Supporting Information

Three Centered Hydrogen Bond of the type C=O···H(N)···X-C in diphenyloxamide derivatives involving halogens and a rotating CF$_3$ group: NMR, QTAIM, NCI and NBO Studies

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2D $^1$H-$^{15}$N HSQC experimental parameters

<table>
<thead>
<tr>
<th>parameter</th>
<th>F$_1$ ($^{15}$N)</th>
<th>F$_2$ ($^1$H)</th>
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</thead>
<tbody>
<tr>
<td>Number of data points</td>
<td>256</td>
<td>2048</td>
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<tr>
<td>Spectral width (Hz)</td>
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<td>Window function used</td>
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</table>

Pulse sequence used:  hsqcetgp

Pulse width: 14.30μs

2D $^1$H-$^{19}$F HOESY experimental parameters

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<th>parameter</th>
<th>F$_1$ ($^{19}$F)</th>
<th>F$_2$ ($^1$H)</th>
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<td>Number of data points</td>
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<td>Spectral width (Hz)</td>
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</table>

S8
Table: $^{1}J_{\text{NH}}$ and $^{15}$N chemical shift values measured from $^{1}$H-$^{15}$N HSQC Spectra.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>$^{1}J_{\text{NH}}$ (CDCl$_3$)</th>
<th>$^{15}$N chemical shift of amide proton (in ppm)</th>
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<tbody>
<tr>
<td>1</td>
<td>-91.3</td>
<td>123.5</td>
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<tr>
<td>2</td>
<td>-92.9</td>
<td>110.4</td>
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<tr>
<td>3</td>
<td>-92.0</td>
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<td>4</td>
<td>-91.8</td>
<td>123.7</td>
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<td>5</td>
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<td>132.1</td>
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<tr>
<td>6</td>
<td>-93.1</td>
<td>115.8</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Coupling values</th>
<th>Molecule 2</th>
<th>Molecule 6</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CDCl$_3$(Hz)</td>
<td>DMSO(Hz)</td>
</tr>
<tr>
<td>$J_{\text{FH}}$</td>
<td>-2.9</td>
<td>+0.85</td>
</tr>
<tr>
<td>$J_{\text{NF}}$</td>
<td>-0.4</td>
<td>-1.25</td>
</tr>
</tbody>
</table>
Experimental:

All the reagents were purchased from Aldrich and used without further purification. The investigated molecules were synthesized according to the following procedure. The spectra were recorded using Bruker 400 and 500 MHz NMR spectrometers. The Eurotherm temperature control unit was utilized to set the temperature to an accuracy of ±1.0 K. The $^1$H chemical shifts were referenced relative to TMS. $^{15}$N spectra are referenced to external nitromethane, $^{19}$F spectra are referenced to trifluoroacetic acid.

Synthesis Procedure:

All the investigated molecules 1-8 were synthesizes using the following procedure.

The substituted aniline (4mM, 2 eq) was dissolved in chloroform (4ml) and it was added drop by drop to Oxalyl chloride (2mM, 1 eq ) at 0°C. After stirring for nearly 10 min the white solid formed was washed with distilled water, and the compound was recrystallized from chloroform.
G09 Reference: