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***N,N'*-(*p*-Phenylene)bis(2,2,2-trifluoroacetamide)**

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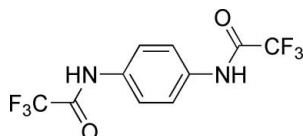
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Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.041; wR factor = 0.101; data-to-parameter ratio = 11.4.

The molecule of the title compound, $\text{C}_{10}\text{H}_6\text{F}_6\text{N}_2\text{O}_2$, is centrosymmetric. The structure exhibits a weak intramolecular $\text{N}-\text{H}\cdots\text{F}$ contact and a stronger $\text{N}-\text{H}\cdots\text{O}$ interaction connecting molecules into chains parallel to $[100]$.

Related literature

For the preparation of the title compound, see: Guo *et al.* (2005). For related literature, see: Allen *et al.* (1987); Frederick & Liu (1999).



Experimental

Crystal data

 $\text{C}_{10}\text{H}_6\text{F}_6\text{N}_2\text{O}_2$ $M_r = 300.17$ Triclinic, $P\bar{1}$ $a = 5.0900$ (3) Å $b = 5.4159$ (3) Å $c = 10.1413$ (6) Å $\alpha = 97.959$ (2)° $\beta = 90.397$ (2)° $\gamma = 92.271$ (2)° $V = 276.63$ (3) Å³ $Z = 1$ Mo $K\alpha$ radiation $\mu = 0.19$ mm⁻¹ $T = 294$ (2) K

0.10 × 0.10 × 0.06 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1997)
 $T_{\min} = 0.96$, $T_{\max} = 0.99$

2883 measured reflections
1080 independent reflections
995 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.041$ $wR(F^2) = 0.102$ $S = 1.08$

1080 reflections

95 parameters

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^i$	0.83 (3)	2.15 (3)	2.9086 (18)	153 (2)
$\text{N1}-\text{H1}\cdots\text{F3}$	0.83 (3)	2.23 (3)	2.6325 (18)	110 (2)

Symmetry code: (i) $x - 1, y, z$.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2127).

References

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supplementary materials

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***N,N'*-(*p*-Phenylene)bis(2,2,2-trifluoroacetamide)**

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Comment

It has been reported that benzamide derivatives display broad, weak, Stokes-shifted fluorescence in nonpolar solvents at room temperature (Frederick *et al.*, 1999). In this paper, we report the crystal structure of the title compound $C_{10}H_6F_6N_2O_2$ (I) (Fig. 1). Bond lengths and angles are in normal ranges (Allen *et al.*, 1987). Fig. 2 presents a packing view showing the main H bonding interactions in the structure (Table 1): a weak intramolecular N—H···F contact, somehow anchoring the rotation of the C—F₃ group, and a stronger intermolecular N—H···O H-bond, linking molecules into chains along [100]. The O···H distance of 2.15 (3) Å is similar to values reported in related compounds [2.14 (1) Å; Guo *et al.*, 2005].

Experimental

The title compound was synthesized according to the procedure of Guo, *et al.* (2005). Crystals of (I) suitable for X-ray data collection were obtained by slow evaporation of a CH₂Cl₂ and MeOH solution in a ratio of 2:1 at 293 K.

Refinement

H atoms bonded to C atoms were positioned geometrically with C—H = 0.93 Å, The H atom bonded to N was found in a Fourier difference map and freely refined. In all cases, $U_{iso}(H) = 1.2U_{eq}(Host)$.

Figures

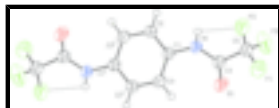


Fig. 1. Molecular view of (I) showing the atom-labelling scheme and, in dashed lines, the intramolecular N—H···F contacts. Displacement ellipsoids are drawn at the 30% probability level. (i): 1 - x, 1 - y, 1 - z.

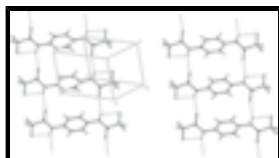


Fig. 2. Packing view of (I). Intermolecular N—H···O and intramolecular N—H···F hydrogen bonds are shown as dashed lines.

***N,N'*-(*p*-Phenylene)bis(2,2,2-trifluoroacetamide)**

Crystal data

$C_{10}H_6F_6N_2O_2$

$M_r = 300.17$

Triclinic, *P*1

Hall symbol: -P1

$Z = 1$

$F_{000} = 150$

$D_x = 1.802 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

supplementary materials

$a = 5.0900 (3) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 5.4159 (3) \text{ \AA}$	Cell parameters from 2167 reflections
$c = 10.1413 (6) \text{ \AA}$	$\theta = 3.8\text{--}28.0^\circ$
$\alpha = 97.959 (2)^\circ$	$\mu = 0.19 \text{ mm}^{-1}$
$\beta = 90.397 (2)^\circ$	$T = 294 (2) \text{ K}$
$\gamma = 92.271 (2)^\circ$	Block, colorless
$V = 276.63 (3) \text{ \AA}^3$	$0.10 \times 0.10 \times 0.06 \text{ mm}$

Data collection

Bruker SMART 4K CCD area-detector diffractometer	1080 independent reflections
Radiation source: fine-focus sealed tube	995 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.038$
$T = 294(2) \text{ K}$	$\theta_{\text{max}} = 26.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1997)	$h = -6 \rightarrow 6$
$T_{\text{min}} = 0.96, T_{\text{max}} = 0.99$	$k = -6 \rightarrow 6$
2883 measured reflections	$l = -11 \rightarrow 12$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.041$	$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.1245P]$
$wR(F^2) = 0.102$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1080 reflections	$\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
95 parameters	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL, $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.30 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.5159 (3)	0.6999 (3)	0.60141 (16)	0.0346 (4)
C2	0.3196 (3)	0.5153 (3)	0.60134 (17)	0.0405 (4)
H2	0.1975	0.5259	0.6695	0.049*
C3	0.3041 (3)	0.3151 (3)	0.50044 (18)	0.0408 (4)
H3	0.1729	0.1909	0.5012	0.049*
C4	0.7350 (3)	1.0283 (3)	0.75876 (17)	0.0392 (4)
C5	0.6875 (3)	1.2389 (3)	0.87289 (18)	0.0431 (5)
F1	0.7988 (3)	1.4501 (2)	0.84711 (14)	0.0733 (5)
F2	0.7916 (3)	1.1896 (3)	0.98453 (13)	0.0782 (5)
F3	0.4361 (2)	1.2787 (3)	0.89411 (14)	0.0732 (5)
N1	0.5199 (3)	0.9037 (3)	0.70675 (14)	0.0381 (4)
O1	0.9608 (2)	0.9925 (3)	0.72602 (15)	0.0606 (5)
H1	0.377 (5)	0.947 (5)	0.738 (2)	0.073*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0267 (7)	0.0358 (8)	0.0391 (9)	0.0026 (6)	-0.0013 (6)	-0.0029 (6)
C2	0.0300 (8)	0.0469 (10)	0.0415 (9)	-0.0034 (7)	0.0076 (7)	-0.0036 (7)
C3	0.0312 (8)	0.0412 (9)	0.0468 (10)	-0.0079 (6)	0.0037 (7)	-0.0030 (7)
C4	0.0291 (8)	0.0420 (9)	0.0434 (9)	0.0004 (6)	0.0008 (7)	-0.0041 (7)
C5	0.0346 (8)	0.0459 (10)	0.0450 (10)	-0.0027 (7)	-0.0002 (7)	-0.0056 (8)
F1	0.0871 (10)	0.0449 (7)	0.0818 (10)	-0.0153 (6)	0.0158 (7)	-0.0088 (6)
F2	0.1004 (11)	0.0829 (10)	0.0477 (7)	0.0171 (8)	-0.0164 (7)	-0.0064 (6)
F3	0.0407 (6)	0.0806 (9)	0.0836 (9)	0.0031 (6)	0.0085 (6)	-0.0410 (7)
N1	0.0254 (7)	0.0405 (8)	0.0443 (8)	0.0005 (6)	0.0032 (6)	-0.0078 (6)
O1	0.0259 (6)	0.0735 (10)	0.0720 (10)	-0.0011 (6)	0.0033 (6)	-0.0256 (8)

Geometric parameters (\AA , $^\circ$)

C1—C3 ⁱ	1.382 (2)	C4—O1	1.214 (2)
C1—C2	1.385 (2)	C4—N1	1.329 (2)
C1—N1	1.425 (2)	C4—C5	1.536 (2)
C2—C3	1.383 (2)	C5—F2	1.312 (2)
C2—H2	0.9300	C5—F1	1.316 (2)
C3—C1 ⁱ	1.382 (2)	C5—F3	1.321 (2)
C3—H3	0.9300	N1—H1	0.83 (3)
C3 ⁱ —C1—C2	119.78 (15)	N1—C4—C5	115.34 (14)
C3 ⁱ —C1—N1	122.26 (14)	F2—C5—F1	107.26 (15)
C2—C1—N1	117.95 (14)	F2—C5—F3	107.70 (16)
C3—C2—C1	120.34 (15)	F1—C5—F3	107.06 (16)

supplementary materials

C3—C2—H2	119.8	F2—C5—C4	110.75 (16)
C1—C2—H2	119.8	F1—C5—C4	110.38 (15)
C1 ⁱ —C3—C2	119.87 (15)	F3—C5—C4	113.43 (14)
C1 ⁱ —C3—H3	120.1	C4—N1—C1	125.29 (14)
C2—C3—H3	120.1	C4—N1—H1	117.4 (18)
O1—C4—N1	127.08 (16)	C1—N1—H1	117.4 (18)
O1—C4—C5	117.58 (15)		
C3 ⁱ —C1—C2—C3	0.5 (3)	O1—C4—C5—F3	174.47 (18)
N1—C1—C2—C3	179.07 (16)	N1—C4—C5—F3	-5.8 (2)
C1—C2—C3—C1 ⁱ	-0.5 (3)	O1—C4—N1—C1	0.4 (3)
O1—C4—C5—F2	-64.3 (2)	C5—C4—N1—C1	-179.27 (15)
N1—C4—C5—F2	115.44 (18)	C3 ⁱ —C1—N1—C4	-33.6 (3)
O1—C4—C5—F1	54.3 (2)	C2—C1—N1—C4	147.82 (18)
N1—C4—C5—F1	-125.92 (17)		

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 ⁱⁱ —O1 ⁱⁱ	0.83 (3)	2.15 (3)	2.9086 (18)	153 (2)
N1—H1 ⁱⁱ —F3	0.83 (3)	2.23 (3)	2.6325 (18)	110 (2)

Symmetry codes: (ii) $x-1, y, z$.

Fig. 1

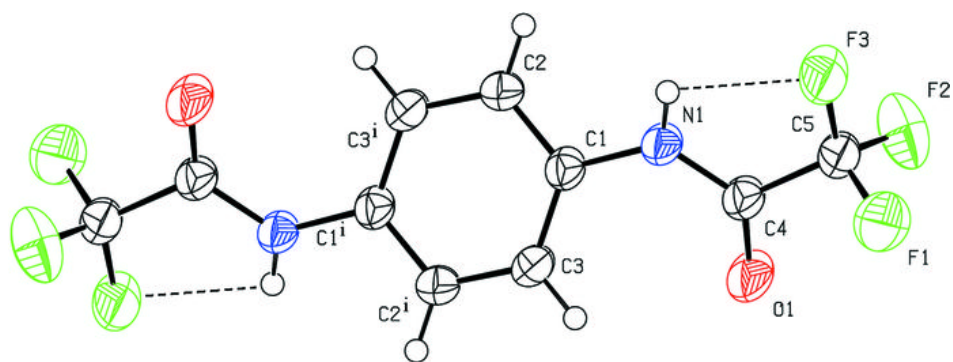


Fig. 2

