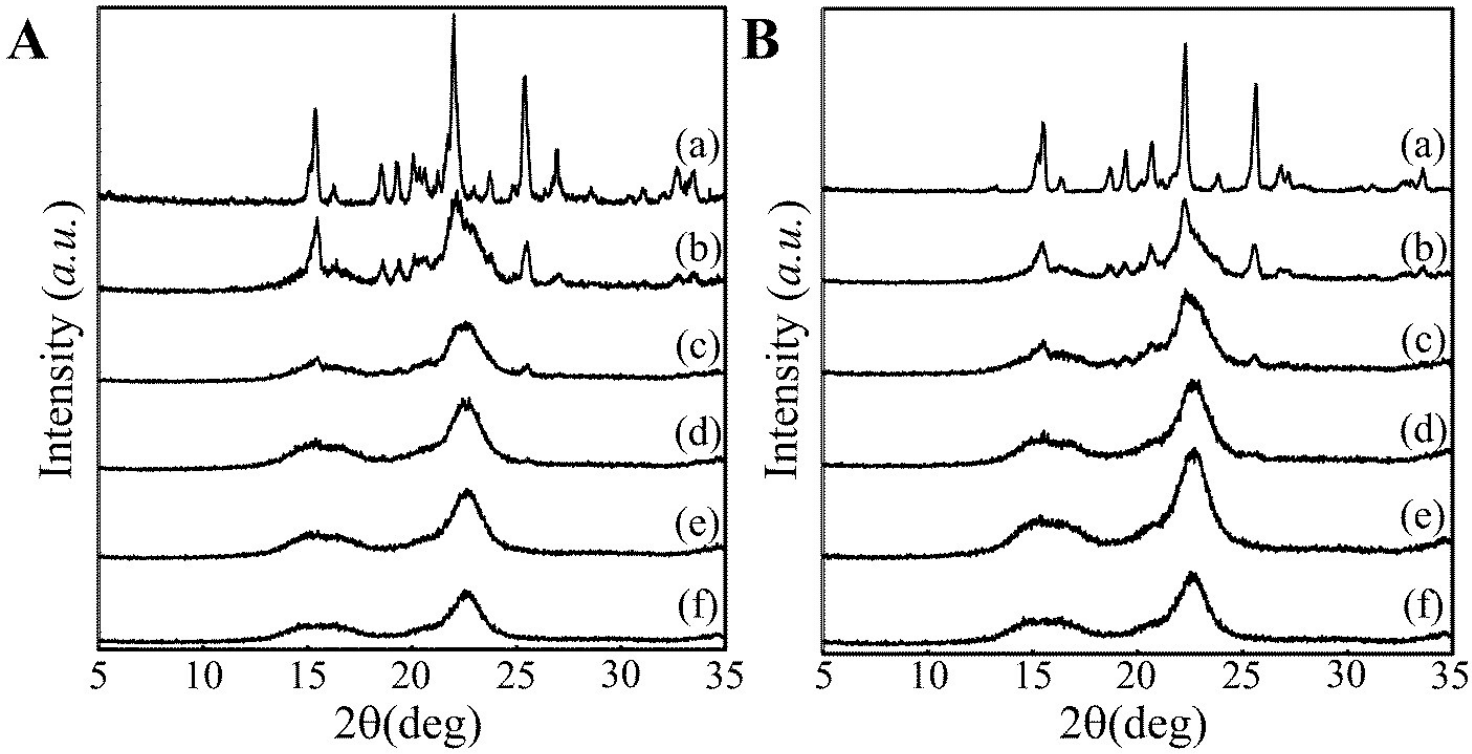
Supplementary Information 5. PXRD patterns of physical mixtures of forms III and IV crystals in various ratios.

The ratio of Form III : Form IV = (a) 100 : 0, (b) 90 : 10, (c) 80 : 20, (d) 70 : 30, (e) 60 : 40, (f) 50 : 50, (g) 40 : 60, (h) 30 : 70, (i) 20 : 80, (j) 10 : 90 and (k) 0 : 100.



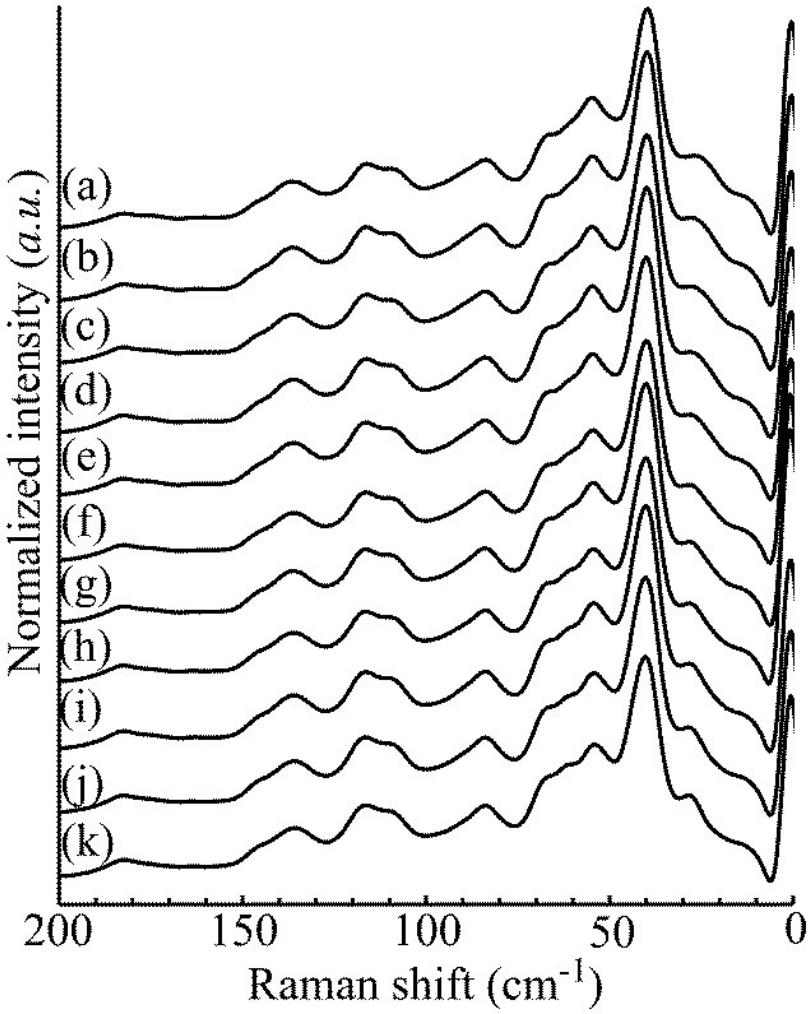
Supplementary Information 6. Averaged Raman spectra of the polytypic physical mixtures in the LF region.

The ratio of Form III : Form IV = (a) 100 : 0, (b) 90 : 10, (c) 80 : 20, (d) 70 : 30, (e) 60 : 40, (f) 50 : 50, (g) 40 : 60, (h) 30 : 70, (i) 20 : 80, (j) 10 : 90, and (k) 0 : 100. These Raman spectra were obtained by averaging twenty-five sub-spectra of the physical mixtures.



Supplementary Information 7. PXRD patterns of the model formulations of Forms III (A) and IV crystals (B) at various API content.

(a) 100% API powder, (b) 30% API powder, (c) 10% API powder, (d) 3% API powder, (e) 1% API powder and (f) microcrystalline cellulose powder.



Supplementary Information 8. Averaged Raman spectra of the model formulations in the LF region.

The ratio of Form III : Form IV = (a) 100 : 0, (b) 90 : 10, (c) 80 : 20, (d) 70 : 30, (e) 60 : 40, (f) 50 : 50, (g) 40 : 60, (h) 30 : 70, (i) 20 : 80, (j) 10 : 90, and (k) 0 : 100. These Raman spectra were obtained by averaging twenty-five sub-spectra of the model formulations.