Supporting information for article:

Role of halogen-involved intermolecular interactions and existence of isostructurality in the crystal packing of —CF3 and halogen (Cl or Br or I) substituted benzamides

Pradip Kumar Mondal, Rahul Shukla, Subha Biswas and Deepak Chopra
**Table S1**

The possible intermolecular interactions and interaction energies (kJ/mol) for the different molecular pair of the benzamides obtained from the PIXEL method.

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| II  | -x+2,-y+1,-z | 4.973 | -16.2 | -7.8  | -46.5 | 34.7 | -35.8 | C6–H6⋯π(C8-C9) | C5–H5⋯π(C10) | 2.69, 129 | 2.87, 144 |
| III | -x+1,-y,-z  | 8.041 | -16.8 | -7.1  | -39.2 | 27.7 | -35.5 | C2–H2⋯Cl1  | N1⋯Cl1   | 2.80, 155 | 3.499(3), 99 |
| IV  | -x+1,-y+1,-z | 5.557 | -9.0  | -5.9  | -39.5 | 27.7 | -26.7 | C10–H10⋯F2 | C9–H9⋯π(C6) | 2.63, 160 | 2.76, 160 |
| V   | -x+1,-y+1,-z+1 | 9.231 | -6.1  | -2.6  | -16.2 | 8.0  | -16.8 | H3⋯H3   | C3–H3⋯F1  | 2.3     | 2.76, 131 |
| VI  | -x+2,-y,-z  | 9.072 | -6.3  | -5.2  | -24.3 | 19.3 | -16.5 | C13–H13⋯Cl1 | O1⋯Cl1   | 2.75, 173 | 3.366(3), 145 |
| VII | -x+2,-y+1,-z+1 | 8.658 | 0.6   | -0.4  | -8.8  | 1.6  | -7.1  | F1⋯π(C2)  | 3.482(4), 157 |
| VIII| x+1,y+1,z+1 | 14.561 | -2.0  | -0.4  | -4.9  | 1.7  | -5.6  | C11–H11⋯F2 | 2.66, 130 |
| IX | x,y+1,z+1 | 14.605 | -0.3 | -0.7 | -7.1 | 4.0 | -4.1 | C11–H11···F3 | 2.65, 148 |
| PC42 |  |  |  |  |  |  |  |  |  |
| a…a |  |  |  |  |  |  |  |  |  |
| I | -x+1,-y,-z+1 | 7.018 | -8.6 | -2.1 | -16.3 | 7.6 | -19.5 | C10–H10···F3 | 2.42, 161 |
| II | x,-y+1/2,z+1/2 | 9.616 | -5.4 | -2.2 | -14.8 | 8.1 | -14.4 | C5–H5···π(C12) F2···π(C13) | 2.73, 172 3.375(3), 147 |
| III | -x+1,-y+1,-z+1 | 9.949 | 1.6 | -2.0 | -16.7 | 15.1 | -2.0 | π(C3)···π(C3) | 3.167(3) |
| a…b |  |  |  |  |  |  |  |  |  |
| IV | x,y,z | 4.910 | -42.9 | -17.6 | -45.0 | 51.3 | -54.2 | N1–H1···O2 C9–H9···π(C16–C15–C20) | 1.95, 152 2.59, 146 |
| V | x-1,y,z | 5.018 | -44.6 | -18.0 | -44.9 | 55.3 | -52.1 | N2–H2···O1 C23–H23···π(C2–C1) | 1.91, 153 2.66, 155 |
| VI | -x+1,-y,-z+1 | 7.610 | -16.0 | -4.9 | -31.0 | 18.1 | -33.8 | C17–H17···O1 C16–H16···π(C11) | 2.51, 154 2.79, 138 |
| VII | -x+1,-y+1,-z+1 | 7.809 | -16.5 | -5.6 | -31.1 | 21.6 | -31.6 | C3–H3···π(C27–C22) C2–H2A···π(C25) | 2.72, 145 2.79, 129 |
| VIII | -x+1,y+1/2,-z+1/2 | 11.295 | -0.4 | -0.9 | -7.7 | 6.6 | -2.4 | F2···Cl2 F3···Cl2 | 3.132(2), 100, 173 3.373(1), 89, 149 |
| IX | -x+1,y+1/2,-z+1/5 | 13.251 | -0.7 | -0.1 | -0.3 | 0.0 | -1.1 | F4···Cl1 F5···Cl1 | 3.084(2), 108, 162 3.397(2), 94, 146 |
| b…b |  |  |  |  |  |  |  |  |  |
| X | -x+2,-y+1,-z+1 | 7.246 | -6.2 | -1.5 | -13.4 | 3.2 | -17.9 | C24–H24···F6 | 2.65, 165 |
### XI
x-\(y+1/2,z-1/2\)

\[
\begin{align*}
9.584 & \quad -6.1 & \quad -2.3 & \quad -16.3 & \quad 8.8 & \quad -15.9 & \quad C19-\text{H19} \cdots \pi(C25) \\
& & & & & & \quad C18-\text{H18} \cdots \text{Cl2}
\end{align*}
\]

3.82, 145

3.11, 122

### XII
-x+2,-y,-z+1

\[
\begin{align*}
9.804 & \quad 2.5 & \quad -1.9 & \quad -15.7 & \quad 10.6 & \quad -4.5 & \quad \pi(C17) \cdots \pi(C17)
\end{align*}
\]

3.401(3)

### PC43

#### I
x-\(y+1/2,z+1/2\)

\[
\begin{align*}
4.882 & \quad -60.6 & \quad -25.2 & \quad -42.5 & \quad 85.0 & \quad -43.3 & \quad \text{N1-\text{H1} \cdots \text{O1}} \\
& & & & & & \quad \text{C2-\text{H2} \cdots \text{O1}}
\end{align*}
\]

1.92, 162

2.28, 132

#### II
-x+1,-y+1,-z+1

\[
\begin{align*}
8.560 & \quad -39.7 & \quad -13.4 & \quad -51.3 & \quad 85.8 & \quad -18.6 & \quad \pi(C8) \cdots \pi(C10) \\
& & & & & & \quad \pi(C9) \cdots \pi(C11) \\
& & & & & & \quad \text{Cl1} \cdots \pi(C7)
\end{align*}
\]

3.408(2)

3.417(3)

3.546(2), 99

#### III
-x,-y,-z+1

\[
\begin{align*}
8.302 & \quad -15.5 & \quad -3.6 & \quad -20.0 & \quad 25.7 & \quad -13.4 & \quad \text{F3A} \cdots \pi(C2)
\end{align*}
\]

3.199(3), 123

#### IV
x-\(y+1.5,z-1/2\)

\[
\begin{align*}
11.146 & \quad -3.6 & \quad -1.9 & \quad -12.5 & \quad 7.9 & \quad -10.1 & \quad \text{C12-\text{H12} \cdots \pi(C10)} \\
& & & & & & \quad \text{C10-\text{H10} \cdots \text{Cl1}}
\end{align*}
\]

2.99, 144

3.20, 141

#### V
x,y+1,z

\[
\begin{align*}
10.386 & \quad -10.3 & \quad -3.9 & \quad -17.6 & \quad 23.7 & \quad -8.1 & \quad \pi(C3) \cdots \pi(C12) \\
& & & & & & \quad \text{Cl} \cdots \pi(C2)
\end{align*}
\]

3.438(3)

3.614(3), 100

#### VI
-x-\(y-1/2,-z+1.5\)

\[
\begin{align*}
8.724 & \quad -5.9 & \quad -1.6 & \quad -10.4 & \quad 10.2 & \quad -7.7 & \quad \text{C6-\text{H6} \cdots \text{F3A}} \\
& & & & & & \quad \text{O1} \cdots \text{F3A}
\end{align*}
\]

2.37, 139

3.195(2), 132

#### VII
-x+1,y-1/2,-z+1/2

\[
\begin{align*}
10.950 & \quad -2.2 & \quad -2.1 & \quad -8.9 & \quad 5.5 & \quad -7.7 & \quad \text{C9-\text{H9} \cdots \text{Cl1}}
\end{align*}
\]

2.90, 145

#### VIII
x,-y-1/2,z-1/2

\[
\begin{align*}
11.796 & \quad -2.7 & \quad -1.2 & \quad -6.2 & \quad 5.8 & \quad -4.3 & \quad \text{C4-\text{H4} \cdots \text{F2A}}
\end{align*}
\]

2.39, 131

#### IX
1-x,2-y,1-z

\[
\begin{align*}
16.779 & \quad -1.4 & \quad -1.1 & \quad -6.5 & \quad 6.1 & \quad -2.9 & \quad \text{Cl1} \cdots \text{Cl1}
\end{align*}
\]

3.531(1), 156, 156

### PC44

#### a\...a

#### I
x,\(-y\),1,z

\[
\begin{align*}
5.252 & \quad -37.8 & \quad -12.5 & \quad -45.1 & \quad 45.3 & \quad -50.0 & \quad \text{N1-\text{H1} \cdots \text{O1}} \\
& & & & & & \quad \text{C9-\text{H9} \cdots \text{O1}}
\end{align*}
\]

2.11, 153

2.48, 125

#### II
-x+2,y-1/2,-z+1/2

\[
\begin{align*}
7.949 & \quad -10.1 & \quad -5.8 & \quad -39.2 & \quad 25.3 & \quad -29.8 & \quad \text{C13-\text{H13} \cdots \pi(C12-C13)} \\
& & & & & & \quad \text{C2-\text{H2A} \cdots \text{Cl1}} \\
& & & & & & \quad \text{C12-\text{H12} \cdots \text{N1}}
\end{align*}
\]

2.67, 147

2.96, 147

2.73, 135

#### a\...b
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PB24

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PB32

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**Figure S1** $^1$H-NMR Spectra of the newly synthesized bulk benzamide compounds
**Figure S2** DSC traces of the newly synthesized bulk benzamide compounds @5 °C/min.
Onset Temperature = 125 °C

Onset Temperature = 177 °C

Onset Temperature = 150 °C
Onset Temperature = 118 °C

Onset Temperature = 111 °C

Onset Temperature = 152 °C
Onset Temperature = 151 °C

Onset Temperature = 124 °C
**Figure S3** Electrostatic potential map on the Hirshfeld surface of N-chlorophenyl-trifluoromethyl-benzamide. The ranges of ESP are from −0.05 a.u. (red) to 0.05 a.u. (blue). (i) PC22 (ii) PC23 (iii) PC24 (iv) PC32 (v) PC33 (vi) PC34 (vii) PC42 (viii) PC43 (ix) PC44.

**Figure S4** Electrostatic potential map on the Hirshfeld surface of N-bromophenyl-trifluoromethyl-benzamide. The ranges of ESP are from −0.05 a.u. (red) to 0.05 a.u. (blue). (i) PB23 (ii) PB24 (iii) PB32 (iv) PB34 (v) PB43 (vi) PB44.
Figure S5  Electrostatic potential map on the Hirshfeld surface of N-iodophenyl-trifluoromethylbenzamide. The ranges of ESP are from −0.05 a.u. (red) to 0.05 a.u. (blue). (i) PI22 (ii) PI23 (iii) PI24 (iv) PI32 (v) PI33 (vi) PI34 (vii) PI43 (viii) PI44.
Figure S6  The 2D and 1D supramolecular constructs obtained from XPac analysis for (i) PC23 and PI23, (ii) PB34 and PC24, (iii) PC34 and PC44, (iv) PB44 and PC34, (v) PC34 and PI44, (vi) PC44 and PI44, (two packing diagrams from the 2:1 seed) (vii) PC44 and PI44, (two packing diagrams from the 1:1 seed) (viii) PB44 and PI44 (two packing diagrams from the 1:1 seed).