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2,2,2-Trifluoro-*N*-(isoquinolin-5-ylmethyl)acetamide

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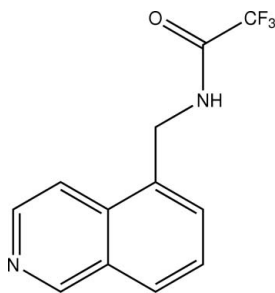
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Key indicators: single-crystal X-ray study; $T = 123$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; disorder in main residue; R factor = 0.051; wR factor = 0.133; data-to-parameter ratio = 10.8.

The molecular structure of the title compound at 123 K, $\text{C}_{12}\text{H}_9\text{F}_3\text{N}_2\text{O}$, presents a rotationally disordered CF_3 group. Hydrogen bonds between the amide NH group and the N atom of the isoquinoline form a chain in the b -axis direction. The packed structure forms alternate layers of isoquinoline and amide groups parallel to the ab plane.

Related literature

In the search for biologically active compounds in the area of anti-inflammatory and pain relief drugs, we have found a class of compounds that act as potent antagonists or agonists of the vanilloid VR1 receptor. These have been shown to be useful in the treatment and prevention of inflammatory and other pain conditions in mammals, see: Jetter *et al.* (2007, 2008); Codd *et al.* (2003). The title compound was prepared as a precursor for more complex compounds. For analysis of the structures of analogous naphthalenes, see: Weinstein & Leiserowitz (1980). For a discussion on disorder in crystal structures, see: Müller (2009).



Experimental

Crystal data

 $\text{C}_{12}\text{H}_9\text{F}_3\text{N}_2\text{O}$ $M_r = 254.21$

Monoclinic, $P2_1/c$
 $a = 7.2308$ (7) Å
 $b = 8.3498$ (11) Å
 $c = 18.157$ (2) Å
 $\beta = 90.583$ (9)°
 $V = 1096.2$ (2) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.14$ mm⁻¹
 $T = 123$ K
 $0.45 \times 0.12 \times 0.02$ mm

Data collection

Oxford Diffraction Xcalibur S diffractometer
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
 $T_{\min} = 0.717$, $T_{\max} = 1.000$

4377 measured reflections
 2071 independent reflections
 1346 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.133$
 $S = 1.06$
 2071 reflections
 191 parameters
 111 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.30$ e Å⁻³
 $\Delta\rho_{\min} = -0.45$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1N}\cdots\text{N2}^i$	0.84 (3)	2.05 (3)	2.847 (3)	158 (3)

Symmetry code: (i) $-x, y - \frac{1}{2}, -z + \frac{3}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2599).

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2,2,2-Trifluoro-*N*-(isoquinolin-5-ylmethyl)acetamide

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Comment

In the search for novel biologically active compounds in the area of anti-inflammatory and pain relief drugs, we have found a class of compounds acting as potent antagonists or agonists of the vanilloid VR1 receptor. These have been shown to be useful in the treatment and prevention of inflammatory and other pain conditions in mammals (Jetter *et al.*, 2007; Jetter *et al.*, 2008; Codd *et al.*, 2003). The title compound was prepared as an important precursor for more complex compounds. Surprisingly, reaction of *n*-hydroxymethyl trifluoroacetamide with isoquinoline in the presence of sulfuric acid afforded a single positional isomer after purification by column chromatography.

The plane of the quinolene ring forms a dihedral angle of 76.2 (2)° with the amide plane, see Fig. 1. Similar conformations were found in a study of similar naphthalene derivatives - though the analogous CF₃ compound had an angle of 89° (Weinstein & Leiserowitz, 1980). The CF₃ group is disordered by rotation about the C—CF₃ bond (Müller, 2009).

A major difference between the naphthalene derivatives and the present compound is seen in the intermolecular contacts. The naphthalenes bond through amide to amide (N—H···O) hydrogen bonds. However, in the quinolene, the presence of a hetero atom enables N—H···N bonds. These form extended chains running along the *b* direction, see Fig. 2.

The packing diagram, Fig. 3, illustrates the layered nature of this structure. Traveling along the *c* direction there are alternate quinolene layers and amide layers. The closest π interaction, connecting molecules along the *a* direction, in the quinolene layer is slightly outside the sum of van der Waals distances (C5···C12 3.486 (4) Å).

Experimental

Isoquinoline (1.29 g, 10 mmol) in concentrated sulfuric acid (50 ml) was cooled to 293 K. *n*-Hydroxymethyl trifluoroacetamide (1.43 g, 10.00 mmol) was added in portions. After 15 min, the reaction mixture was allowed to warm to room temperature and stirred for 16 h. The clear light-brown reaction mixture was then poured onto 200 g of ice, then concentrated ammonium hydroxide was added dropwise until the reaction mixture was basic to pH paper. After extraction with 100 ml of dichloromethane, the organic layer was washed (2 x 100 ml brine), dried over MgSO₄ and then evaporated under reduced pressure. The residue was applied to a silica gel column and eluted with 1:2 ethyl acetate:hexane [*R*_F = 1/5]. This gave the product as a crystalline solid (2.03 g, 80%), m.p. 435 - 438 K. IR (KBr): 1716, 1624, 1563, 1380, 1211, 1141, 1034, 832, 755, 707 cm⁻¹. ¹H NMR (DMSO-*d*₆): 10.08 (1*H*, s), 9.35 (1*H*, d, *J* = 0.8 Hz), 8.57 (1*H*, d, *J* = 6.0 Hz), 8.10 (1*H*, dd, *J* = 6.9 & 1.9 Hz), 7.96 (1*H*, d, *J* = 6.0 Hz), 7.71–7.65 (2*H*, m), 4.85 (2*H*, s) ppm.

Refinement

The F atoms of the CF₃ group are disordered by rotation about the C2—C1 bond. After several trial calculations, a model with three separate groups of F atom positions was adopted. Site occupancy factors are 0.5 for F1 to F3, 0.3 for F4 to F6

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and 0.2 for F7 to F9. Only F1 to F3 were refined anisotropically. Restraints were placed on the C—F distances (1.33 Å) and to encourage similarity in the F atom U_{ij} values (Müller, 2009).

The amide-H atom was found by difference synthesis and refined isotropically. All other H atoms were positioned geometrically at distances of 0.95 and 0.99 Å from the parent C atom for CH and CH₂ groups respectively. For these atoms, a riding model was used with $U_{iso}(H)$ values constrained to be 1.2 times U_{eq} of the parent C atom.

Figures

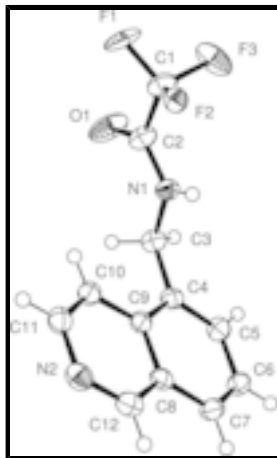


Fig. 1. The molecular structure and atomic labelling, showing 40% probability displacement ellipsoids. H atoms are shown as spheres of arbitrary radius. Minor disorder components are not shown.

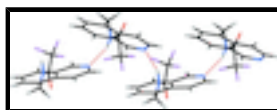


Fig. 2. Part of the hydrogen bonded chains formed along the b direction. O atoms are red, N atoms blue, F atoms pink and C-atoms are black. Hydrogen bonds are shown as dashed lines.

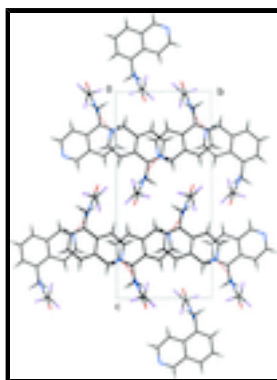


Fig. 3. Packed structure viewed down the *a*-axis.

2,2,2-Trifluoro-*N*-(isoquinolin-5-ylmethyl)acetamide

Crystal data

$C_{12}H_9F_3N_2O$

$M_r = 254.21$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.2308 (7) \text{ \AA}$

$F(000) = 520$

$D_x = 1.540 \text{ Mg m}^{-3}$

Melting point = 435–438 K

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1879 reflections

$b = 8.3498 (11) \text{ \AA}$	$\theta = 2.7\text{--}30.1^\circ$
$c = 18.157 (2) \text{ \AA}$	$\mu = 0.14 \text{ mm}^{-1}$
$\beta = 90.583 (9)^\circ$	$T = 123 \text{ K}$
$V = 1096.2 (2) \text{ \AA}^3$	Blade, colourless
$Z = 4$	$0.45 \times 0.12 \times 0.02 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur S diffractometer	2071 independent reflections
Radiation source: fine-focus sealed tube graphite	1346 reflections with $I > 2\sigma(I)$
Detector resolution: $16.0268 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.031$
ω scans	$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 2.7^\circ$
Absorption correction: multi-scan (<i>Crys.Alis RED</i> ; Oxford Diffraction, 2007)	$h = -8 \rightarrow 8$
$T_{\text{min}} = 0.717$, $T_{\text{max}} = 1.000$	$k = -10 \rightarrow 9$
4377 measured reflections	$l = -21 \rightarrow 22$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.051$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.133$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 0.0571P]$
2071 reflections	where $P = (F_o^2 + 2F_c^2)/3$
191 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
111 restraints	$\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.45 \text{ e \AA}^{-3}$

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 $F^2 > \sigma(F^2)$ is used only for calculating 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.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
F1	-0.3651 (5)	0.3984 (6)	1.0372 (2)	0.0468 (10)	0.50
F2	-0.3741 (5)	0.3253 (6)	0.92452 (18)	0.0266 (10)	0.50
F3	-0.3909 (5)	0.1505 (5)	1.0096 (3)	0.0490 (10)	0.50
F4	-0.3837 (11)	0.2632 (9)	0.9261 (3)	0.042 (2)*	0.30
F5	-0.3858 (10)	0.2219 (12)	1.0445 (4)	0.0590 (19)*	0.30
F6	-0.3263 (9)	0.4512 (6)	1.0002 (4)	0.0530 (17)*	0.30
F7	-0.3639 (12)	0.3146 (15)	1.0568 (3)	0.031 (2)*	0.20
F8	-0.3620 (17)	0.3826 (12)	0.9363 (5)	0.044 (3)*	0.20
F9	-0.3770 (13)	0.1449 (9)	0.9730 (6)	0.043 (2)*	0.20
O1	-0.0083 (3)	0.3065 (3)	1.04575 (11)	0.0574 (7)	
N1	-0.0214 (3)	0.2113 (3)	0.92904 (12)	0.0269 (5)	
N2	0.2036 (3)	0.5534 (3)	0.69021 (12)	0.0323 (6)	
C1	-0.3025 (3)	0.2895 (3)	0.98984 (12)	0.0345 (7)	
C2	-0.0925 (4)	0.2699 (3)	0.99042 (14)	0.0323 (7)	
C3	0.1779 (3)	0.1840 (3)	0.92121 (13)	0.0291 (6)	
H3A	0.2135	0.0859	0.9485	0.035*	
H3B	0.2465	0.2752	0.9431	0.035*	
C4	0.2312 (3)	0.1660 (3)	0.84124 (13)	0.0248 (6)	
C5	0.2834 (3)	0.0198 (3)	0.81357 (14)	0.0285 (6)	
H5	0.2895	-0.0697	0.8458	0.034*	
C6	0.3287 (3)	-0.0013 (4)	0.73828 (13)	0.0297 (6)	
H6	0.3651	-0.1039	0.7211	0.036*	
C7	0.3203 (3)	0.1237 (3)	0.69074 (13)	0.0294 (6)	
H7	0.3497	0.1090	0.6403	0.035*	
C8	0.2672 (3)	0.2763 (3)	0.71693 (13)	0.0249 (6)	
C9	0.2235 (3)	0.2993 (3)	0.79266 (13)	0.0230 (6)	
C10	0.1718 (3)	0.4552 (3)	0.81438 (13)	0.0264 (6)	
H10	0.1419	0.4768	0.8642	0.032*	
C11	0.1651 (3)	0.5738 (3)	0.76334 (14)	0.0305 (6)	
H11	0.1314	0.6780	0.7794	0.037*	
C12	0.2528 (3)	0.4093 (4)	0.66921 (14)	0.0306 (6)	
H12	0.2805	0.3935	0.6187	0.037*	
H1N	-0.089 (4)	0.189 (4)	0.8928 (16)	0.038 (8)*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0389 (18)	0.068 (3)	0.0337 (18)	0.0250 (19)	0.0054 (15)	-0.022 (2)
F2	0.0278 (17)	0.020 (2)	0.0314 (19)	0.0033 (19)	0.0001 (12)	0.0036 (17)
F3	0.0405 (18)	0.048 (2)	0.058 (2)	-0.0050 (16)	0.0009 (18)	0.038 (2)
O1	0.0464 (13)	0.094 (2)	0.0313 (11)	0.0251 (12)	-0.0109 (9)	-0.0248 (12)
N1	0.0266 (11)	0.0317 (14)	0.0223 (11)	0.0007 (10)	0.0021 (9)	-0.0017 (11)
N2	0.0275 (11)	0.0318 (16)	0.0376 (13)	-0.0004 (10)	0.0000 (9)	0.0053 (12)
C1	0.0418 (16)	0.0372 (19)	0.0247 (14)	0.0078 (14)	0.0052 (11)	0.0029 (13)

C2	0.0382 (15)	0.0337 (18)	0.0250 (14)	0.0089 (13)	0.0028 (11)	0.0004 (13)
C3	0.0300 (13)	0.0301 (17)	0.0271 (13)	0.0042 (12)	0.0006 (10)	0.0016 (12)
C4	0.0197 (12)	0.0290 (17)	0.0258 (13)	0.0025 (11)	-0.0001 (9)	-0.0002 (12)
C5	0.0279 (13)	0.0236 (16)	0.0340 (14)	0.0044 (11)	0.0000 (10)	0.0032 (13)
C6	0.0286 (14)	0.0272 (16)	0.0335 (14)	0.0035 (11)	0.0035 (10)	-0.0048 (13)
C7	0.0263 (13)	0.0356 (18)	0.0263 (13)	0.0000 (12)	0.0042 (10)	-0.0055 (13)
C8	0.0203 (12)	0.0283 (15)	0.0262 (13)	-0.0023 (11)	0.0014 (9)	0.0011 (12)
C9	0.0182 (11)	0.0253 (15)	0.0255 (13)	-0.0007 (10)	-0.0007 (9)	-0.0004 (12)
C10	0.0235 (13)	0.0270 (16)	0.0286 (13)	0.0004 (11)	-0.0003 (10)	-0.0024 (12)
C11	0.0246 (13)	0.0273 (17)	0.0396 (15)	0.0002 (11)	0.0001 (10)	-0.0013 (13)
C12	0.0264 (13)	0.0371 (18)	0.0284 (13)	-0.0021 (12)	0.0013 (10)	0.0029 (13)

Geometric parameters (Å, °)

F1—C1	1.334 (3)	C3—H3A	0.9900
F2—C1	1.324 (4)	C3—H3B	0.9900
F3—C1	1.374 (4)	C4—C5	1.374 (4)
F4—C1	1.311 (5)	C4—C9	1.421 (4)
F5—C1	1.295 (5)	C5—C6	1.420 (3)
F6—C1	1.375 (5)	C5—H5	0.9500
F7—C1	1.316 (5)	C6—C7	1.356 (4)
F8—C1	1.314 (5)	C6—H6	0.9500
F9—C1	1.356 (5)	C7—C8	1.414 (4)
O1—C2	1.209 (3)	C7—H7	0.9500
N1—C2	1.326 (3)	C8—C12	1.412 (4)
N1—C3	1.467 (3)	C8—C9	1.427 (3)
N1—H1N	0.84 (3)	C9—C10	1.411 (4)
N2—C12	1.312 (3)	C10—C11	1.357 (4)
N2—C11	1.370 (3)	C10—H10	0.9500
C1—C2	1.527 (4)	C11—H11	0.9500
C3—C4	1.514 (3)	C12—H12	0.9500
C2—N1—C3	121.9 (2)	C4—C3—H3B	109.3
C2—N1—H1N	121 (2)	H3A—C3—H3B	108.0
C3—N1—H1N	117.2 (19)	C5—C4—C9	118.5 (2)
C12—N2—C11	117.0 (2)	C5—C4—C3	120.8 (2)
F5—C1—F4	113.3 (6)	C9—C4—C3	120.6 (2)
F8—C1—F7	118.6 (8)	C4—C5—C6	122.0 (2)
F2—C1—F1	106.9 (3)	C4—C5—H5	119.0
F8—C1—F9	103.5 (7)	C6—C5—H5	119.0
F7—C1—F9	102.3 (7)	C7—C6—C5	120.5 (3)
F2—C1—F3	104.2 (3)	C7—C6—H6	119.7
F1—C1—F3	104.2 (3)	C5—C6—H6	119.7
F5—C1—F6	105.3 (5)	C6—C7—C8	119.4 (2)
F4—C1—F6	103.3 (5)	C6—C7—H7	120.3
F5—C1—C2	114.7 (4)	C8—C7—H7	120.3
F4—C1—C2	115.1 (4)	C12—C8—C7	121.4 (2)
F8—C1—C2	112.7 (6)	C12—C8—C9	118.0 (2)
F7—C1—C2	110.8 (4)	C7—C8—C9	120.6 (2)
F2—C1—C2	114.2 (2)	C10—C9—C4	123.9 (2)

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F1—C1—C2	114.4 (2)	C10—C9—C8	117.1 (2)
F9—C1—C2	107.4 (5)	C4—C9—C8	119.0 (2)
F3—C1—C2	111.9 (3)	C11—C10—C9	119.3 (2)
F6—C1—C2	103.3 (3)	C11—C10—H10	120.3
O1—C2—N1	126.5 (3)	C9—C10—H10	120.3
O1—C2—C1	118.1 (2)	C10—C11—N2	124.4 (3)
N1—C2—C1	115.3 (2)	C10—C11—H11	117.8
N1—C3—C4	111.6 (2)	N2—C11—H11	117.8
N1—C3—H3A	109.3	N2—C12—C8	124.2 (2)
C4—C3—H3A	109.3	N2—C12—H12	117.9
N1—C3—H3B	109.3	C8—C12—H12	117.9
C3—N1—C2—O1	-0.3 (5)	N1—C3—C4—C9	69.5 (3)
C3—N1—C2—C1	-179.4 (2)	C9—C4—C5—C6	-0.3 (4)
F5—C1—C2—O1	-52.4 (6)	C3—C4—C5—C6	178.1 (2)
F4—C1—C2—O1	173.4 (5)	C4—C5—C6—C7	-0.4 (4)
F8—C1—C2—O1	122.9 (6)	C5—C6—C7—C8	0.5 (4)
F7—C1—C2—O1	-12.8 (7)	C6—C7—C8—C12	-178.7 (2)
F2—C1—C2—O1	148.2 (4)	C6—C7—C8—C9	0.3 (3)
F1—C1—C2—O1	24.5 (5)	C5—C4—C9—C10	179.9 (2)
F9—C1—C2—O1	-123.8 (5)	C3—C4—C9—C10	1.5 (4)
F3—C1—C2—O1	-93.7 (4)	C5—C4—C9—C8	1.0 (3)
F6—C1—C2—O1	61.6 (4)	C3—C4—C9—C8	-177.4 (2)
F5—C1—C2—N1	126.8 (6)	C12—C8—C9—C10	-1.0 (3)
F4—C1—C2—N1	-7.4 (5)	C7—C8—C9—C10	-180.0 (2)
F8—C1—C2—N1	-57.9 (7)	C12—C8—C9—C4	178.0 (2)
F7—C1—C2—N1	166.4 (6)	C7—C8—C9—C4	-1.0 (3)
F2—C1—C2—N1	-32.7 (4)	C4—C9—C10—C11	-178.6 (2)
F1—C1—C2—N1	-156.3 (4)	C8—C9—C10—C11	0.3 (3)
F9—C1—C2—N1	55.4 (5)	C9—C10—C11—N2	0.8 (4)
F3—C1—C2—N1	85.5 (4)	C12—N2—C11—C10	-1.1 (3)
F6—C1—C2—N1	-119.2 (4)	C11—N2—C12—C8	0.3 (4)
C2—N1—C3—C4	-162.6 (2)	C7—C8—C12—N2	179.7 (2)
N1—C3—C4—C5	-108.9 (3)	C9—C8—C12—N2	0.8 (4)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1N \cdots N2 ⁱ	0.84 (3)	2.05 (3)	2.847 (3)	158 (3)

Symmetry codes: (i) $-x, y-1/2, -z+3/2$.

Fig. 1

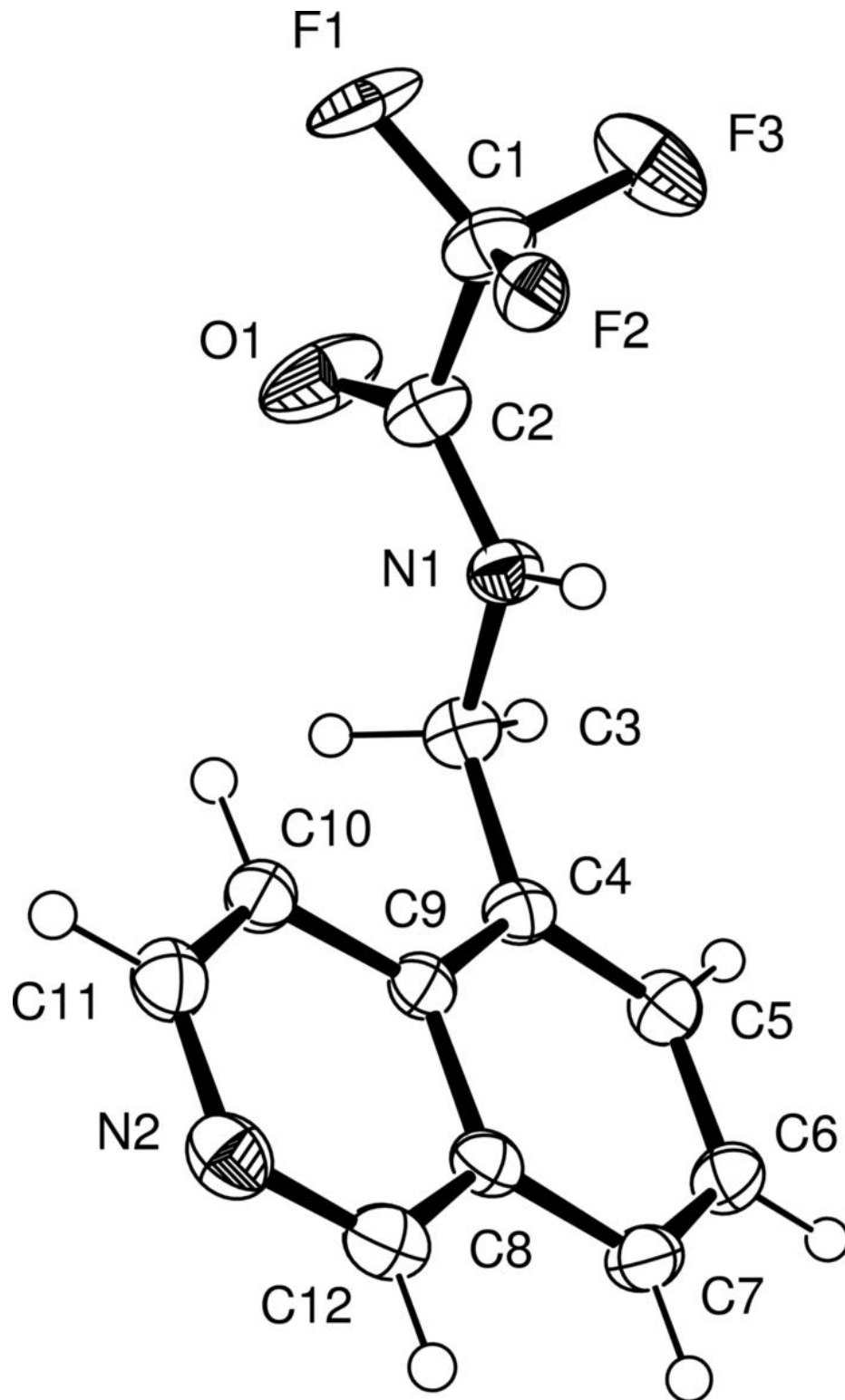


Fig. 2

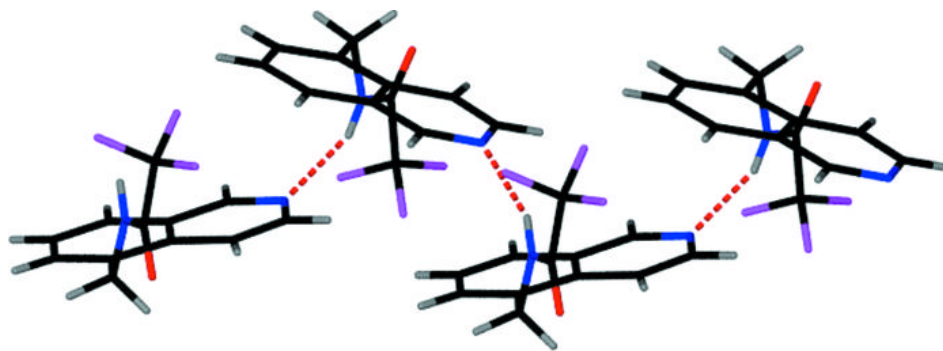


Fig. 3

