Electronic Supplementary Material for CrystEngComm

Solvent mediated centric/non-centric polymorph pairs of an indole derivative: Subtle variation of C-H···O hydrogen bonds and C-H···π interactions

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Table 1: Crystal Data

	Polymorph 1	**Polymorph 2**
Formula	$C_{22}H_{20}NOF$	$C_{22}H_{20}NOF$
Solvent	Dichloromethane/hexane	Acetone
Morphology	rectangular blocks	rhombohedral blocks
Crystal System	Monoclinic	Monoclinic
a/Å	12.874(8)	7.892(5)
b/Å	6.713(4)	10.861(6)
c/Å	20.311(15)	10.786(2)
β/°	94.65(1)	109.99(8)
V/Å^3	1749.5(2)	868.9(3)
Z	4	2
Space Group	$P2_1/n$	$P2_1$
Temp/K	90.0(2)	90.0(2)
Density (calc)/gcm^{-3}	1.266	1.274
Radiation	MoK_α	MoK_α
Structure Solution	Direct methods SIR92	Direct methods SIR92
Diffractometer	Bruker AXS	Bruker AXS
Detector	SMART APEX CCD	SMART APEX CCD
F_{000}	703.9	351.9
μ/mm^{-1}	0.84	0.83
Scan Mode	ω/ϕ	ω/ϕ
2θ range	1.8-25.3°	2.0-25.4°
Total No. of Reflections	12157	6405
Unique Reflections	3196	3154
No. of Parameters	306	306
R, R_w	0.039, 0.121	0.027, 0.072
$\Delta\rho_{min,\ max}$/eÅ^{-3}	-0.223, 0.260	-0.174, 0.155
g.o.f	1.033	1.034

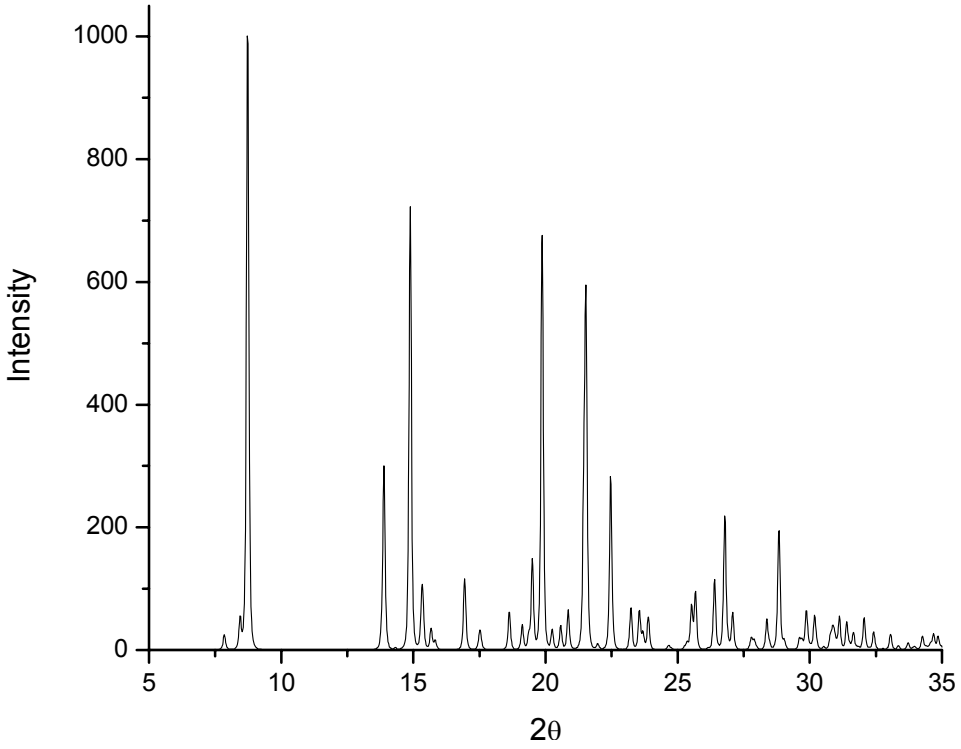

Figure 1a: Simulated PXRD of the form I

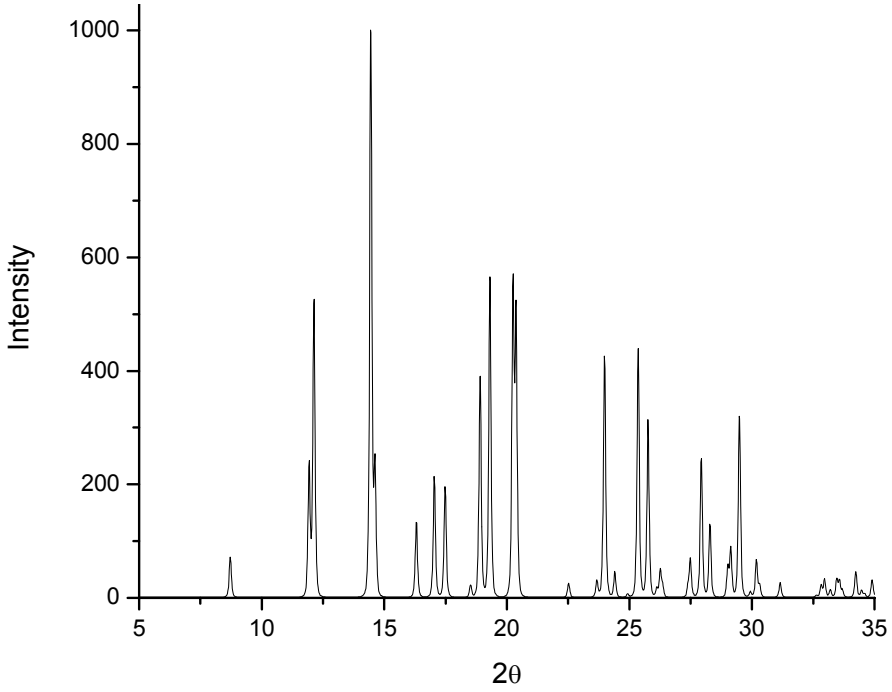

Figure 1b: Simulated PXRD of the form II

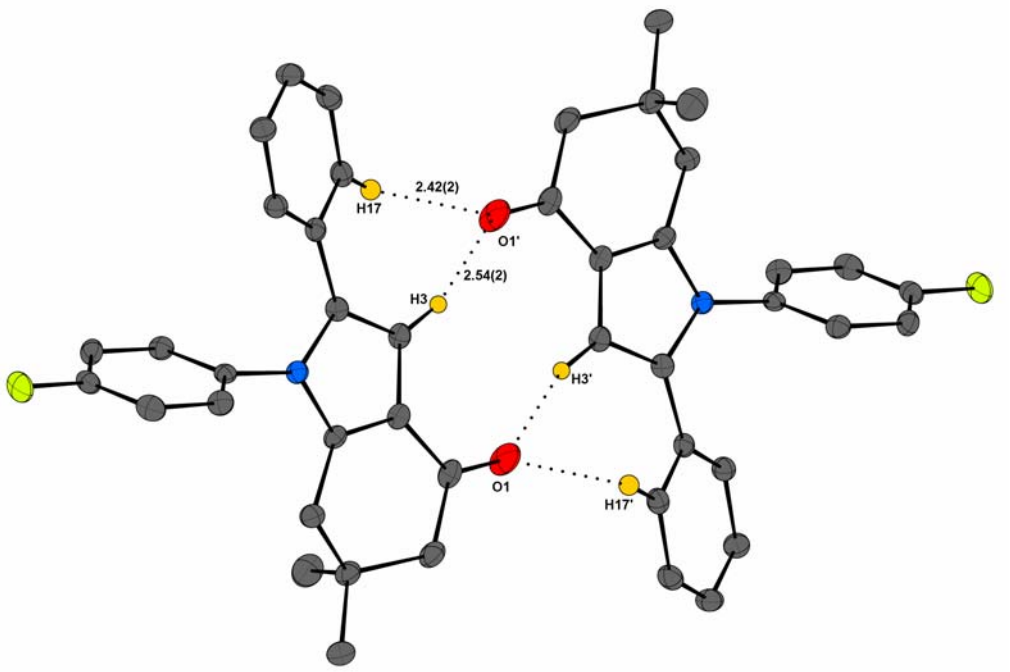

Figure 2a: Molecular dimer via bifurcated C-H…O'=C' interaction in form I, molecules at (x, y, z) and (- x, 2 – y, - z) are shown.

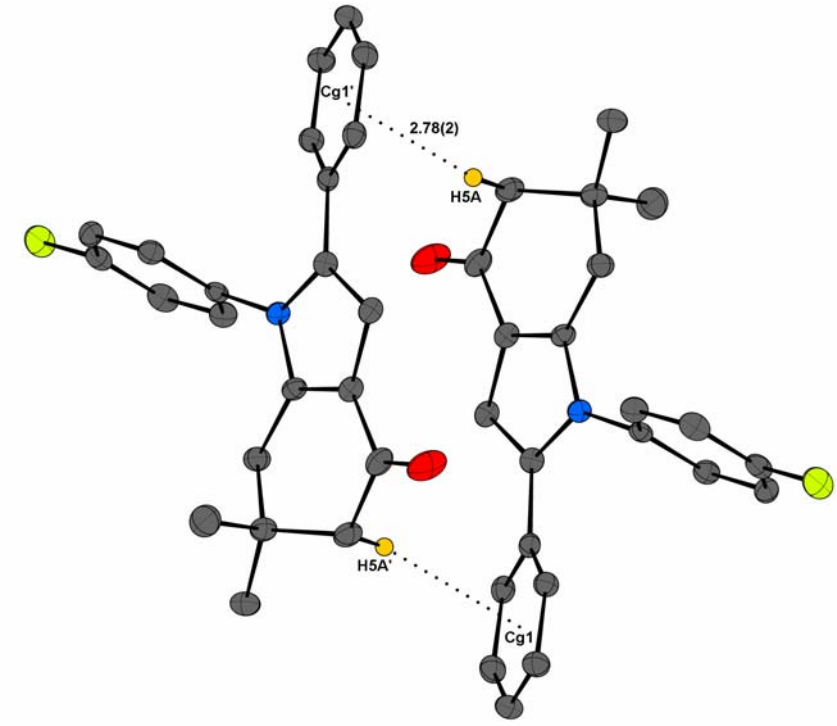

Figure 2b: Molecular dimer via C-H…π interaction involving C5-H5A…Cg1' in form I, molecules at (x, y, z) and (- x, 1 – y, - z) are shown.

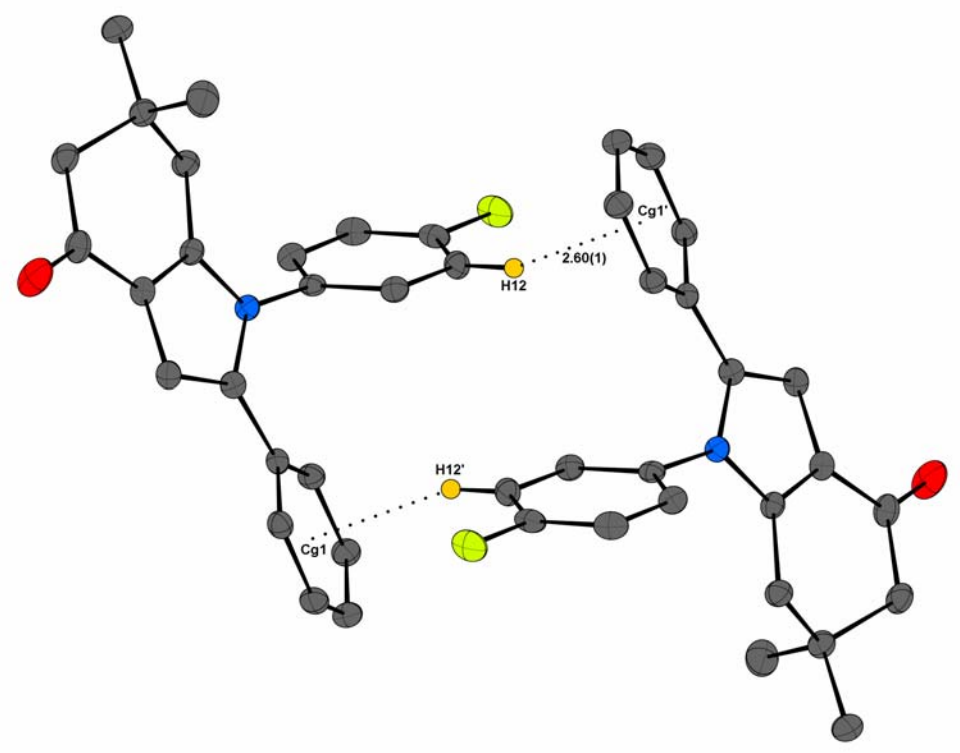

Figure 2c: Molecular dimer via C-H…π interaction involving C12-H12…Cg1' in form I, molecules at (x, y, z) and (1 – x, 1 – y, - z) are shown.

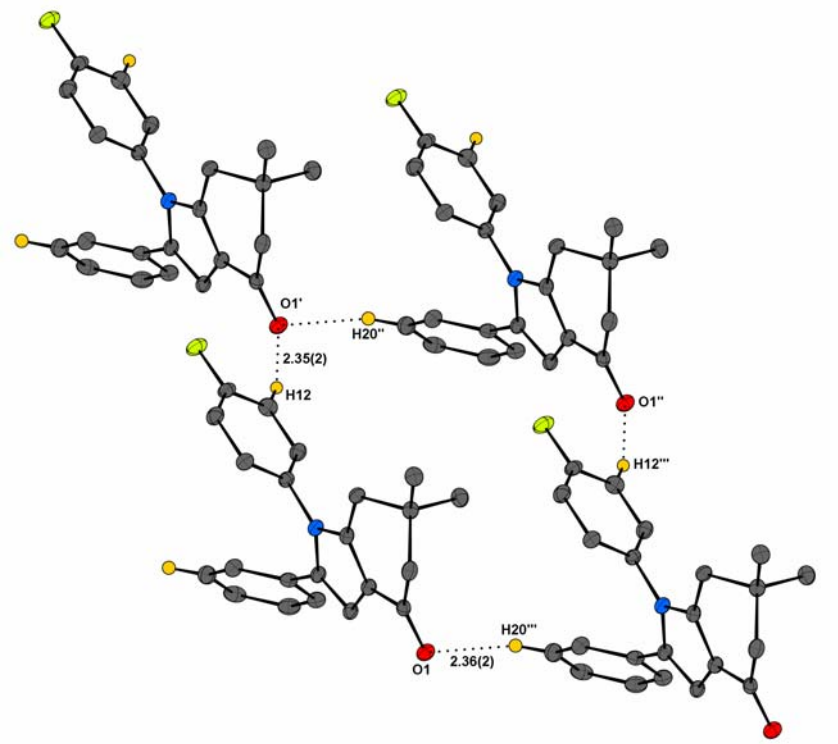

Figure 3a: Molecular sheet via bifurcated C-H…O'=C' interactions in form II

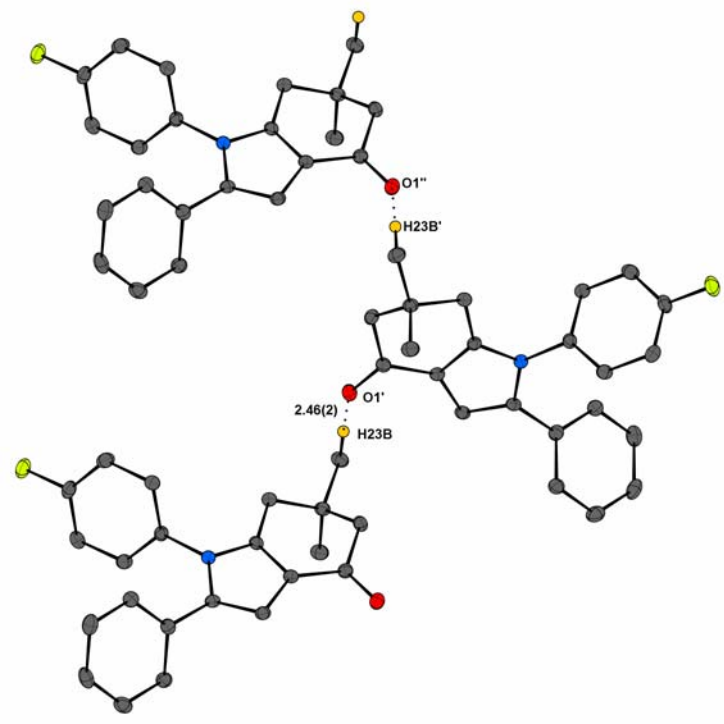

Figure 3b: Molecular chain down via C-H…O'=C' interactions in form II, molecules at (2 – x, y – ½, 1 – z) and (x, y – 1, z) are shown as (') and ('') respectively.

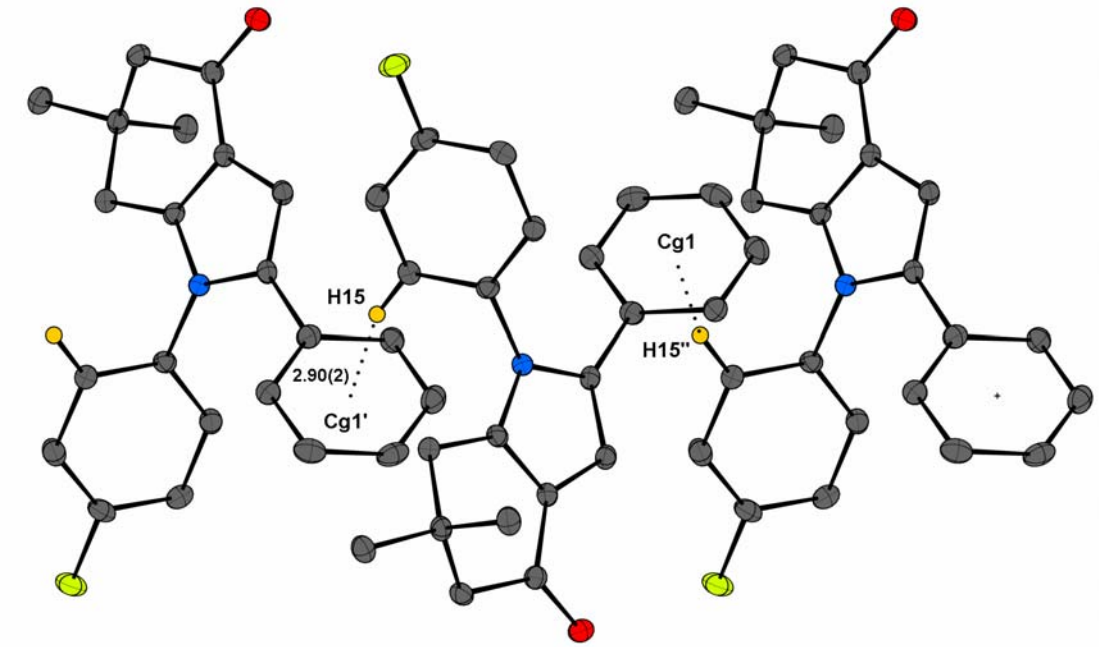

Figure 3c: Molecular chain down '*a*' axis via C-H…π interactions in form II, molecules at (- x, y – ½, 2 - z) and (1 – x, y – ½, 2 - z) are shown as (') and ('') respectively.