Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Polymorphism and porosity in 4-[(4-hydroxy-3, 5-dimethylphenyl) (5-methyl-1H-imidazol-4-yl) methyl]-2, 6- dimethylphenol

Bhaskar Nath, Jubaraj B. Baruah*

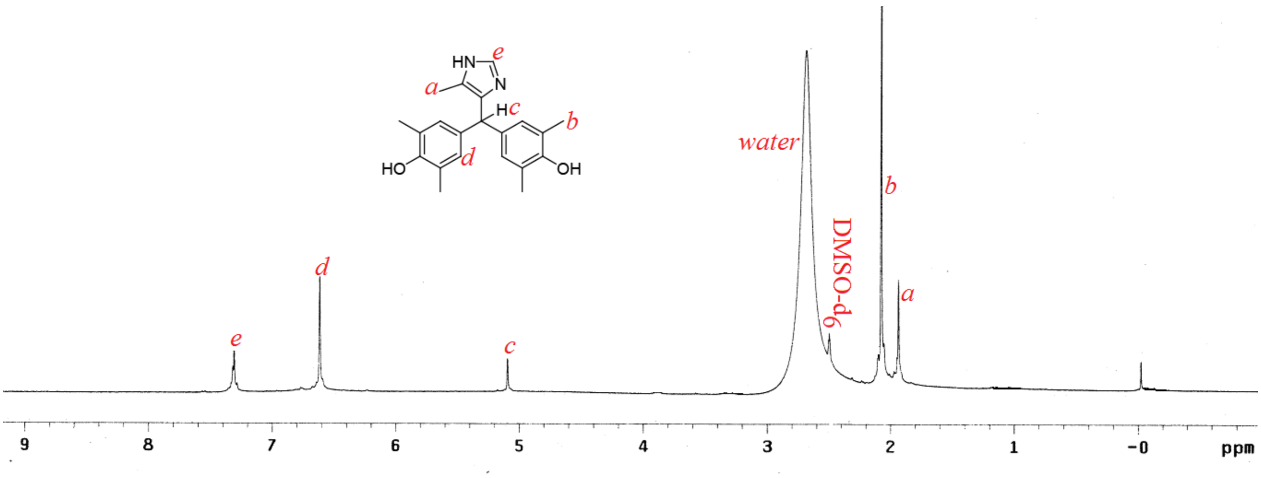

Figure S1: ^{1}H-NMR (4oo MHz) of **Imbp** in DMSO-d_6

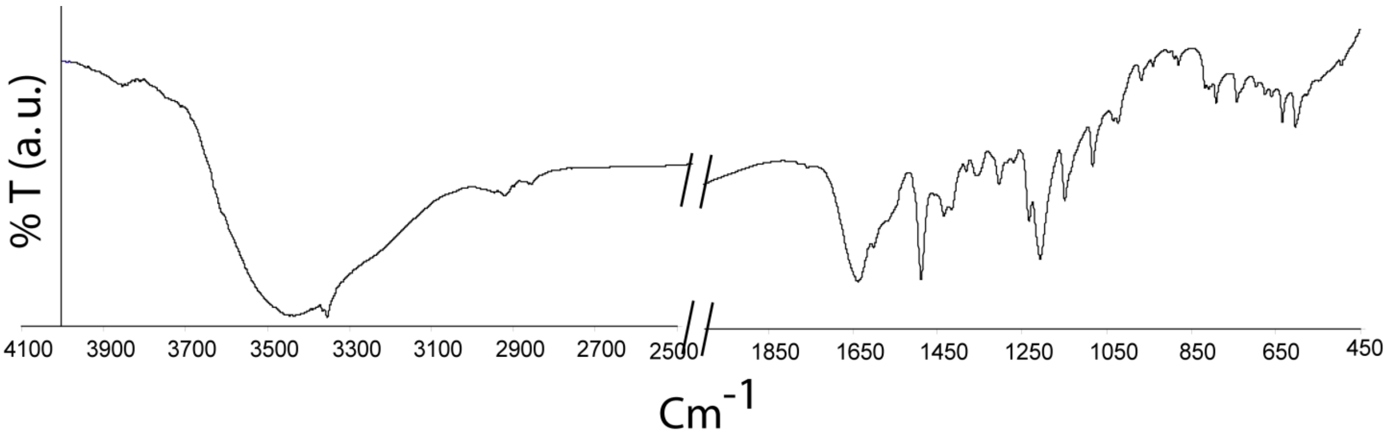

Figure S2: FT-IR spectra (KBr, cm $^{-1}$) of the **polymorph I**

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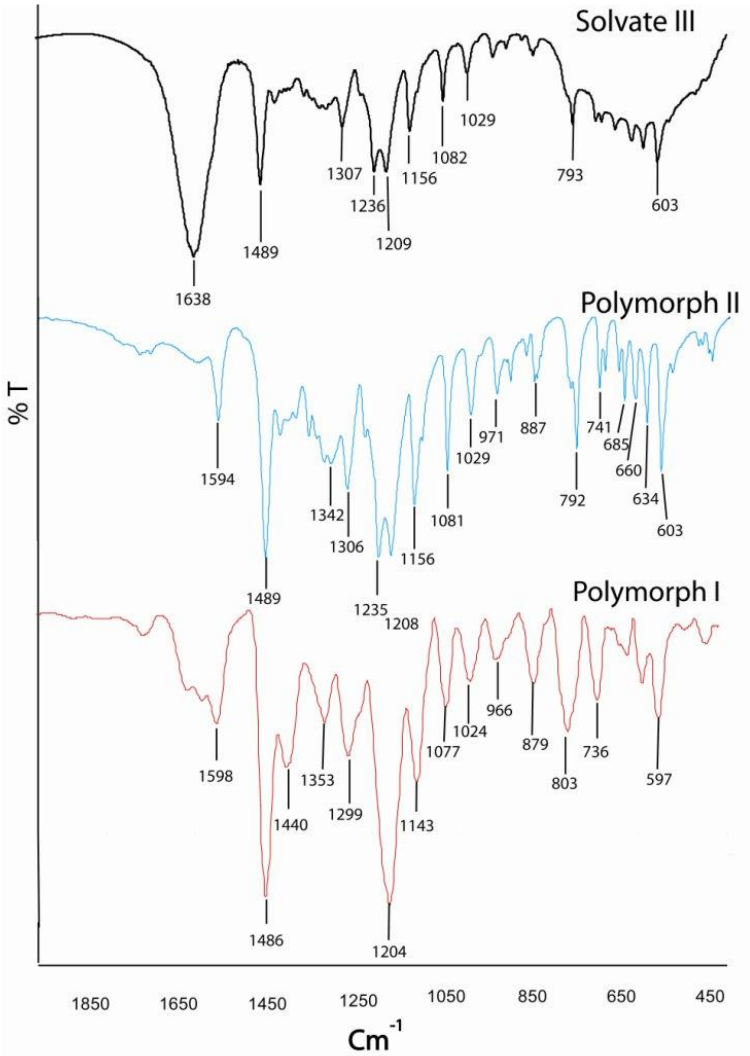


Figure S3: Comparison of solid state IR (KBr, cm $^{-1}$) spectra of polymorph **I** (bottom, red) and polymorph **II** (middle, blue) and solvate **III** (top, black) in the region of 2000-450 cm $^{-1}$.

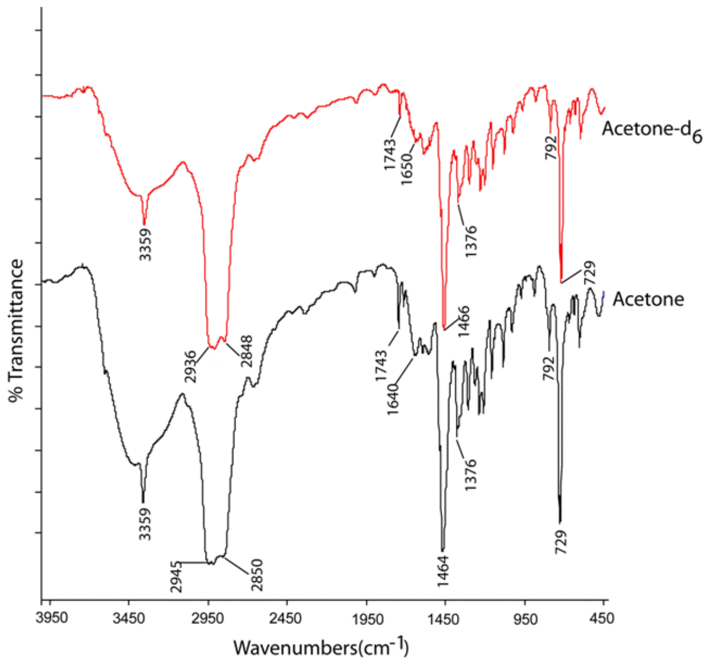


Figure S4: FT-IR spectra (Film) of acetone-**Imbp** and acetone-d_6-**Imbp** solvate.

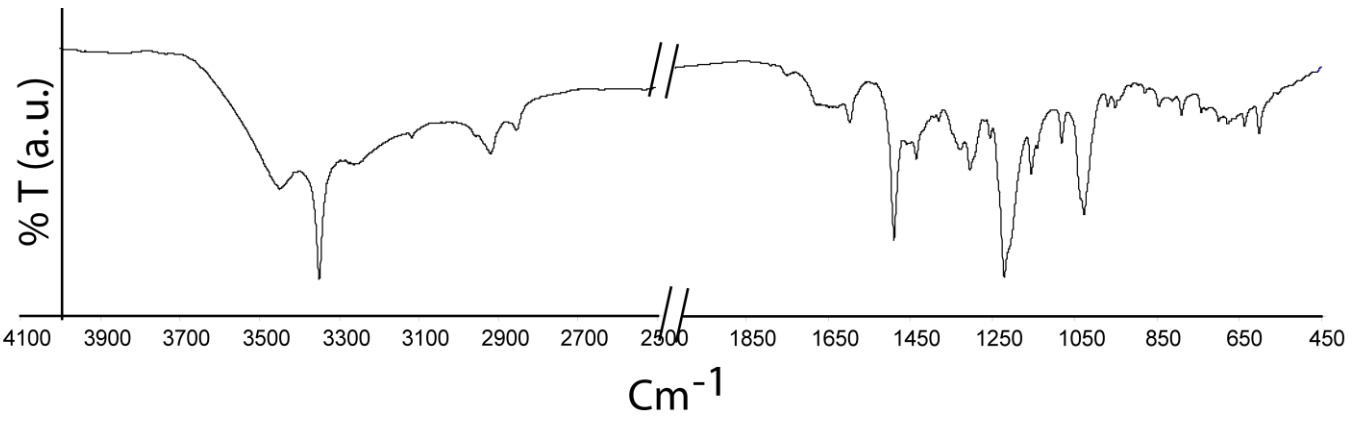


Figure S5: FT-IR spectra (KBr, cm^{-1}) of the solvate **IV**

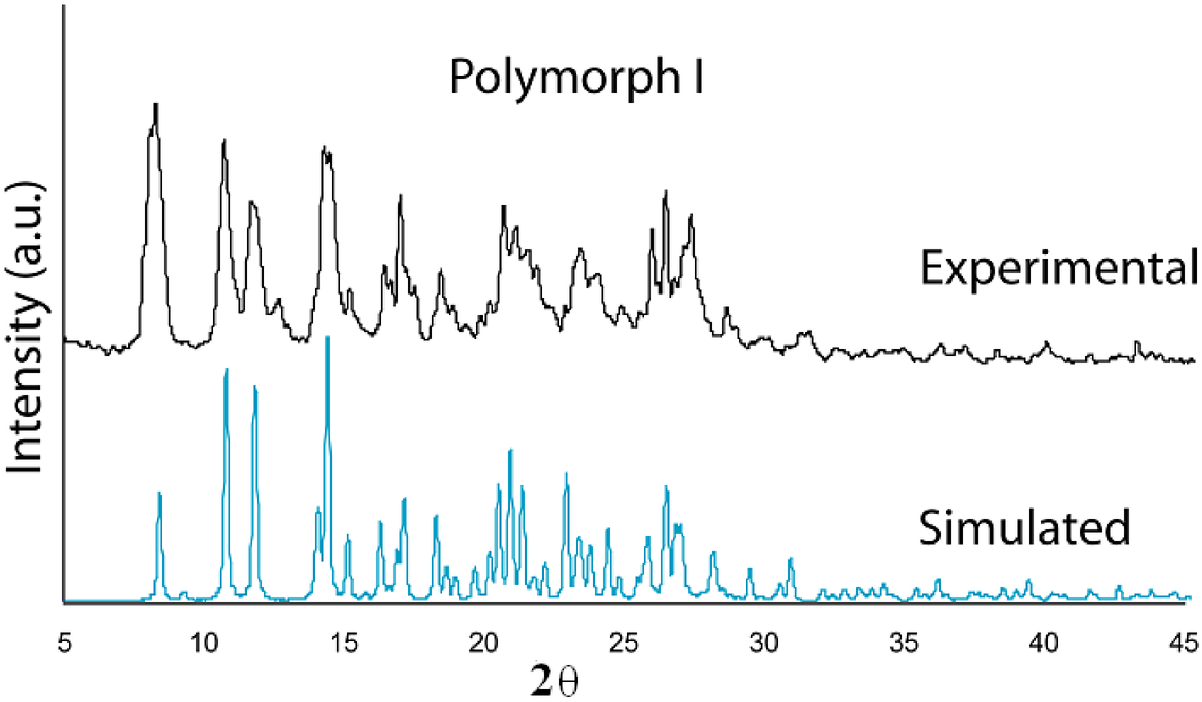


Figure S6: Comparison of the simulated and experimental PXRD pattern of solvate **III.**

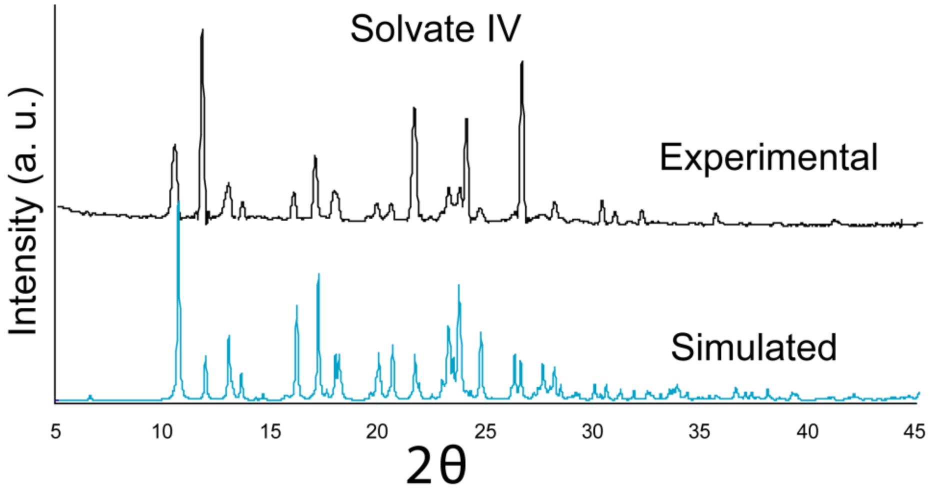


Figure S7: Comparison of the simulated and experimental PXRD pattern of solvate **IV.**

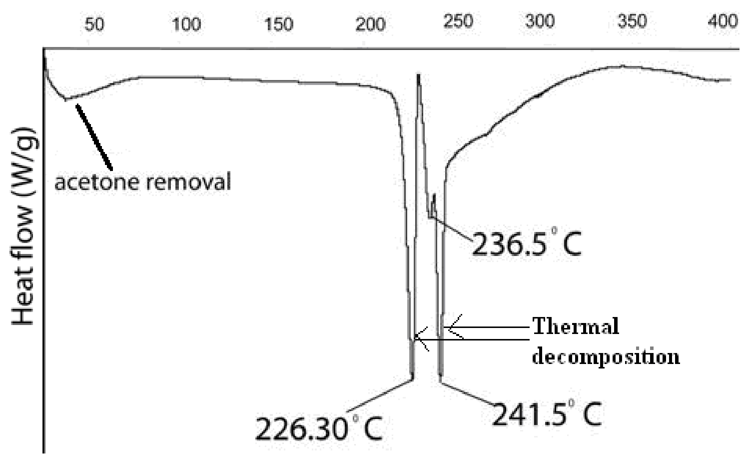


Figure S8: DSC of the **solvate III (heating rate 5°C/min).**

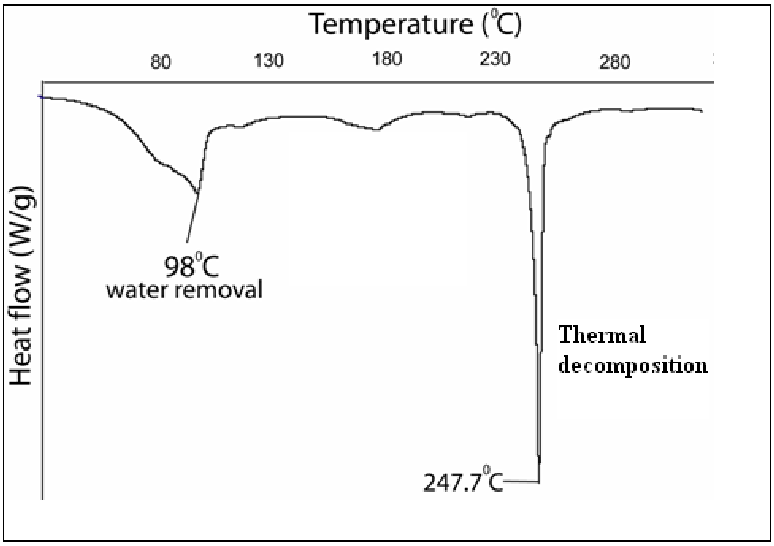


Figure S9: DSC of the **solvate IV** (heating rate 5°C/min)

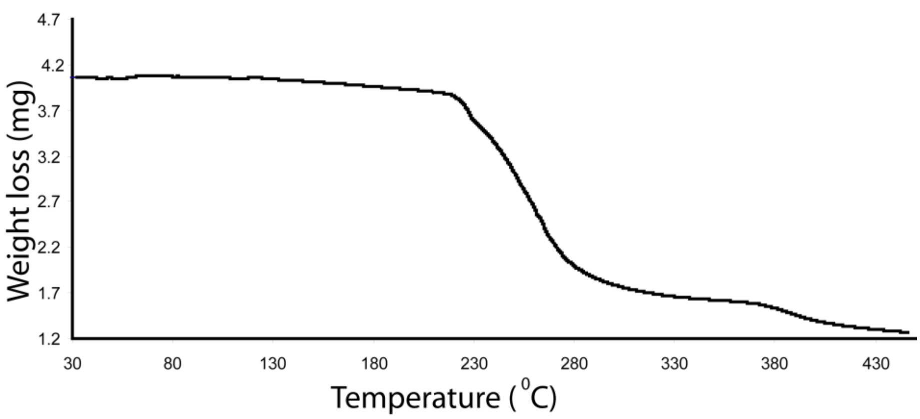


Figure S10: TGA of the **polymorph II** showing the absence of disordered solvent molecules in the voids (heating rate 5°C/min).

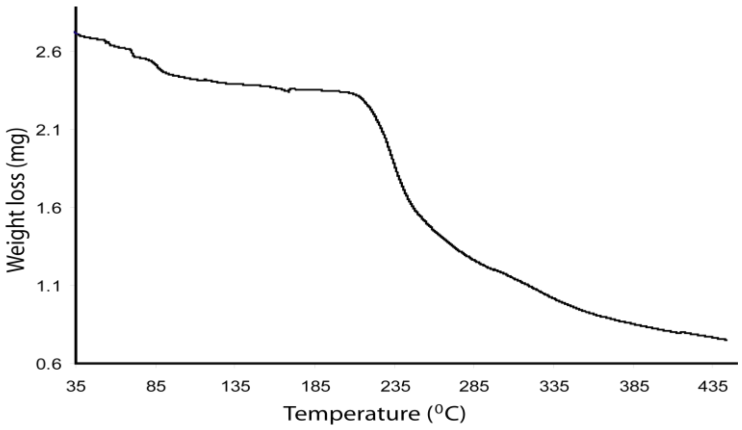


Figure S11: TGA of the **solvate III** (heating rate 5° C / min).

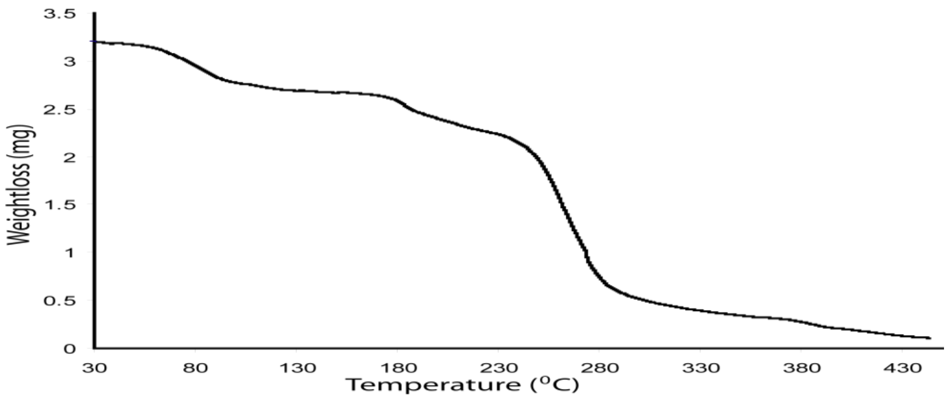


Figure S12: TGA of the **solvate IV** (heating rate 5° C / min)

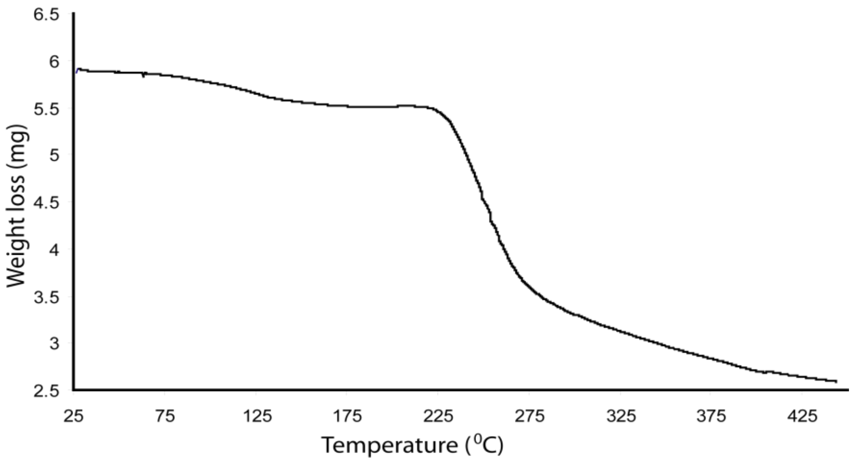
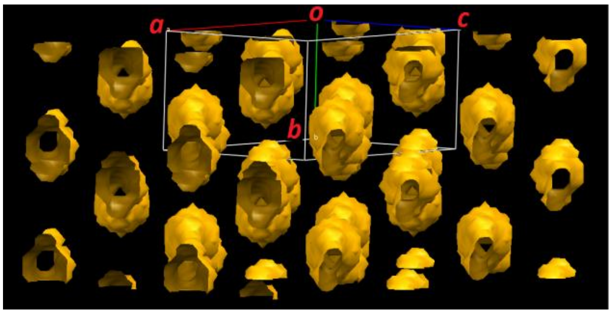
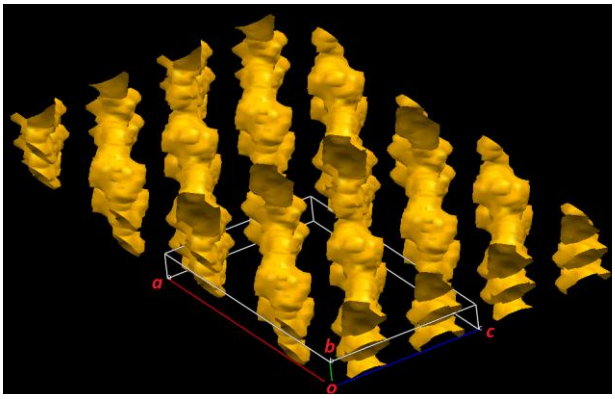


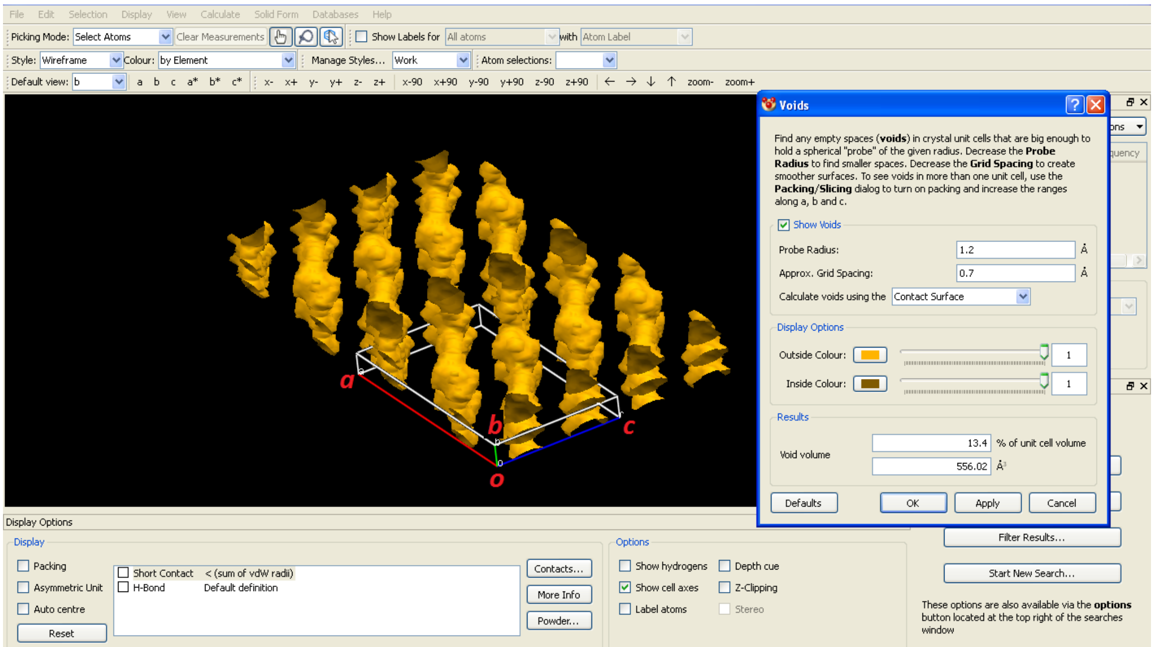
Figure S13: TGA of the polymorph **II** after exposing it to acetone vapour for 2 hours. (heating rate 5° C / min)


a
o
c
b

(a)


a
b
c
o

(b)


File Edit Selection Display View Calculate Solid Form Databases Help
Picking Mode: Select Atoms
Clear Measurements
Show Labels for All atoms with Atom Label
Style: Wireframe Colour: by Element Manage Styles... Work Atom selections:
Default view: b a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 zoom- zoom+
a
b
c
o
Voids
Find any empty spaces (voids) in crystal unit cells that are big enough to hold a spherical "probe" of the given radius. Decrease the Probe Radius to find smaller spaces. Decrease the Grid Spacing to create smoother surfaces. To see voids in more than one unit cell, use the Packing/Slicing dialog to turn on packing and increase the ranges along a, b and c.
Show Voids
Probe Radius: 1.2 Å
Approx. Grid Spacing: 0.7 Å
Calculate voids using the Contact Surface
Display Options
Outside Colour: 1
Inside Colour: 1
Results
Void volume 13.4 % of unit cell volume
556.02 Å³
Defaults OK Apply Cancel
Display Options
Display
Packing
Asymmetric Unit
Auto centre
Reset
Short Contact < (sum of vdW radii)
H-Bond Default definition
Contacts...
More Info
Powder...
Options
Show hydrogens
Show cell axes
Label atoms
Depth cue
Z-Clipping
Stereo
Filter Results...
Start New Search...
These options are also available via the options button located at the top right of the searches window

(c)

Figure S14: Presentation of the voids in the polymorph **II** from different directions.

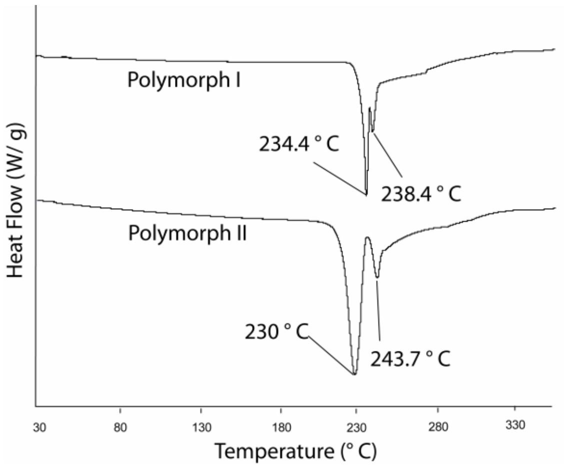


Figure S15: DSC of the polymorph **I** and **II** (heating rate 5° C/ minute).

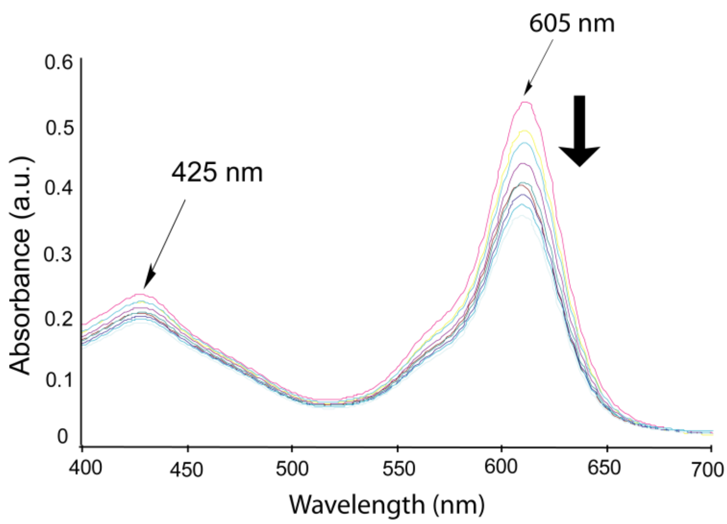


Figure S16: UV-visible spectra of DMSO solvate (1.2×10^{-2} M, 2 mL) with 50 µL incremental addition of acetone.

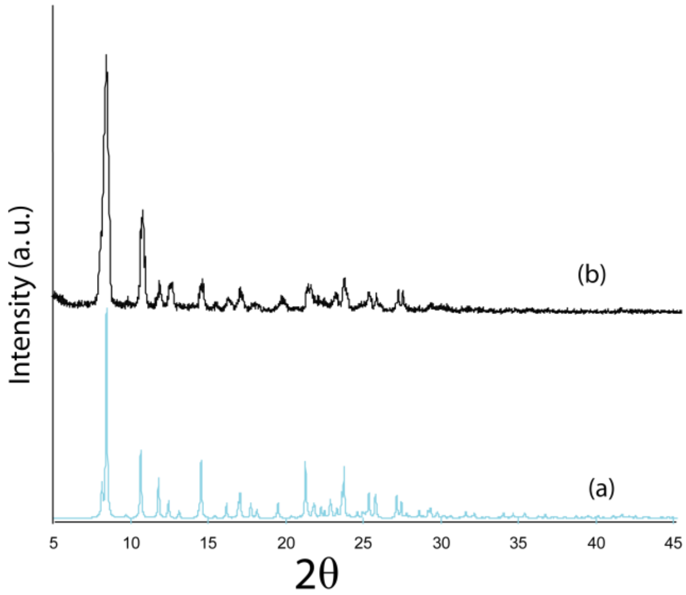


Figure S17: The PXRD of the (a) acetone solvate **III** (simulated) and the (b) PXRD of the polymorph **II** after exposure to acetone vapour (*suggests transformation of* ***II*** *to* ***III***).

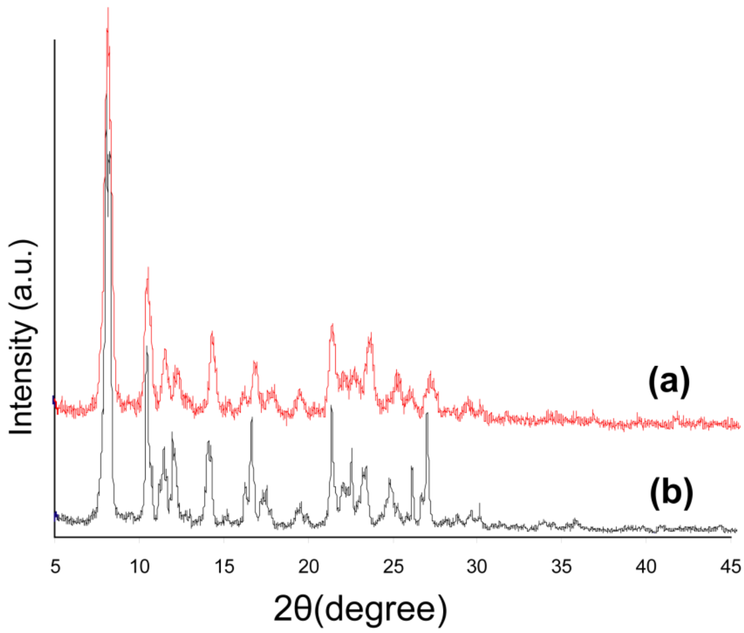


Figure S18: The experimentally observed PXRD of the (a) DMSO solvate **IV** after heating up to 200°C and the (b) polymorph **II** (*Suggesting conversion of* ***IV*** *to* ***II***).

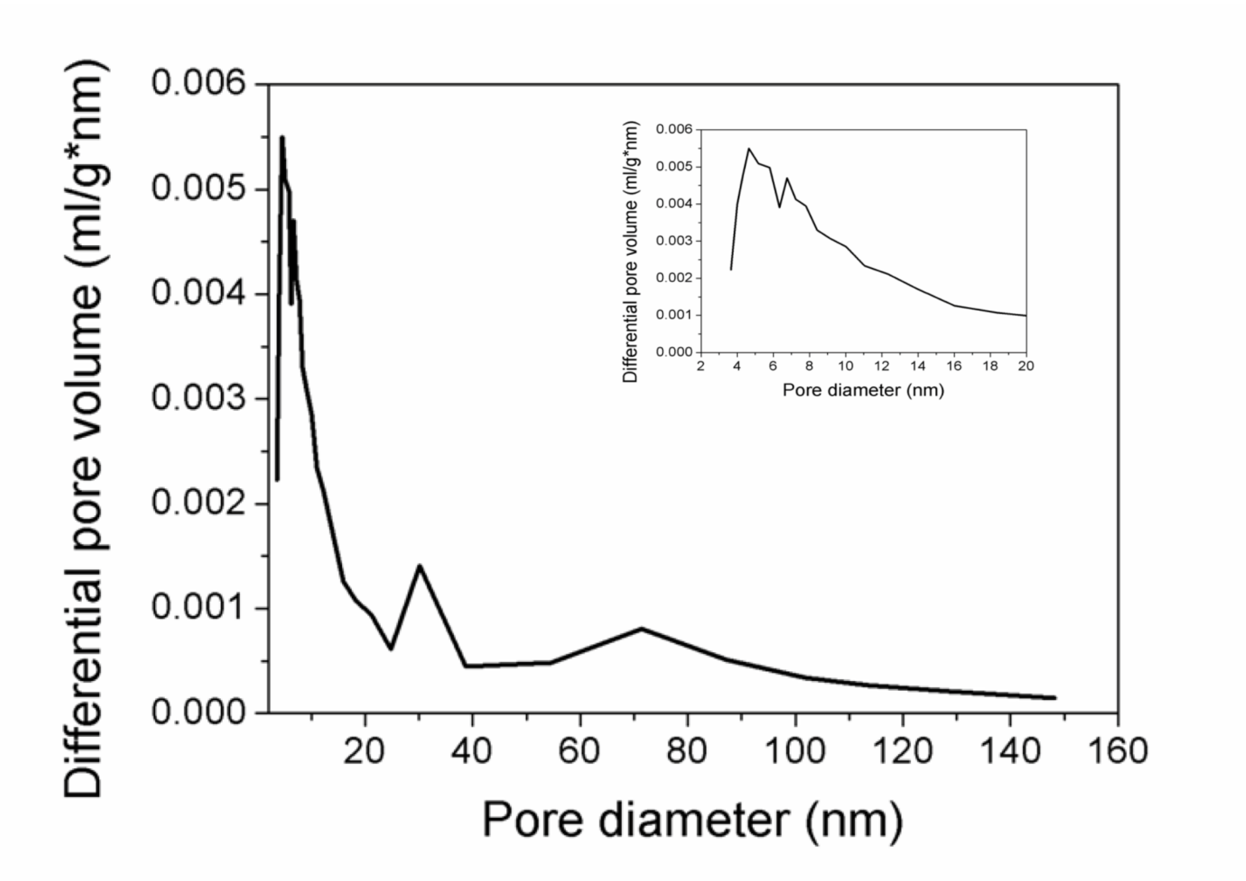


Figure S19: Plot for pore size distribution of the polymorph **II**

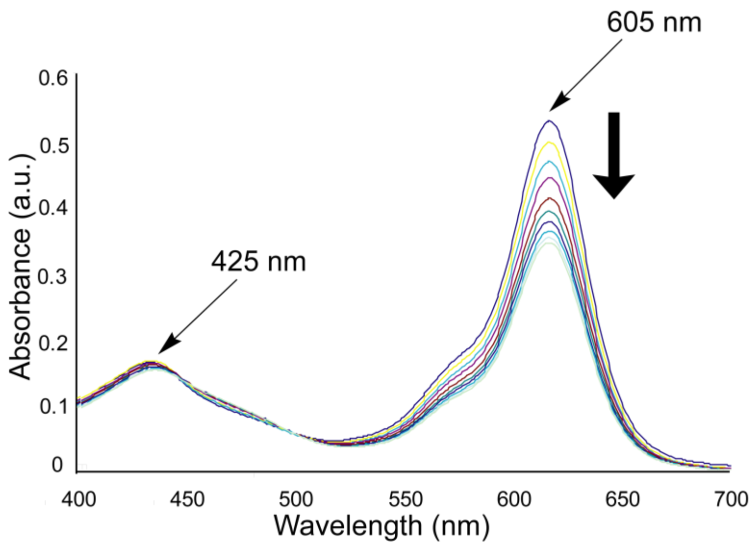


Figure S20: The changes of UV-vis spectra of **II** in DMSO (2×10^{-2} M, 2 mL,) on 50 μL incremental addition of DMSO.

Table S1: Some relevant hydrogen-bond parameters of **I-IV**.

Compound	D-H···A	$d_{D-H(Å)}$	$d_{H\cdots A(Å)}$	$d_{D\cdots A(Å)}$	∠D-H···A(°)

I	O(1)-H···O (2) [x, 3/2-y,1/2+z]	0.82	1.95	2.705 (2)	152
	O(2)-H···N(2) [1-x, 2-y, -z]	0.82	1.91	2.669(3)	154
II	O(1)-H···O (2) [1/2+x, 1/2-y,1/2+z]	0.82	1.89	2.680(8)	161
	O(2)-H···N(2) [-x, 1-y, 1-z]	0.82	1.84	2.617(7)	157
III	O(1)-H···N(2) [1-x,-y,-z]	0.82	1.86	2.6241	155
	O(2)-H···O(1) [-1/2+x,1/2-y,-1/2+z]	0.82	1.92	2.6750	153
	C(13)-H···O3	0.96	2.71	3.633	160.74
IV	O(1)-H···N(2) [1-x,1-y,-z]	0.86(6)	1.87(6)	2.721(5)	169(5)
	O(2)-H···O(4)	0.87(6)	1.91(4)	2.702(6)	151(5)
	O(4)-H···O(2)	0.84(5)	2.24(13)	2.702(6)	114(10)
	O(4)-H···O(1) [x,1/2-y,1/2+z]	0.87(3)	2.04(4)	2.889(6)	164(4)
	C(12)-H···O(3)	0.929	2.696	3.520	148.24
	C(15)-H···O(1) [1-x,1-y,-z]	0.93	2.57	3.490(5)	172