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2-[3-(Trifluoromethyl)phenyl]furo[2,3-*c*]-pyridine

Viktor Vrábel,[a]* Ľubomír Švorc,[a] Ivana Bradiaková,[b] Jozef Kožíšek[c] and Alžbeta Krutošíková[b]

[a]Institute of Analytical Chemistry, Faculty of Chemical and Food Technology, Slovak Technical University, Radlinského 9, SK-812 37 Bratislava, Slovak Republic, [b]Department of Chemistry, Faculty of Natural Sciences, University of St. Cyril and Methodius, 917 01 Trnava, Slovak Republic, and [c]Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak Technical University, Radlinského 9, SK-812 37 Bratislava, Slovak Republic
Correspondence e-mail: viktor.vrabel@stuba.sk

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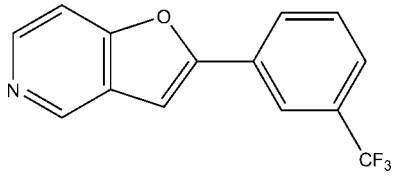
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.065; wR factor = 0.137; data-to-parameter ratio = 13.5.

In the molecular structure of the title compound, $C_{14}H_8F_3NO$, the furopyridine ring system and the benzene ring are almost coplanar, making a dihedral angle of 5.5 (1)°. In the crystal structure, molecules are linked into layers parallel to the *ab* plane by intermolecular C—H···N and C—H···F hydrogen bonds. Weak π–π interactions are observed between the furan and benzene rings [centroid–centroid distance = 3.829 (2) Å] of molecules in adjacent layers, resulting in the formation of a three-dimensional network.

Related literature

For related literature, see: Abadi & Brun (2003); Baran *et al.* (2005); Bravo *et al.* (1994); Jung *et al.* (2002); Kücükgüzel *et al.* (2000); Miklovič *et al.* (2004); Navarrete-Vazquez *et al.* (2006); Vrábel *et al.* (2007*a*,*b*). For preparation, see: Bradiaková *et al.* (2008); Gajdoš *et al.* (2006).



Experimental

Crystal data

$C_{14}H_8F_3NO$
M_r = 263.21
Monoclinic, $P2_1/c$
a = 13.4075 (16) Å
b = 12.1237 (9) Å
c = 7.3008 (10) Å
β = 104.754 (13)°
V = 1147.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 298 (2) K
0.51 × 0.17 × 0.02 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: analytical (Clark & Reid, 1995)
T_{min} = 0.960, T_{max} = 0.997
32658 measured reflections
2335 independent reflections
1185 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.137
S = 1.03
2335 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6A···N4^{i}	0.93	2.47	3.397 (5)	171
C5—H5A···F17^{ii}	0.93	2.56	3.432 (5)	156

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2498).

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supplementary materials

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2-[3-(Trifluoromethyl)phenyl]furo[2,3-*c*]pyridine

V. Vrábel, L. Svorc, I. Bradiaková, J. Kozísek and A. Krutosíková

Comment

In recent years, fluorinated compounds have been very important in the pharmaceutical field. Incorporation of an F atom instead of an H atom can alter the course of the reaction as well as biological activities. Introduction of further F atoms in a CF_3 group provides better lipophilicity and the compounds might be pharmacologically more interesting compared to their non-fluorinated analogues. Many heterocyclic compounds, which bear the trifluoromethyl group, possess a wide range of biological activity (Navarrete-Vazquez *et al.*, 2006), as herbicides (Bravo *et al.*, 1994), fungicides (Jung *et al.*, 2002) and inhibitors for platelet aggregation (Kücükgüzel *et al.*, 2000). 7-(Trifluoromethyl)-quinoline derivatives have been evaluated for *in vitro* activity against some parasites in blood (Abadi & Brun, 2003). Furo[3,2-*c*]pyridine and its derivatives represent isoquinoline isosters, in which the benzene ring is replaced by the furan. The pyridine ring of this system can be readily coordinated to metal centers through N-donor atom. Structural characterization of isothiocyanate nickel(II) complexes with furo[3,2-*c*]pyridine and its 2-methyl, 2,3-dimethyl analogues, and [1]benzofuro[3,2-*c*]pyridine (Bzfupy) have been reported (Miklovič *et al.*, 2004; Baran *et al.*, 2005). We report here the crystal structure of the title compound, which is used as an important starting material for the synthesis of tetra-μ-acetato-bis[(benzofuro[3,2-*c*] pyridine)copper(II)] and bis(1-benzofuro[3,2-*c*]pyridine-κ*N*) dichlorocobalt(II), the structures of which have already been reported (Vrábel *et al.*, 2007*a*,b).

The molecular structure of title compound is shown in Fig. 1. The furo[3,2-*c*]pyridine ring system is essentially planar, with an r.m.s. deviation of 0.007 Å. The dihedral angle between the furo[3,2-*c*]pyridine ring system and the benzene ring is 5.5 (1)°. As can be seen from Fig. 2, the intermolecular C6—H6···N4 and C5—H5···F17 interactions (Table 1) link the molecules into layers parallel to the *ab* plane. Neighboring planes of molecules are connected through additional ring stacking interactions [shortest contact is C10···C15 (x, 1/2 − y, 1/2 + z), 3.370 (6) Å], resulting in a three-dimensional framework structure.

Experimental

2-[3-(Trifluoromethyl)phenyl]furo[3,2-*c*]pyridine was prepared by five step synthesis according to literature procedures of Gajdoš *et al.* (2006) and Bradiaková *et al.* (2008).

Refinement

All H atoms were placed in geometrically calculated positions and allowed to ride on their parent atoms, with C—H distances of 0.93 Å and U_{iso} set at 1.2U_{eq} of the parent atom.

Figures

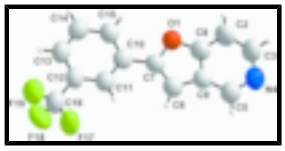

Fig. 1. The molecular structure of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

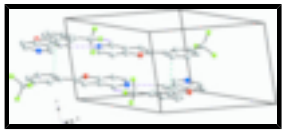

Fig. 2. Part of the crystal packing of the title compound. Dashed lines indicate intermolecular C—H···N and C—H···F hydrogen bonds, and short C···C contacts.

2-[3-(Trifluoromethyl)phenyl]furo[2,3-*c*]pyridine

Crystal data

$C_{14}H_8F_3NO$	F_{000} = 536
M_r = 263.21	D_x = 1.523 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9171 reflections
a = 13.4075 (16) Å	θ = 3.3–29.4°
b = 12.1237 (9) Å	μ = 0.13 mm^{-1}
c = 7.3008 (10) Å	T = 298 (2) K
β = 104.754 (13)°	Needle, colourless
V = 1147.6 (2) Å^3	0.51 × 0.17 × 0.02 mm
Z = 4	

Data collection

Oxford Diffraction Gemini R CCD diffractometer	2335 independent reflections
Radiation source: fine-focus sealed tube	1185 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.058
Detector resolution: 10.4340 pixels mm^{-1}	θ_{max} = 26.4°
T = 298(2) K	θ_{min} = 4.4°
Rotation method data acquisition using ω and φ scans	h = −16→16
Absorption correction: analytical (Clark & Reid, 1995)	k = −15→15
T_{min} = 0.960, T_{max} = 0.997	l = −9→9
32658 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.065	$w = 1/[\sigma^2(F_o^2) + (0.0009P)^2 + 2.196P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.137$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.21$ e Å^{-3}
2335 reflections	$\Delta\rho_{min} = -0.19$ e Å^{-3}
173 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0070 (4)
Secondary atom site location: difference Fourier map	

Special details

Experimental. face-indexed (*CrysAlis RED*; Oxford Diffraction, 2006)

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 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C2	0.6800 (4)	0.6145 (3)	0.1799 (7)	0.0839 (14)
H2A	0.7327	0.6565	0.1537	0.101*
C3	0.5935 (4)	0.6607 (4)	0.2109 (8)	0.0884 (15)
H3A	0.5884	0.7372	0.2030	0.106*
C5	0.5215 (3)	0.4974 (4)	0.2603 (7)	0.0748 (12)
H5A	0.4677	0.4578	0.2881	0.090*
C6	0.6366 (3)	0.3280 (3)	0.2264 (6)	0.0625 (11)
H6A	0.5994	0.2664	0.2463	0.075*
C7	0.7296 (3)	0.3280 (3)	0.1896 (5)	0.0551 (10)
C8	0.6841 (3)	0.5019 (3)	0.1900 (6)	0.0636 (11)
C9	0.6055 (3)	0.4405 (3)	0.2292 (6)	0.0595 (10)
C10	0.8025 (3)	0.2409 (3)	0.1813 (5)	0.0540 (10)
C11	0.7755 (3)	0.1315 (3)	0.2039 (5)	0.0583 (10)
H11A	0.7107	0.1150	0.2205	0.070*
C12	0.8443 (3)	0.0486 (3)	0.2016 (6)	0.0600 (11)
C13	0.9415 (3)	0.0716 (4)	0.1779 (6)	0.0699 (12)
H13A	0.9881	0.0147	0.1790	0.084*
C14	0.9688 (3)	0.1781 (4)	0.1528 (6)	0.0713 (12)
H14A	1.0335	0.1936	0.1345	0.086*
C15	0.8995 (3)	0.2631 (3)	0.1548 (6)	0.0633 (11)
H15A	0.9183	0.3355	0.1383	0.076*
C16	0.8184 (4)	−0.0687 (4)	0.2311 (8)	0.0783 (13)
N4	0.5155 (3)	0.6069 (3)	0.2514 (6)	0.0838 (11)
O1	0.7619 (2)	0.4357 (2)	0.1668 (4)	0.0671 (8)
F17	0.7194 (2)	−0.0846 (2)	0.2133 (6)	0.1261 (14)
F18	0.8665 (3)	−0.1046 (2)	0.4027 (5)	0.1156 (11)

F19	0.8467 (2)	−0.1372 (2)	0.1143 (5)	0.1072 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.086 (3)	0.044 (2)	0.132 (4)	−0.004 (2)	0.045 (3)	−0.002 (3)
C3	0.094 (4)	0.047 (2)	0.133 (5)	0.003 (3)	0.044 (3)	−0.003 (3)
C5	0.067 (3)	0.056 (3)	0.104 (3)	−0.001 (2)	0.027 (3)	−0.001 (3)
C6	0.061 (3)	0.045 (2)	0.081 (3)	−0.0037 (19)	0.018 (2)	0.003 (2)
C7	0.058 (3)	0.041 (2)	0.065 (3)	−0.0053 (18)	0.014 (2)	0.0015 (18)
C8	0.065 (3)	0.045 (2)	0.083 (3)	−0.005 (2)	0.025 (2)	−0.006 (2)
C9	0.059 (2)	0.048 (2)	0.073 (3)	0.002 (2)	0.019 (2)	0.003 (2)
C10	0.051 (2)	0.050 (2)	0.059 (2)	−0.0002 (18)	0.0107 (19)	−0.0034 (18)
C11	0.054 (2)	0.051 (2)	0.070 (3)	0.0008 (19)	0.015 (2)	0.001 (2)
C12	0.056 (2)	0.049 (2)	0.073 (3)	0.0077 (19)	0.013 (2)	0.001 (2)
C13	0.058 (3)	0.063 (3)	0.091 (3)	0.013 (2)	0.023 (2)	0.000 (2)
C14	0.055 (3)	0.071 (3)	0.091 (3)	−0.001 (2)	0.023 (2)	−0.001 (2)
C15	0.060 (3)	0.052 (2)	0.078 (3)	−0.002 (2)	0.019 (2)	0.001 (2)
C16	0.071 (3)	0.061 (3)	0.106 (4)	0.013 (2)	0.029 (3)	0.002 (3)
N4	0.088 (3)	0.052 (2)	0.116 (3)	0.012 (2)	0.034 (2)	0.001 (2)
O1	0.0642 (17)	0.0433 (15)	0.099 (2)	−0.0034 (13)	0.0309 (16)	0.0001 (14)
F17	0.0762 (19)	0.0539 (16)	0.258 (4)	−0.0001 (14)	0.061 (2)	0.012 (2)
F18	0.147 (3)	0.080 (2)	0.120 (3)	0.0169 (19)	0.035 (2)	0.0299 (18)
F19	0.125 (2)	0.0591 (16)	0.148 (3)	0.0073 (16)	0.055 (2)	−0.0197 (17)

Geometric parameters (Å, °)

C2—C3	1.357 (6)	C10—C11	1.395 (5)
C2—C8	1.368 (5)	C10—C15	1.389 (5)
C2—H2A	0.93	C11—C12	1.367 (5)
C3—N4	1.329 (6)	C11—H11A	0.93
C3—H3A	0.93	C12—C13	1.385 (5)
C5—N4	1.331 (5)	C12—C16	1.493 (6)
C5—C9	1.388 (5)	C13—C14	1.366 (6)
C5—H5A	0.93	C13—H13A	0.93
C6—C7	1.341 (5)	C14—C15	1.390 (5)
C6—C9	1.428 (5)	C14—H14A	0.93
C6—H6A	0.93	C15—H15A	0.93
C7—O1	1.399 (4)	C16—F17	1.314 (5)
C7—C10	1.451 (5)	C16—F19	1.313 (5)
C8—O1	1.360 (4)	C16—F18	1.328 (5)
C8—C9	1.378 (5)		
C3—C2—C8	115.3 (4)	C12—C11—C10	120.1 (4)
C3—C2—H2A	122.4	C12—C11—H11A	120.0
C8—C2—H2A	122.4	C10—C11—H11A	120.0
N4—C3—C2	126.1 (4)	C11—C12—C13	120.8 (4)
N4—C3—H3A	117.0	C11—C12—C16	121.1 (4)
C2—C3—H3A	117.0	C13—C12—C16	118.1 (4)

N4—C5—C9	121.9 (4)	C14—C13—C12	120.0 (4)
N4—C5—H5A	119.0	C14—C13—H13A	120.0
C9—C5—H5A	119.0	C12—C13—H13A	120.0
C7—C6—C9	107.0 (3)	C13—C14—C15	119.8 (4)
C7—C6—H6A	126.5	C13—C14—H14A	120.1
C9—C6—H6A	126.5	C15—C14—H14A	120.1
C6—C7—O1	110.8 (3)	C14—C15—C10	120.6 (4)
C6—C7—C10	132.8 (4)	C14—C15—H15A	119.7
O1—C7—C10	116.3 (3)	C10—C15—H15A	119.7
O1—C8—C9	111.0 (3)	F17—C16—F19	107.1 (4)
O1—C8—C2	127.1 (4)	F17—C16—F18	106.3 (4)
C9—C8—C2	121.9 (4)	F19—C16—F18	104.7 (4)
C8—C9—C5	117.4 (4)	F17—C16—C12	113.1 (4)
C8—C9—C6	105.8 (3)	F19—C16—C12	113.1 (4)
C5—C9—C6	136.8 (4)	F18—C16—C12	111.9 (4)
C11—C10—C15	118.7 (4)	C3—N4—C5	117.4 (4)
C11—C10—C7	119.3 (3)	C8—O1—C7	105.4 (3)
C15—C10—C7	122.0 (3)		
C8—C2—C3—N4	0.9 (9)	C10—C11—C12—C16	178.2 (4)
C9—C6—C7—O1	−0.3 (5)	C11—C12—C13—C14	−1.2 (7)
C9—C6—C7—C10	175.4 (4)	C16—C12—C13—C14	−179.2 (4)
C3—C2—C8—O1	−179.3 (4)	C12—C13—C14—C15	1.2 (7)
C3—C2—C8—C9	−0.1 (7)	C13—C14—C15—C10	−0.2 (7)
O1—C8—C9—C5	178.7 (4)	C11—C10—C15—C14	−0.7 (6)
C2—C8—C9—C5	−0.6 (7)	C7—C10—C15—C14	178.1 (4)
O1—C8—C9—C6	−1.1 (5)	C11—C12—C16—F17	15.2 (7)
C2—C8—C9—C6	179.6 (4)	C13—C12—C16—F17	−166.9 (4)
N4—C5—C9—C8	0.6 (7)	C11—C12—C16—F19	137.1 (4)
N4—C5—C9—C6	−179.7 (5)	C13—C12—C16—F19	−45.0 (6)
C7—C6—C9—C8	0.8 (5)	C11—C12—C16—F18	−104.9 (5)
C7—C6—C9—C5	−178.9 (5)	C13—C12—C16—F18	73.1 (5)
C6—C7—C10—C11	4.2 (7)	C2—C3—N4—C5	−1.0 (9)
O1—C7—C10—C11	179.7 (3)	C9—C5—N4—C3	0.2 (7)
C6—C7—C10—C15	−174.6 (4)	C9—C8—O1—C7	0.9 (5)
O1—C7—C10—C15	0.9 (6)	C2—C8—O1—C7	−179.8 (5)
C15—C10—C11—C12	0.6 (6)	C6—C7—O1—C8	−0.4 (4)
C7—C10—C11—C12	−178.2 (4)	C10—C7—O1—C8	−176.8 (3)
C10—C11—C12—C13	0.3 (6)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6A···N4^{i}	0.93	2.47	3.397 (5)	171
C5—H5A···F17^{ii}	0.93	2.56	3.432 (5)	156

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1, *y*+1/2, −*z*+1/2.

Fig. 1

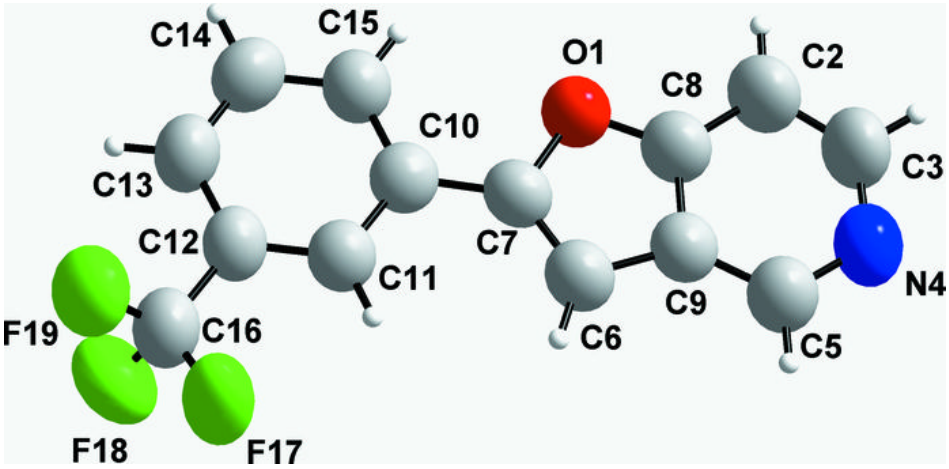

Fig. 2