

Short Note

# *N*-(2,4-Difluorophenyl)-2-fluorobenzamide

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**Abstract:** The title compound *N*-(2,4-difluorophenyl)-2-fluorobenzamide (**Fo24**) was synthesized in high yield (1.09 g; 87%) using standard synthetic procedures from the condensation reaction of 2-fluorobenzoyl chloride with 2,4-difluoroaniline. Crystals of **Fo24** were grown from CH<sub>2</sub>Cl<sub>2</sub> at room temperature. The **Fo24** crystal structure was determined using single-crystal X-ray diffraction methods at 294 (1) K in space group *Pn* (No. 7). **Fo24** is the second regular tri-fluorinated benzamide with the formula C<sub>13</sub>H<sub>8</sub>F<sub>3</sub>N<sub>1</sub>O<sub>1</sub> to be reported and contrasts with the more common difluorinated and tetra-fluorinated analogues. In **Fo24**, both aromatic rings are effectively coplanar with an interplanar angle of 0.7(2)°. The central amide group plane is oriented by 23.04(18)° and 23.69(17)° from both aromatic rings, forming an intramolecular contact with an *ortho*-F12 atom with H1 ··· F12 = 2.12(4) Å. The primary hydrogen bonds are 1D amide–amide interactions that form along the *b*-axis direction. In addition, weaker C-H ··· F/O interactions are noted: a *R*<sup>2</sup><sub>2</sub>(12) synthon involving two C-H, a N-H and two C-F groups, with C-F ··· C ring–ring stacking contacts completing the interactions.

**Keywords:** amide; crystal structure; fluorine; hydrogen bonding; molecular stacking; ring stacking

## 1. Introduction

Fluorinated molecules have attracted extensive research interest in medicinal chemistry and pharmaceuticals over the past several decades, with the development of new drugs and therapies [1,2]. Moreover, structural analyses of fluorinated benzamides have increased, with advances demonstrated in the enormous increase in benzamide datasets, structures and published papers [3–9], as archived on databases and repositories such as the Cambridge Structural Database (CSD) [3].

In this short study, we expand on the structural knowledge of halogenated benzamides and report the chemistry and crystal structure of *N*-(2,4-difluorophenyl)-2-fluorobenzamide, (**Fo24**), an isomer of the recently reported 2,3-difluorinated analogue **Fo23** [10].

**Fo24** is a compound of the larger 18 isomer grid containing three sets of six **FpXY**, **FmXY** and **FoXY** isomers (where *p*, *m*, *o* are the *para*-, *meta*-, *ortho*- substitution of the monofluoro-substituted aromatic ring). The *XY* labels (*X* = 2 or 3; *Y* = 3, 4, 5 or 6) represent the six disubstituted fluorinated aromatic groups as 2,3-; 2,4-; 2,5-; 2,6-; 3,4- and 3,5-F<sub>2</sub>. Additionally, the amide reversed series represent 18 more compounds, resulting in a 36-isomer grid. Beyond this, more isomers are possible where trifluoro-aromatic substitution results in another 20 isomers. As such, completion of entire isomer grids is desirable for a thorough physicochemical analysis and full representation of the 3D structural space around a particular compound. In reporting the **Fo24** crystal structure herein, we highlight once again the gap that exists in the available structural data for tri-fluorinated benzamides. This contrasts with their di-fluorinated and tetra-fluorinated counterparts which have been well documented to date [3–6,9].

## 2. Experimental

### 2.1. Materials and Characterisation

The chemicals, materials, spectroscopic, X-ray diffraction methods and analytical equipment are as reported in previous research [7–9]. Chemicals in the **Fo24** synthesis



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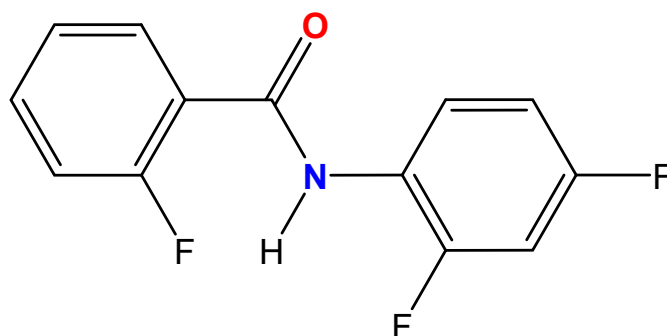
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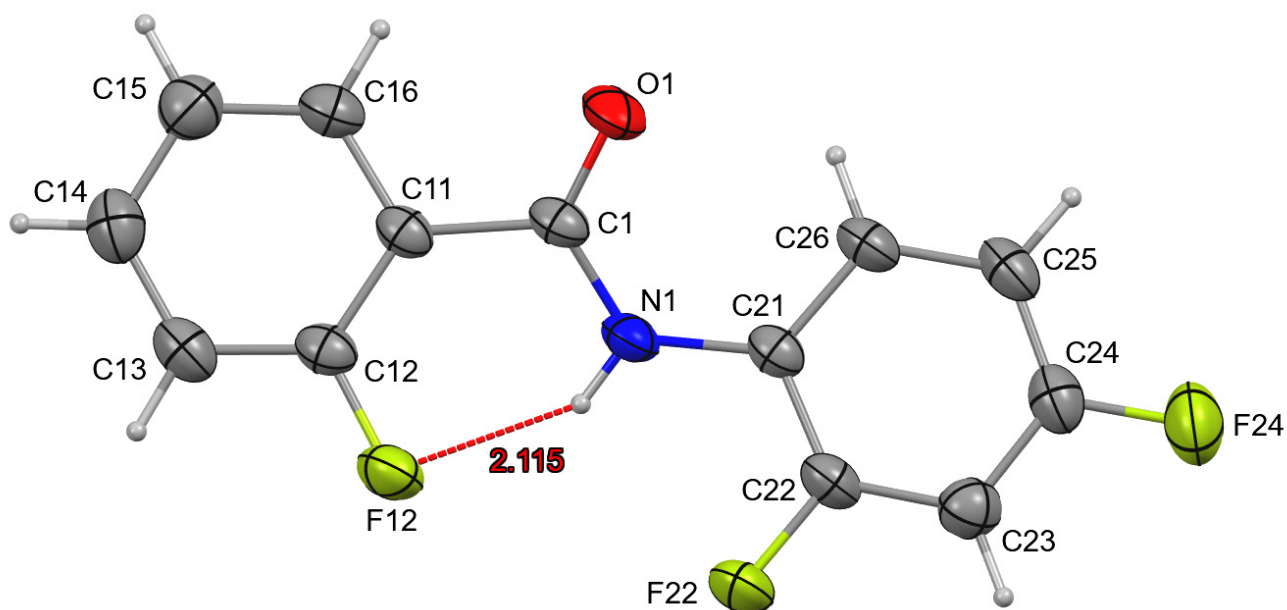


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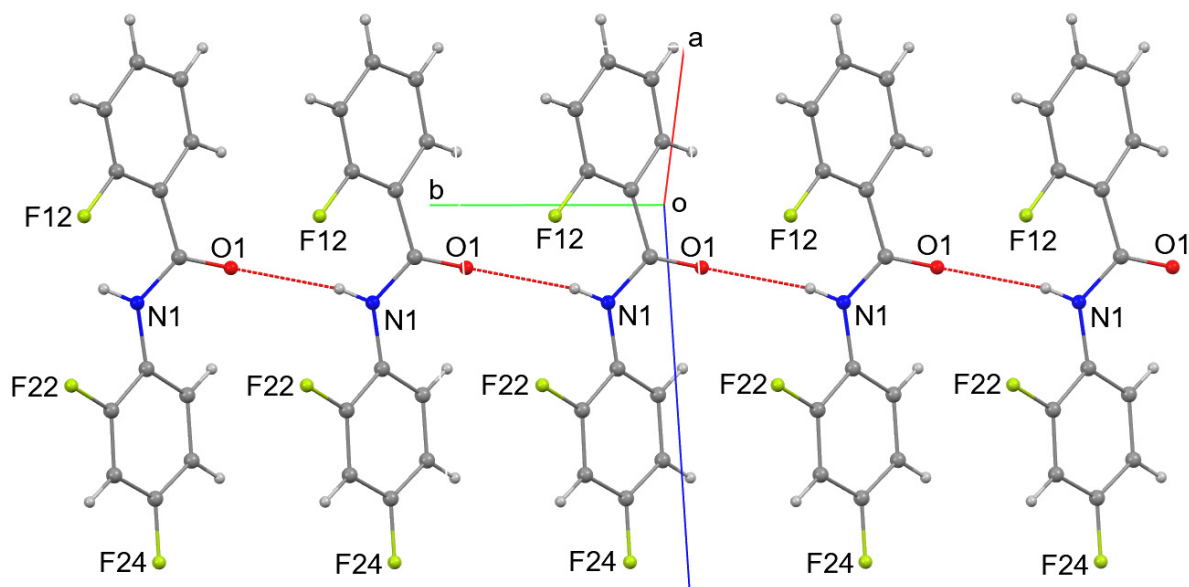
(Scheme 1) were used as purchased from Sigma Aldrich. The synthetic approaches are standard, (ESI) [4–9]. The single crystal X-ray diffraction methods and data collection procedures for the **Fo24** crystal structure (Scheme 1, Figure 1) are routine [9,11]. Data collection, reduction, structure solution and refinement were performed using the CrysAlisPro [11] and SHELXS, SHELXL14 programs [12]. The molecular structure and hydrogen bonding diagrams (Figures 1–4) were made using the Mercury program [13]. Geometric analysis of **Fo24** was accomplished using the SHELXL14 output [12] and CALC ALL function in the PLATON package [14]. CSD structural analyses and comparisons were performed with version 5.45 [Conquest 2023.3.0—Build 392256] on 19 December 2023 [3].



**Scheme 1.** **Fo24** or (*N*-(2,4-difluorophenyl)-2-fluorobenzamide).



**Figure 1.** An ORTEP diagram of the **Fo24** structure with displacement ellipsoids at the 30% probability level and highlighting the intramolecular N1-H1···F12 interaction.



**Figure 2.** A view of the amide...amide interaction along the *b*-axis direction in Fo24 with unit cell axes.

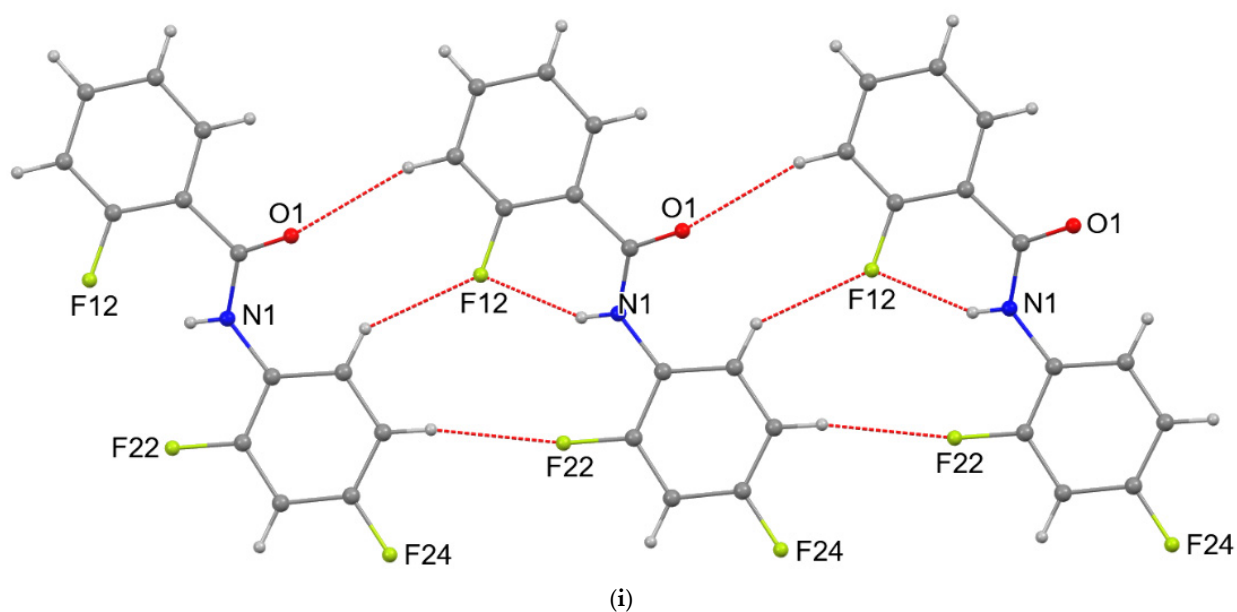
## 2.2. Reaction Procedure and Characterisation: Experimental and Spectroscopic Data

Synthetic yield (%) = 87%. Melting point range of 110–112 °C.

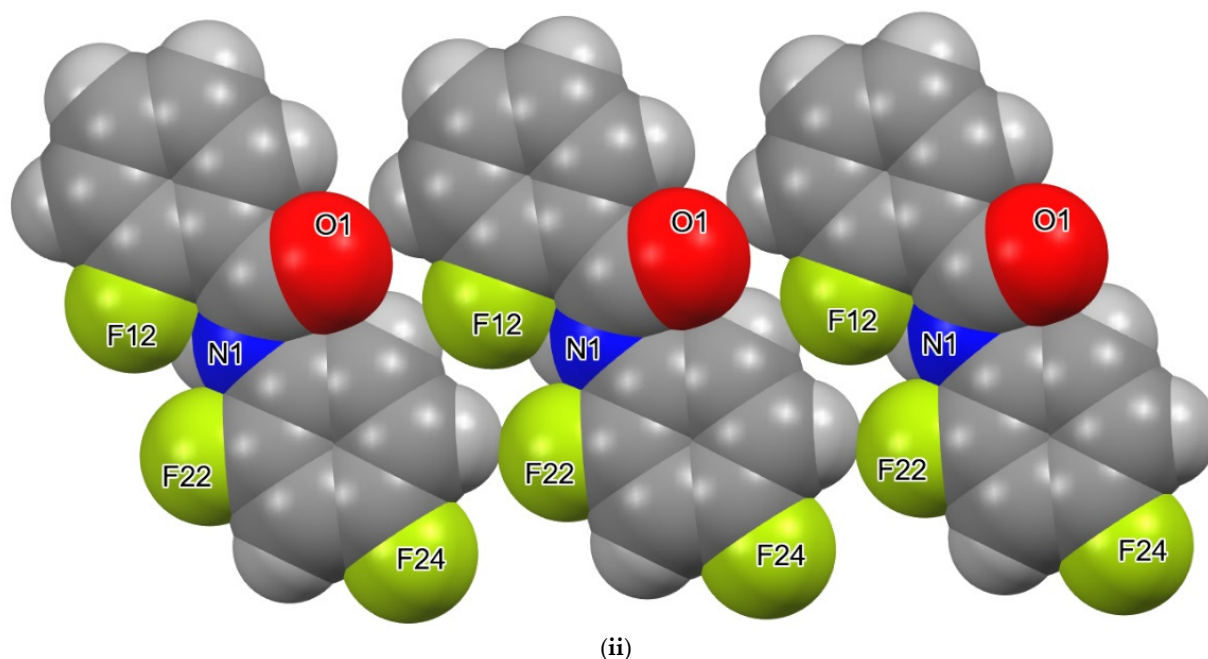
Experimental (Calculated) CHN Analysis (%): C = 62.4% (62.2); H = 3.1% (3.2); N = 5.9% (5.6).

<sup>1</sup>H NMR data (CDCl<sub>3</sub>): 6.85 (2H, m), 7.14 (1H, dd, <sup>3</sup>J = 8.5, <sup>4</sup>J = 1), 7.26 (1H, td, <sup>3</sup>J = 7.6, <sup>4</sup>J = 1), 7.48 (1H, m), 8.11 (1H, td, <sup>3</sup>J = 7.6, <sup>4</sup>J = 1.8), 8.37 (1H, td, <sup>3</sup>J = 8.5, <sup>4</sup>J = 6), 8.61 (1H, d, <sup>3</sup>J = 16.4).

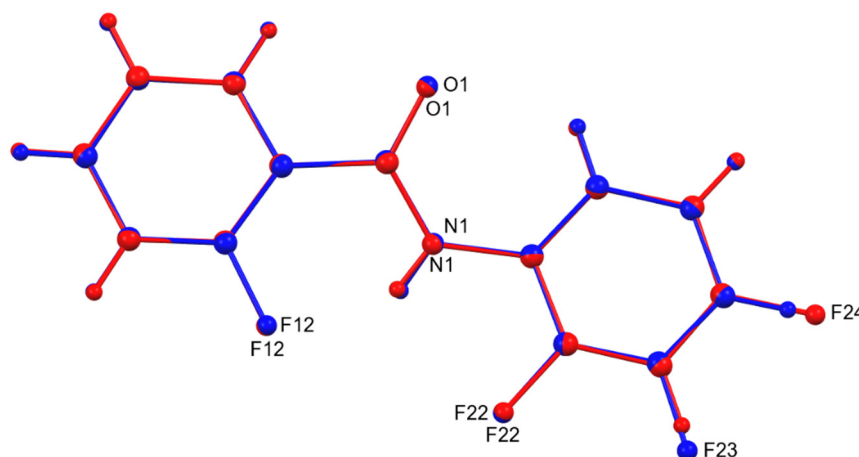
<sup>1</sup>H NMR data (*d*<sup>6</sup>-DMSO): 7.13 (1H, t, <sup>3</sup>J = 8.5), 7.36 (3H, m), 7.60 (1H, q, <sup>3</sup>J = 7.1, <sup>4</sup>J = 1.5), 7.73 (2H, m), 10.16 (1H, br. s). <sup>19</sup>F NMR data (*d*<sup>6</sup>-DMSO) (ppm): −114, −115, −118. IR (ATR): 3375 (m), 3070 (m), 1656 (m), 1610 (m), 1481 (m), 1285 (m), 1216 (m), 1086 (m), 961 (m), 846 (s). The <sup>13</sup>C spectral data diagrams are available in the supplementary information (ESI).



**Figure 3.** Cont.



**Figure 3.** (i) A view of the C-H...O/F interactions between three **Fo24** molecules involving O1, F12 and F22 and (ii) a view with atoms drawn as their van der Waals spheres.



**Figure 4.** A view of the overlap between **Fo23** [10] and **Fo24**, highlighting the similar molecular geometry.

**Fo24** crystal structure data collected using a Xcalibur Sapphire 3 (Gemini Ultra) [11].

Chemical formula:  $C_{13}H_8F_3O_1N_1$ ; Mr 251.20; crystal system and space group, monoclinic  $Pn$  (No. 7); T = 294 (2) K;  $a = 5.6756(3)$ ,  $b = 4.9829(2)$ ,  $c = 19.3064(12)$  Å,  $\beta = 91.197(5)^\circ$ ,  $V = 545.88(5)$  Å<sup>3</sup>; radiation Mo- $K\alpha$ ;  $\mu = 0.13$  mm<sup>-1</sup>; crystal size 0.93 × 0.39 × 0.07 mm; analytical absorption correction,  $T_{min,max} = 0.933, 0.991$ ; number of measured, independent, observed [ $I > 2\sigma(I)$ ] reflections and parameters, 3717, 1799, 1615 and 168, with 2 restraints;  $R_{int} = 0.019$ ;  $R[F^2 > 2\sigma(F^2)] = 0.038$ ,  $wR(F^2) = 0.091$ , Goodness of fit = 1.04; hydrogen atoms treated by a mixture of independent (N-H) and constrained (C-H) refinement;  $\Delta\rho_{max}, \Delta\rho_{min}$  (as e Å<sup>-3</sup>) = 0.18, -0.14; the absolute structure = -0.5(7).

### 3. Results and Discussion

The **Fo24** compound was synthesized in high yield using standard condensation procedures as reported for **Fo23** and related compounds [9,10]. The spectroscopic data are as predicted, and inspection of the <sup>1</sup>H NMR spectrum of **Fo24** attests to its overall high purity. The <sup>13</sup>C and <sup>19</sup>F spectra are as expected when compared with similar fluorinated

compounds. For the  $^{19}\text{F}$  NMR, the peaks at  $-114$ ,  $-115$  and  $-118$  ppm are typical of the fluorine substitution patterns expected in aromatic systems [15,16].

The **Fo24** crystal structure is notable (Figure 1) in that it is essentially isomorphous with its **Fo23** isomer (they crystallize in the same space group  $Pn$ ). The unit cell dimensions (with an  $a$ - and  $b$ -axis swap) and cell volumes are similar. The overlay of **Fo23** [10] and **Fo24** molecules, therefore, attests to the structural similarity (Figure 4). The **Fo24** molecular structure is essentially planar with respect to the aromatic rings, with both  $\text{C}_6$  rings mutually oriented at an interplanar angle of  $0.7(2)^\circ$  (Figure 1). The amide group ( $\text{C} = \text{ONH}$ ) is at an interplanar angle with the aromatic ring planes of  $23.04(18)^\circ$  and  $23.69(17)^\circ$  and arises with 1D amide–amide hydrogen bonding in the  $b$ -axis direction (Figure 2). An intramolecular contact is present between the amido N1 and *ortho*-F12, with  $\text{N1} \cdots \text{F12} = 2.745(3) \text{ \AA}$ . The amide H1 was refined with isotropic displacement parameters and results in an intramolecular  $\text{H1} \cdots \text{F12}$  distance =  $2.12(4) \text{ \AA}$ , with  $\text{N1-H1} \cdots \text{F12}$  angle =  $132(3)^\circ$ . This distance is short [3], but not as short as the intramolecular  $\text{H} \cdots \text{F}$  distances of ca.  $1.95 \text{ \AA}$  from CSD datasets [3,17], and as reported by Leckta et al. in several naphthalenylbenzamide structures [18]. In this study of **Fo24**, an auxiliary intramolecular  $\text{C26-H26} \cdots \text{O1}$  interaction is also noted, with a  $\text{C26} \cdots \text{O1}$  distance of  $2.858(5) \text{ \AA}$ .

The primary intermolecular hydrogen bond is the amide–amide interaction linking **Fo24** molecules into 1D chains along the  $b$ -axis direction ( $\text{N1} \cdots \text{O1}^i = 3.092(3) \text{ \AA}$ ; symmetry code:  $i = x, 1 + y, z$ ) (Figure 2). There is also a synthon with longer intermolecular  $\text{C-H} \cdots \text{F}^{ii}$  contacts involving two C-Hs (H25, H26) forming a cyclic hydrogen-bonded  $R^2_2(12)$  motif with the F12 and F22 atoms on a nearby **Fo24** molecule (symmetry code:  $ii = x - 1, y - 1, z$ ;  $\text{H} \cdots \text{F}^{ii} = 2.49, 2.57 \text{ \AA}$ ). This involves the N-H group positioned *syn*- to the F12 and F22 atoms (Figure 3). This type of composite interaction is noted in  $N,N'$ -(2-fluoro-5-methylbenzene-1,2-diyl)-bis(2-fluorobenzamide), **PIHQUT** [3,19] with  $\text{H} \cdots \text{F}$  distances of  $2.54 \text{ \AA}$ , and **YAZBOT** ( $N$ -(2,4-difluorophenyl)-2,5-difluorobenzamide) [6] ( $\text{H} \cdots \text{F} = 2.42, 2.49 \text{ \AA}$ ). In **Fo24**, the non-hydrogen atoms in the cyclical hydrogen-bonded arrangement are coplanar and parallel to the  $(1 -1 2)$  plane.

The molecular similarity with **Fo23** is remarkable, with an RMSD of  $0.02 \text{ \AA}$  and a maximum deviation =  $0.05 \text{ \AA}$  (Figure 4). This is not surprising, and the differences between the molecules involves the peripheral F23 (**Fo23**) and F24 (**Fo24**) atoms that have little impact on the molecular geometries in their respective structures. This demonstrates the similarities and differences that can arise in closely related structures. Acquiring as many crystal structures as possible in molecular series is desirable to fill known gaps in the CSD [3]. Rationalizing why similarities and differences in series of molecules (isomers) requires entire, completed structural sequences at different temperatures and polymorphic grids assessed so as to gain a systematic insight into the overall structural behaviour.

It is noted from a CSD review that 2-chloro- $N$ -(4-chloro-2-fluorophenyl)benzamide or **XEHZOD** crystallizes in space group  $Pna2_1$  and differs by replacing the two F atoms (in **Fo24**) with two Cl atoms [3,20]. The 2-bromo- $N$ -(2,4-dichlorophenyl)benzamide or **ZAJWUF** structure in space group  $Pbca$  is another related crystal structure [21]. Both structural examples are the only equivalent halo-substituted structures available on the CSD, where the three F atoms in **Fo24** are replaced by any X = halogen atoms [3]. However, in terms of isostructural behaviour, the crystal structures that are noted for being similar to **Fo24** are **Fo23** [10], **YAZBIN** (in space group  $Pn$ ) and **YAZBOT** (in space group  $P2_1$ ) [6].

#### 4. Overall Structural Results and Related Literature

Tri-fluorinated benzamides with the  $\text{C}_6\text{CONHC}_6$  skeleton are relatively rare on the CSD [3,10]. Analysis using the formula  $\text{C}_{13}\text{H}_8\text{F}_3\text{O}_1\text{N}_1$  reveals that only **Fo23** (with which it is essentially isomorphous) [3,10] is available for direct comparisons with **Fo24**. It does not matter if the compound is trisubstituted fluorine on one  $\text{C}_6$  aromatic ring or in any combination of *o*-/*m*-/*p*-monosubstituted F and disubstituted  $\text{F}_2$  as [2,3-; 2,4-; 2,5-; 2,6-; 3,4-; 3,5- $\text{F}_2$ ] on the second ring. These tri-fluorinated aromatic crystal structures of the formula  $\text{C}_{13}\text{H}_8\text{F}_3\text{O}_1\text{N}_1$  have not been reported. In contrast, many di- and



tetra-fluorinated analogues are available for structural comparisons [3–6,9]. Analysis of a benzamide search [ $C_{13}H_8X_3O_1N_1$  formula;  $X = F, Cl, Br, I$  and  $C_6CONHC_6$  skeleton] and reviewing various trihalide ( $X$ ) combinations shows that the majority are chloro-derivatives. The chloro-derivatives provide ten CSD structural ‘hits’ and structures, as listed by CANYAV, CANYEZ [3,22], ENUKAA [23], JOFHAO [24], KODTUT [25], LAQDOY [26], XEHZOD [20], YODDUR [27], YOVMIG [28] and ZAJWUF [21].

We anticipate that many tri-fluorinated benzamide structures will be reported in the literature shortly and archived in the CSD [3]. The crystal structure of **Fo24** is the second tri-fluorinated crystal structure reported by our group [10].

## 5. Conclusions and Future Work

The benzamide crystal structures reported in the Cambridge Structural Database [3] facilitate analysis of physicochemical research trends and patterns. Ongoing research is directed towards the development of larger  $n \times m$  benzamide isomer grids and correlating properties such as melting points, spectroscopic and structural data [3–10,20–28]. Even when analyzing relatively small molecules such as benzamides, there are gaps in our structural knowledge where crystal structure prediction can potentially be used to fill the spaces [29]. However, it is better if the structural data become available for as many compounds as possible as this is the definitive structural proof. As in any broad structure class of organic compound, there are gaps in the published/archived structural data, as noted for tri-fluorinated and mixed halogenated benzamides [3]. Given the frequency of disorder and crystallographic twinning [9] that occurs in benzamides, it is not surprising that there is a lack of datasets with many structures not reported due to high  $R$ -factors, etc. [3]. We hope to substantially increase the number of benzamide structures in the near future. This approach and the developing computational methods [29] will assist the scientific community in future endeavors regarding structural systematics [3].

**Supplementary Materials:** The following are available online: the  $^1H$ ,  $^{13}C$  and  $^{19}F$  NMR spectral data, supplementary diagram, CSD analyses, Interaction Table and the **Fo24** CheckCIF report.

**Author Contributions:** N.H. synthesized, characterized, crystallized **Fo24** and collated the preliminary data; J.F.G. performed the single-crystal X-ray diffraction experiment and analyzed the crystallographic data; J.F.G. edited and submitted the **Fo24** manuscript and supplementary ESI. All authors have read and agreed to the published version of the manuscript.

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**Conflicts of Interest:** The authors declare no conflicts of interest.

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