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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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Electronic Supplementary material
Table 1: Crystal Data

<table>
<thead>
<tr>
<th></th>
<th>Polymorph 1</th>
<th>Polymorph 2</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Formula</strong></td>
<td>$\text{C}<em>{22}\text{H}</em>{20}\text{NOF}$</td>
<td>$\text{C}<em>{22}\text{H}</em>{20}\text{NOF}$</td>
</tr>
<tr>
<td><strong>Solvent</strong></td>
<td>Dichloromethane/hexane</td>
<td>Acetone</td>
</tr>
<tr>
<td><strong>Morphology</strong></td>
<td>rectangular blocks</td>
<td>rhombohedral blocks</td>
</tr>
<tr>
<td><strong>Crystal System</strong></td>
<td>Monoclinic</td>
<td>Monoclinic</td>
</tr>
<tr>
<td><strong>$a/\text{Å}$</strong></td>
<td>12.874(8)</td>
<td>7.892(5)</td>
</tr>
<tr>
<td><strong>$b/\text{Å}$</strong></td>
<td>6.713(4)</td>
<td>10.861(6)</td>
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<tr>
<td><strong>$c/\text{Å}$</strong></td>
<td>20.311(15)</td>
<td>10.786(2)</td>
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<tr>
<td><strong>$\beta/\text{o}$</strong></td>
<td>94.65(1)</td>
<td>109.99(8)</td>
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<tr>
<td><strong>$V/\text{Å}^3$</strong></td>
<td>1749.5(2)</td>
<td>868.9(3)</td>
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<tr>
<td><strong>$Z$</strong></td>
<td>4</td>
<td>2</td>
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<tr>
<td><strong>Space Group</strong></td>
<td>$P_{21}/n$</td>
<td>$P_{21}$</td>
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<tr>
<td><strong>Temp/K</strong></td>
<td>90.0(2)</td>
<td>90.0(2)</td>
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<tr>
<td><strong>Density (calc)/gcm$^{-3}$</strong></td>
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<td>1.274</td>
</tr>
<tr>
<td><strong>Radiation</strong></td>
<td>MoK$_\alpha$</td>
<td>MoK$_\alpha$</td>
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<tr>
<td><strong>Structure Solution</strong></td>
<td>Direct methods SIR92</td>
<td>Direct methods SIR92</td>
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<tr>
<td><strong>Diffractometer</strong></td>
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<td>Bruker AXS</td>
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<tr>
<td><strong>Detector</strong></td>
<td>SMART APEX CCD</td>
<td>SMART APEX CCD</td>
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<tr>
<td><strong>$F_{000}$</strong></td>
<td>703.9</td>
<td>351.9</td>
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<tr>
<td><strong>$\mu/\text{mm}^{-1}$</strong></td>
<td>0.84</td>
<td>0.83</td>
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<td><strong>Scan Mode</strong></td>
<td>$\omega/\phi$</td>
<td>$\omega/\phi$</td>
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<tr>
<td><strong>2$\theta$ range</strong></td>
<td>1.8-25.3$^\circ$</td>
<td>2.0-25.4$^\circ$</td>
</tr>
<tr>
<td><strong>Total No. of Reflections</strong></td>
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<td>6405</td>
</tr>
<tr>
<td><strong>Unique Reflections</strong></td>
<td>3196</td>
<td>3154</td>
</tr>
<tr>
<td><strong>No. of Parameters</strong></td>
<td>306</td>
<td>306</td>
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<tr>
<td><strong>$R$, $R_w$</strong></td>
<td>0.039, 0.121</td>
<td>0.027, 0.072</td>
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<tr>
<td><strong>$\Delta\rho_{\text{min, max}}/e\text{Å}^3$</strong></td>
<td>-0.223, 0.260</td>
<td>-0.174, 0.155</td>
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<tr>
<td><strong>g.o.f</strong></td>
<td>1.033</td>
<td>1.034</td>
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</table>
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 \((2 - x, y - \frac{1}{2}, 1 - z)\) 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.