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Crystal structure of 2-cyano-*N*-(furan-2-ylmethyl)acetamide

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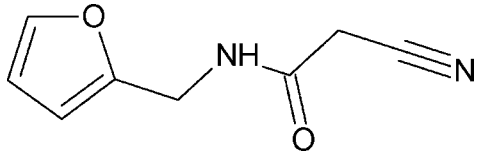
In the title compound, $C_8H_8N_2O_2$, the acetamide unit is inclined to the furan ring by 76.7 (1)°. In the crystal, molecules are linked by N—H···O and C—H···O hydrogen bonds, generating $C(4)$ chains along [100]. The carbonyl O atom is a bifurcated acceptor and an $R_2^1(6)$ ring is formed.

Keywords: crystal structure; furan; acetamide; cyano; bifurcated hydrogen bonding..

CCDC reference: 1404031

1. Related literature

For examples of biological properties of furan derivatives, see: Anupam *et al.* (2011). For the biological activities of some heterocyclic derivatives containing the acetamide moiety, see: Fallah-Tafti *et al.* (2011); Shams *et al.* (2011). For a related acetamide structure, see: Jasinski *et al.* (2013). For the crystal structure of similar compound, 2-cyano-*N*-furfuryl-3-(2-furyl)acrylamide, see: Pomés Hernández *et al.* (1996).



2. Experimental

2.1. Crystal data

$C_8H_8N_2O_2$
M_r = 164.16
Monoclinic, $P2_1/c$
a = 4.8093 (4) Å
b = 14.9495 (16) Å
c = 11.4969 (11) Å
β = 93.482 (3)°
V = 825.06 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.3 × 0.2 × 0.2 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.946, T_{max} = 0.986
7302 measured reflections
1455 independent reflections
1175 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.111
S = 1.09
1455 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	1.99	2.846 (1)	175
C7—H7A···O2^{i}	0.97	2.55	3.395 (2)	145

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS2014/7* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014*/7 (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2014/7* and *PLATON*.

Acknowledgements

We thank Dr Babu Varghese for the XRD data collection at the Sophisticated Analytical Instrument Facility (SAIF), Indian Institute of Technology, Madras.

Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5145).

References

Anupam, V., Pandeya, S. N. & Shweta, S. (2011). *Int. J. Res. Ayurveda Pharm.* **2**, 1110–1116.
Bruker (2004). *APEX2*, *SAINT*, *XPREP* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fallah-Tafti, A., Foroumadi, A., Tiwari, R., Shirazi, A. N., Hangauer, D. G., Bu, Y., Akbarzadeh, T., Parang, K. & Shafiee, A. (2011). *Eur. J. Med. Chem.* **46**, 4853–4858.
Jasinski, J. P., Guild, C. J., Yathirajan, H. S., Narayana, B. & Samshuddin, S. (2013). *Acta Cryst.* E**69**, o461.

Pomés Hernández, R., Duque Rodríguez, J., Novoa de Armas, H. & Toscano, R. A. (1996). *Acta Cryst.* C**52**, 203–205.
Shams, H. Z., Mohareb, R. M., Helal, M. H. & Mahmoud, A. (2011). *Molecules*, **16**, 52–73.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* A**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2015). E**71**, o455–o456 [doi:10.1107/S2056989015010488]

Crystal structure of 2-cyano-*N*-(furan-2-ylmethyl)acetamide

Shivanna Subhadramma, Budanur Papaiah Siddaraju, Chandra Naveen, Janardhanan Saravanan and Dasararaju Gayathri

S1. Structural commentary

Furan derivatives are gaining importance for their wide pharmacological activities like antibacterial, antitumor, anti-inflammatory, antifungal, and analgesic (Anupam *et al.*, 2011). Acetamide derivatives have been shown to possess various biological properties, and recently, the synthesis and biological activities of some heterocyclic derivatives containing the acetamide moiety have been reported (Fallah-Tafti *et al.*, 2011; Shams *et al.*, 2011). In continuation of our work on the synthesis of acetamide derivatives (Jasinski *et al.*, 2013), we report herein on the synthesis and crystal structure of the title compound.

The title molecule, Fig. 1, is Z-shaped. The furan ring (O1/C1—C4) is nearly perpendicular with the mean plane of the acetamide group (O2/N1/C6/C7) with a dihedral angle of 76.7 (1)°. The acetonitrile moiety is inclined to the mean plane of the acetamide group by 54 (6) °. The bond lengths and angles are close to those reported for a very similar structure, 2-cyano-*N*-furfuryl-3-(2-furyl)acrylamide (Pomés Hernández *et al.*, 1996).

The crystal packing is stabilized by N—H···O and C—H···O hydrogen bonds (Table 1 and Fig. 2). Atoms N1 and C7 act as donors to a bifurcated acceptor O-atom, O2, generating C(4) chains along the *a*-axis and, as a consequence, an $R_2^1(6)$ ring is formed.

S2. Synthesis and crystallization

An equimolar mixture of furfuryl amine and ethyl cyano acetate were mixed in a conical flask and the mixture was heated under microwave irradiation at 700 W for 3 min with an interval of 20 seconds each time. The mixture was then poured to a beaker and cooled giving a solid whose size reduced, washed with ethanol. It was recrystallized from an acetone/water mixture (7:3), yielding colourless block-like crystals on slow evaporation of the solvent.

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The NH and C-bound H atoms were included in calculated positions and refined using a riding model: N—H = 0.86 Å, C—H = 0.93 - 0.97 Å with $U_{iso}(H) = 1.2U_{eq}$ (N,C).

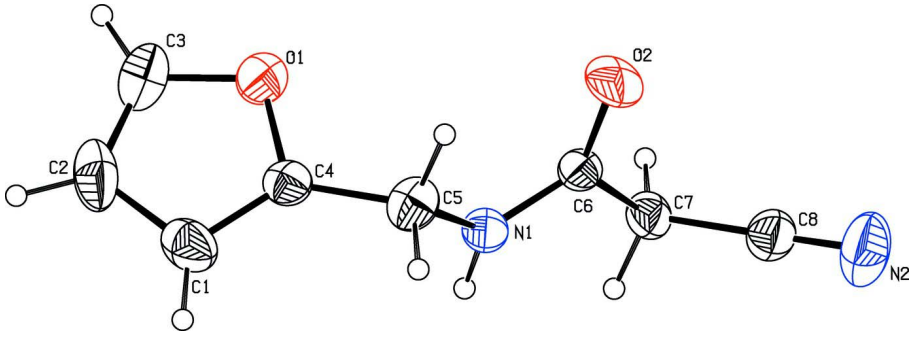


Figure 1

The molecular structure of the title compound, with atom labelling. The displacement ellipsoids are drawn at the 30% probability level.

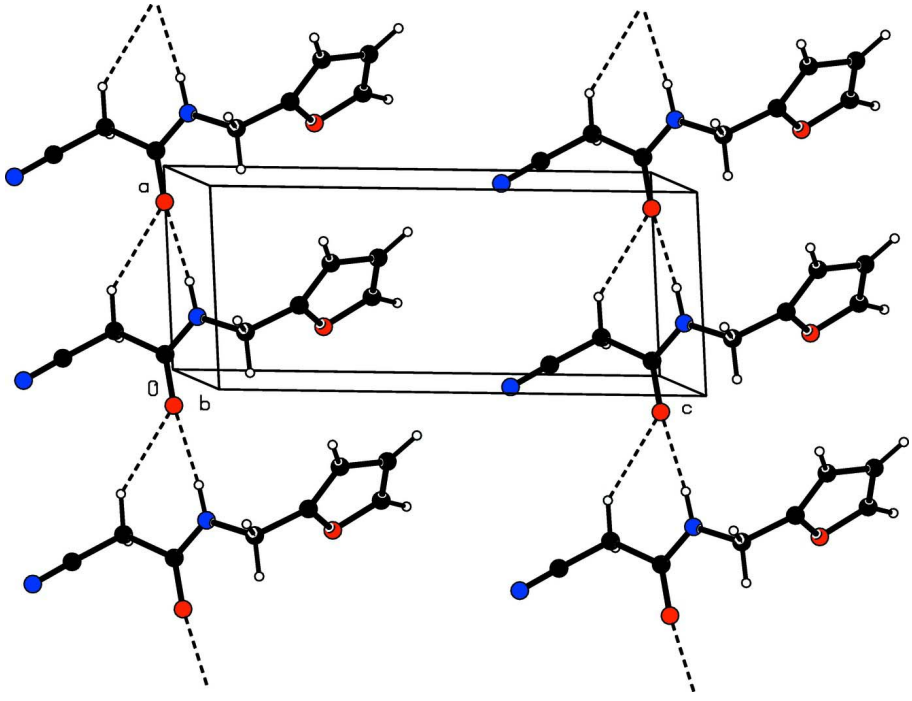


Figure 2

A view along the *b* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1 for details).

2-Cyano-*N*-(furan-2-ylmethyl)acetamide

Crystal data

$C_8H_8N_2O_2$
M_r = 164.16
Monoclinic, $P2_1/c$
a = 4.8093 (4) Å
b = 14.9495 (16) Å
c = 11.4969 (11) Å
β = 93.482 (3)°
V = 825.06 (14) Å^3
Z = 4
$F(000)$ = 344
D_x = 1.322 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1455 reflections
θ = 2.2–25.0°
μ = 0.10 mm^{-1}
T = 293 K
Block, colourless
0.3 × 0.2 × 0.2 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.0216 pixels mm^{-1}
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.946, T_{max} = 0.986

7302 measured reflections
1455 independent reflections
1175 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.0°, θ_{min} = 2.2°
h = −5→5
k = −17→17
l = −12→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.111
S = 1.09
1455 reflections
109 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 0.1342P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6009 (4)	0.71318 (14)	0.26789 (17)	0.0705 (5)
H1A	0.7123	0.7616	0.2502	0.085*
C2	0.6246 (4)	0.65991 (17)	0.37051 (16)	0.0816 (6)
H2	0.7549	0.6667	0.4330	0.098*
C3	0.4271 (5)	0.59926 (15)	0.36003 (17)	0.0777 (6)
H3	0.3942	0.5558	0.4154	0.093*
C4	0.3883 (3)	0.68024 (10)	0.20223 (13)	0.0483 (4)
C5	0.2563 (3)	0.70388 (11)	0.08709 (13)	0.0575 (4)
H5A	0.0559	0.7057	0.0925	0.069*
H5B	0.3170	0.7633	0.0660	0.069*
C6	0.1307 (3)	0.59915 (10)	−0.07049 (12)	0.0443 (4)
C7	0.2372 (3)	0.54182 (11)	−0.16707 (12)	0.0506 (4)
H7A	0.4373	0.5489	−0.1694	0.061*
H7B	0.1983	0.4793	−0.1522	0.061*
C8	0.1019 (4)	0.56845 (11)	−0.27806 (15)	0.0590 (4)
N1	0.3219 (2)	0.64139 (9)	−0.00467 (10)	0.0467 (3)
H1	0.4942	0.6316	−0.0164	0.056*
N2	−0.0079 (5)	0.59089 (12)	−0.36283 (16)	0.0947 (6)
O1	0.2779 (2)	0.60909 (8)	0.25698 (10)	0.0649 (4)
O2	−0.1197 (2)	0.60352 (9)	−0.05760 (11)	0.0713 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0617 (10)	0.0790 (13)	0.0714 (12)	−0.0144 (9)	0.0087 (9)	−0.0277 (10)
C2	0.0772 (13)	0.1118 (17)	0.0535 (11)	0.0191 (13)	−0.0147 (9)	−0.0260 (11)
C3	0.1019 (15)	0.0806 (14)	0.0500 (10)	0.0116 (12)	−0.0012 (10)	−0.0002 (9)
C4	0.0465 (8)	0.0503 (9)	0.0491 (8)	0.0010 (7)	0.0112 (6)	−0.0087 (7)
C5	0.0624 (10)	0.0576 (10)	0.0535 (9)	0.0132 (8)	0.0110 (7)	−0.0042 (7)
C6	0.0312 (7)	0.0565 (9)	0.0455 (8)	0.0070 (6)	0.0038 (6)	0.0080 (7)
C7	0.0404 (7)	0.0614 (10)	0.0497 (9)	0.0038 (7)	0.0004 (6)	−0.0016 (7)
C8	0.0713 (11)	0.0528 (10)	0.0526 (10)	−0.0083 (8)	0.0015 (8)	0.0013 (8)
N1	0.0339 (6)	0.0611 (8)	0.0458 (7)	0.0072 (5)	0.0079 (5)	−0.0030 (6)
N2	0.1407 (18)	0.0789 (12)	0.0611 (10)	−0.0056 (11)	−0.0226 (11)	0.0125 (9)
O1	0.0713 (8)	0.0667 (8)	0.0568 (7)	−0.0098 (6)	0.0037 (6)	0.0023 (6)
O2	0.0304 (6)	0.1024 (10)	0.0816 (9)	0.0076 (6)	0.0088 (5)	−0.0081 (7)

Geometric parameters (Å, º)

C1—C4	1.328 (2)	C5—H5A	0.9700
C1—C2	1.422 (3)	C5—H5B	0.9700
C1—H1A	0.9300	C6—O2	1.2238 (16)
C2—C3	1.314 (3)	C6—N1	1.3162 (18)
C2—H2	0.9300	C6—C7	1.516 (2)
C3—O1	1.355 (2)	C7—C8	1.452 (2)
C3—H3	0.9300	C7—H7A	0.9700
C4—O1	1.3602 (19)	C7—H7B	0.9700
C4—C5	1.476 (2)	C8—N2	1.131 (2)
C5—N1	1.4579 (19)	N1—H1	0.8600
C4—C1—C2	106.51 (18)	C4—C5—H5B	108.9
C4—C1—H1A	126.7	H5A—C5—H5B	107.7
C2—C1—H1A	126.7	O2—C6—N1	124.26 (14)
C3—C2—C1	106.82 (17)	O2—C6—C7	119.83 (13)
C3—C2—H2	126.6	N1—C6—C7	115.90 (12)
C1—C2—H2	126.6	C8—C7—C6	109.59 (13)
C2—C3—O1	110.29 (18)	C8—C7—H7A	109.8
C2—C3—H3	124.9	C6—C7—H7A	109.8
O1—C3—H3	124.9	C8—C7—H7B	109.8
C1—C4—O1	109.60 (15)	C6—C7—H7B	109.8
C1—C4—C5	134.05 (17)	H7A—C7—H7B	108.2
O1—C4—C5	116.34 (13)	N2—C8—C7	178.0 (2)
N1—C5—C4	113.30 (13)	C6—N1—C5	123.31 (12)
N1—C5—H5A	108.9	C6—N1—H1	118.3
C4—C5—H5A	108.9	C5—N1—H1	118.3
N1—C5—H5B	108.9	C3—O1—C4	106.78 (14)
C4—C1—C2—C3	−0.1 (2)	N1—C6—C7—C8	−125.10 (14)
C1—C2—C3—O1	0.5 (2)	O2—C6—N1—C5	−4.5 (2)

C2—C1—C4—O1	−0.39 (19)	C7—C6—N1—C5	175.82 (13)
C2—C1—C4—C5	−179.82 (17)	C4—C5—N1—C6	124.16 (16)
C1—C4—C5—N1	105.9 (2)	C2—C3—O1—C4	−0.7 (2)
O1—C4—C5—N1	−73.48 (17)	C1—C4—O1—C3	0.70 (18)
O2—C6—C7—C8	55.19 (19)	C5—C4—O1—C3	−179.76 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	1.99	2.846 (1)	175
C7—H7*A*···O2^{i}	0.97	2.55	3.395 (2)	145

Symmetry code: (i) *x*+1, *y*, *z*.