Spectroscopic, single crystal XRD structure, DFT and molecular dynamics investigation of 1-(3-Chloro-4-fluorophenyl)-3-[3-(trifluoromethyl)phenyl]thiourea

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Table S1. Geometrical parameters (DFT/XRD/MacroModel (OPLS 2005 force field)) of ANF-2

<table>
<thead>
<tr>
<th>Bond lengths (Å)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C1 - C2</td>
<td>1.4007/1.4015/1.4139</td>
</tr>
<tr>
<td>C1 - H23</td>
<td>1.0808/0.9500/1.0811</td>
</tr>
<tr>
<td>C2 - N7</td>
<td>1.4126/1.4224/1.4214</td>
</tr>
<tr>
<td>C3 - H24</td>
<td>1.0858/0.9500/1.0802</td>
</tr>
<tr>
<td>C4 - C19</td>
<td>1.5052/1.4925/1.5215</td>
</tr>
<tr>
<td>C5 - H26</td>
<td>1.0853/0.9500/1.0805</td>
</tr>
<tr>
<td>N7 - H27</td>
<td>1.0129/0.8800/1.0081</td>
</tr>
<tr>
<td>N8 - C9</td>
<td>1.4174/1.4254/1.4217</td>
</tr>
<tr>
<td>C11 - C12</td>
<td>1.4035/1.3895/1.4147</td>
</tr>
<tr>
<td>C12 - C13</td>
<td>1.3926/1.3815/1.4086</td>
</tr>
<tr>
<td>C13 - C14</td>
<td>1.3887/1.3815/1.4078</td>
</tr>
<tr>
<td>C14 - C15</td>
<td>1.3963/1.3765/1.4102</td>
</tr>
<tr>
<td>C15 - C16</td>
<td>1.3916/1.3975/1.4093</td>
</tr>
<tr>
<td>C16 - H31</td>
<td>1.0844/0.9500/1.0805</td>
</tr>
<tr>
<td>C19 - F21</td>
<td>1.3545/1.3245/1.3322</td>
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<table>
<thead>
<tr>
<th>Bond angles (°)</th>
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</thead>
<tbody>
<tr>
<td>C6-C1-C2</td>
<td>119.5/119.2/120.2340</td>
</tr>
<tr>
<td>H23-C1-C6</td>
<td>120.7/120.4/119.1521</td>
</tr>
<tr>
<td>N7-C2-C1</td>
<td>123.8/122.0/122.2689</td>
</tr>
<tr>
<td>C4-C3-C2</td>
<td>120.2/118.7/120.7084</td>
</tr>
<tr>
<td>H24-C3-C4</td>
<td>119.6/120.7/118.8207</td>
</tr>
<tr>
<td>C19-C4-C3</td>
<td>119.6/119.0/119.7311</td>
</tr>
<tr>
<td>C6-C5-C4</td>
<td>119.0/120.3/120.2422</td>
</tr>
<tr>
<td>H25-C5-C6</td>
<td>120.9/119.1/119.7881</td>
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<tr>
<td>H26-C6-C1</td>
<td>119.0/120.0/119.8736</td>
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<tr>
<td>C8-N7-C2</td>
<td>131.1/127.3/129.1563</td>
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<tr>
<td>H27-N7-C8</td>
<td>115.0/116.3/114.9662</td>
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<tr>
<td>N10-C8-N7</td>
<td>113.9/113.1/112.8811</td>
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<tr>
<td>Bond Angles (°)</td>
<td>C11-N10-C8</td>
</tr>
<tr>
<td></td>
<td>H28-N10-C11</td>
</tr>
<tr>
<td></td>
<td>C16-C11-N10</td>
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<tr>
<td></td>
<td>C13-C12-C11</td>
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<tr>
<td></td>
<td>H29-C12-C13</td>
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<tr>
<td></td>
<td>H30-C13-C12</td>
</tr>
<tr>
<td></td>
<td>C15-C14-C13</td>
</tr>
<tr>
<td></td>
<td>F18-C14-C15</td>
</tr>
<tr>
<td></td>
<td>C17-C15-C14</td>
</tr>
<tr>
<td></td>
<td>C15-C16-C11</td>
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<tr>
<td></td>
<td>H31-C16-C15</td>
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<td>F21-C19-C4</td>
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<td></td>
<td>F22-C19-C4</td>
</tr>
<tr>
<td></td>
<td>F22-C19-F21</td>
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</tbody>
</table>

| Dihedral angles (°) | C1-C2-C3-C4 | -0.3/2.1/−2.2     | C1-C2-N7-C8 | 28.3/130.2/49.4 |
|                     | C1-C6-C5-C4 | -0.0/1.1/−0.2      | C2-C1-C6-C5  | −0.7/0.3/−0.8  |
|                     | C2-C3-C4-C5 | -0.5/−1.3/1.2      | C2-C3-C4-C19 | 177.1/178.9/−179.8 |
|                     | C2-N7-C8-S9 | 5.3/1.2/5.2       | C2-N7-C8-N10 | −176.7/−175.8/−178.5 |
|                     | C3-C2-C1-C6 | 0.8/−1.4/1.9      | C3-C2-N7-C8  | −154.8/−52.7/−134.9 |
|                     | C3-C4-C5-C6 | 0.6/−0.4/0.1      | C3-C4-C19-F20 | 148.3/162.4/160.3 |
|                     | C3-C4-C19-F21 | -92.2/−77.1/−79.6 | C3-C4-C19-F22 | 27.4/38.3/39.7 |
|                     | C4-C3-C2-N7 | −177.3/−179.1/−178.0 | C4-C3-C4-C19-F20 | −34.1/−17.7/−20.8 |
|                     | C5-C4-C19-F21 | 85.4/103.0/99.3 | C5-C4-C19-F22 | −154.9/−141.3/−141.4 |
|                     | C6-C1-C2-N7 | 177.6/178.5/177.6 | C6-C5-C4-C19 | −177.0/−179.6/−179.0 |
|                     | N7-C8-N10-C11 | 7.8/−179.6/8.9 | C8-N10-C11-C12 | 47.9/47.9/47.2 |
|                     | C8-N10-C11-C16 | −134.9/−136.3/−136.3 | C9-C8-N10-C11 | −174.0/−2.9/−174.5 |
|                     | N10-C11-C12-C13 | 178.3/177.2/178.3 | N10-C11-C16-C15 | −176.9/−176.3/−178.4 |
|                     | C11-C12-C13-C14 | −1.5/1.2/−0.8 | C11-C16-C15-C14 | −1.4/1.4/0.7 |
|                     | C11-C16-C15-C17 | 179.6/177.5/−179.3 | C12-C11-C16-C15 | 0.3/0.3/−1.8 |
|                     | C12-C13-C14-C15 | 0.4/0.6/−0.3 | C12-C13-C14-F18 | −179.3/0.0/0.0 |
|                     | C13-C12-C11-C16 | 1.1/1.5/1.8 | C13-C14-C15-C16 | 1.0/1.7/0.4 |
|                     | C13-C14-C15-C17 | −179.9/177.2/−179.6 | C16-C15-C14-F18 | −179.3/−178.8/0.0 |
|                     | C17-C15-C14-F18 | −0.2/2.5/0.1 |                     |                     |