Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyl 3-(2-furylmethylidene)carbazate

Yu-Feng Li

Microscale Science Institute, Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China
Correspondence e-mail: liyufeng8111@163.com

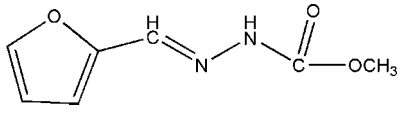
Received 5 December 2010; accepted 6 December 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.072; wR factor = 0.186; data-to-parameter ratio = 17.0.

The asymmetric unit of the title compound, $C_7H_8N_2O_3$, contains two approximately planar molecules (r.m.s. deviations = 0.058 and 0.070 Å). In the crystal, molecules are linked into [010] chains by way of alternating N—H···O and N—H···(N,O) hydrogen-bond linkages.

Related literature

For a related structure, see: Li & Jian (2010).



Experimental

Crystal data

$C_7H_8N_2O_3$
M_r = 168.15
Monoclinic, $C2$
a = 14.668 (5) Å
b = 7.7356 (15) Å
c = 14.720 (3) Å
β = 104.11 (4)°
V = 1619.8 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.25 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
7823 measured reflections
3695 independent reflections
2600 reflections with $I > 2\sigma(I)$
R_{int} = 0.117

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.186
S = 0.89
3695 reflections
217 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O5^{i}	0.86	2.07	2.867 (4)	155
N3—H3A···O2	0.86	2.30	3.085 (4)	152
N3—H3A···N2	0.86	2.53	3.232 (3)	140

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5763).

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, Y. F. & Jian, F.-F. (2010). *Acta Cryst.* E**66**, o1720.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2011). E**67**, o64 [**doi:10.1107/S1600536810051019**]

Methyl 3-(2-furylmethylidene)carbazate

Y.-F. Li

Experimental

A mixture of methyl carbazate (0.1 mol), and furfural (0.1 mol) was stirred in refluxing ethanol (20 mL) for 4 h to afford the title compound (0.085 mol, yield 85%). Colourless blocks of the title compound were obtained by recrystallization from ethanol at room temperature.

Refinement

The absolute structure was indeterminate in the present study. H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H distances = 0.93–0.97 Å; N—H = 0.86Å and with U_{iso}(H) = 1.2U_{eq}(C,*N*) or 1.5U_{eq}(C_{methyl}).

Figures

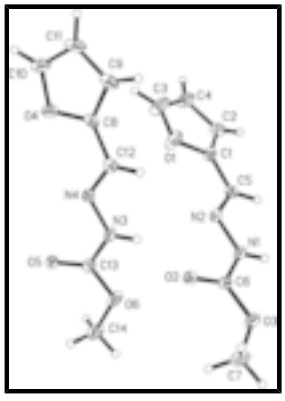


Fig. 1. The structure of the title compound showing 30% probability displacement ellipsoids.

Methyl 3-(2-furylmethylidene)carbazate

Crystal data

$C_7H_8N_2O_3$	F(000) = 704
M_r = 168.15	D_x = 1.379 Mg m^{-3}
Monoclinic, *C*2	Mo *K*α radiation, λ = 0.71073 Å
a = 14.668 (5) Å	Cell parameters from 3695 reflections
b = 7.7356 (15) Å	θ = 3.2–27.5°
c = 14.720 (3) Å	μ = 0.11 mm^{-1}
β = 104.11 (4)°	*T* = 293 K
V = 1619.8 (7) Å^3	Block, colorless
Z = 8	0.25 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer	2600 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.117$
graphite	$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
phi and ω scans	$h = -16\rightarrow18$
7823 measured reflections	$k = -9\rightarrow10$
3695 independent reflections	$l = -19\rightarrow19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.072$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.186$	H-atom parameters constrained
$S = 0.89$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
3695 reflections	$(\Delta/\sigma)_{max} < 0.001$
217 parameters	$\Delta\rho_{max} = 0.37$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.28$ 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.

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O5	0.18498 (16)	0.9708 (3)	0.08083 (14)	0.0286 (5)
N4	0.22925 (19)	0.8558 (3)	0.25908 (17)	0.0242 (5)
N3	0.1797 (2)	0.7585 (3)	0.18594 (17)	0.0281 (6)
H3A	0.1595	0.6572	0.1951	0.034*
O4	0.33569 (18)	1.0262 (3)	0.41175 (15)	0.0358 (6)
O6	0.1200 (2)	0.7115 (3)	0.03597 (15)	0.0397 (7)
C8	0.2972 (2)	0.8690 (4)	0.4211 (2)	0.0276 (7)
C12	0.2438 (2)	0.7836 (4)	0.3391 (2)	0.0260 (7)

H12A	0.2194	0.6741	0.3443	0.031*
C13	0.1635 (2)	0.8259 (4)	0.0994 (2)	0.0261 (7)
C9	0.3199 (3)	0.8194 (5)	0.5124 (2)	0.0376 (9)
H9A	0.3020	0.7180	0.5371	0.045*
C14	0.0973 (4)	0.7748 (5)	−0.0591 (2)	0.0489 (11)
H14A	0.0666	0.6853	−0.1005	0.073*
H14B	0.1539	0.8086	−0.0759	0.073*
H14C	0.0562	0.8728	−0.0640	0.073*
C11	0.3764 (3)	0.9529 (6)	0.5622 (2)	0.0419 (9)
H11A	0.4032	0.9564	0.6263	0.050*
C10	0.3839 (3)	1.0730 (6)	0.4994 (2)	0.0421 (9)
H10A	0.4176	1.1754	0.5137	0.051*
O2	0.04032 (17)	0.4665 (3)	0.19917 (14)	0.0296 (5)
N1	0.1456 (2)	0.2564 (4)	0.18947 (19)	0.0291 (6)
H1A	0.1539	0.1531	0.1715	0.035*
N2	0.22041 (19)	0.3544 (3)	0.23547 (17)	0.0265 (6)
C6	0.0590 (2)	0.3252 (4)	0.1731 (2)	0.0272 (7)
O3	−0.00370 (18)	0.2153 (3)	0.12255 (17)	0.0371 (6)
C5	0.3004 (2)	0.2814 (4)	0.2473 (2)	0.0264 (7)
H5A	0.3037	0.1687	0.2264	0.032*
O1	0.37821 (19)	0.5284 (3)	0.3290 (2)	0.0509 (8)
C1	0.3852 (2)	0.3697 (4)	0.2920 (2)	0.0282 (7)
C2	0.4759 (3)	0.3280 (5)	0.3040 (2)	0.0348 (8)
H2B	0.4995	0.2257	0.2857	0.042*
C7	−0.0995 (3)	0.2726 (6)	0.0996 (3)	0.0501 (10)
H7A	−0.1386	0.1857	0.0629	0.075*
H7B	−0.1046	0.3780	0.0644	0.075*
H7C	−0.1194	0.2924	0.1562	0.075*
C4	0.5291 (3)	0.4693 (6)	0.3499 (3)	0.0463 (10)
H4B	0.5943	0.4781	0.3669	0.056*
C3	0.4682 (3)	0.5862 (6)	0.3638 (3)	0.0587 (13)
H3B	0.4842	0.6924	0.3929	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O5	0.0362 (13)	0.0239 (12)	0.0235 (10)	−0.0029 (10)	0.0033 (9)	−0.0002 (8)
N4	0.0261 (13)	0.0244 (14)	0.0213 (12)	0.0009 (11)	0.0044 (9)	−0.0031 (10)
N3	0.0392 (16)	0.0191 (12)	0.0258 (13)	−0.0054 (11)	0.0074 (11)	−0.0036 (10)
O4	0.0394 (15)	0.0431 (15)	0.0218 (11)	−0.0052 (11)	0.0018 (10)	0.0004 (9)
O6	0.0650 (19)	0.0328 (14)	0.0197 (11)	−0.0137 (12)	0.0070 (11)	−0.0089 (9)
C8	0.0252 (17)	0.033 (2)	0.0244 (15)	0.0089 (13)	0.0056 (12)	0.0049 (12)
C12	0.0236 (15)	0.0287 (17)	0.0274 (15)	0.0047 (12)	0.0093 (12)	0.0010 (12)
C13	0.0276 (16)	0.0272 (17)	0.0249 (15)	−0.0004 (13)	0.0090 (12)	−0.0056 (12)
C9	0.040 (2)	0.049 (2)	0.0234 (16)	0.0136 (17)	0.0078 (14)	0.0077 (14)
C14	0.078 (3)	0.046 (2)	0.0189 (16)	−0.018 (2)	0.0044 (17)	−0.0067 (15)
C11	0.038 (2)	0.064 (3)	0.0198 (15)	0.0132 (18)	0.0010 (14)	−0.0020 (16)
C10	0.044 (2)	0.052 (2)	0.0260 (17)	−0.0013 (18)	0.0013 (15)	−0.0107 (16)

O2	0.0335 (12)	0.0265 (12)	0.0247 (11)	0.0025 (10)	−0.0006 (9)	−0.0045 (9)
N1	0.0292 (15)	0.0200 (13)	0.0360 (14)	−0.0038 (11)	0.0039 (11)	−0.0066 (10)
N2	0.0294 (15)	0.0209 (13)	0.0273 (13)	−0.0028 (11)	0.0035 (10)	−0.0039 (10)
C6	0.0319 (18)	0.0264 (16)	0.0206 (14)	−0.0028 (13)	0.0015 (12)	−0.0025 (12)
O3	0.0319 (14)	0.0315 (14)	0.0434 (14)	−0.0036 (10)	0.0006 (11)	−0.0118 (10)
C5	0.0294 (17)	0.0275 (16)	0.0223 (14)	0.0021 (12)	0.0062 (12)	−0.0001 (11)
O1	0.0242 (14)	0.0374 (15)	0.088 (2)	−0.0019 (11)	0.0086 (13)	−0.0304 (14)
C1	0.0311 (18)	0.0256 (17)	0.0284 (16)	0.0014 (13)	0.0082 (13)	−0.0049 (12)
C2	0.0346 (19)	0.0350 (18)	0.0327 (17)	0.0130 (15)	0.0043 (14)	−0.0072 (14)
C7	0.033 (2)	0.051 (2)	0.058 (2)	−0.0012 (18)	−0.0055 (17)	−0.016 (2)
C4	0.0242 (19)	0.055 (2)	0.055 (2)	0.0022 (17)	0.0021 (16)	−0.023 (2)
C3	0.025 (2)	0.054 (3)	0.093 (3)	−0.0031 (18)	0.006 (2)	−0.035 (2)

Geometric parameters (Å, °)

O5—C13	1.214 (4)	O2—C6	1.211 (4)
N4—C12	1.273 (4)	N1—C6	1.344 (4)
N4—N3	1.368 (3)	N1—N2	1.369 (4)
N3—C13	1.343 (4)	N1—H1A	0.8600
N3—H3A	0.8600	N2—C5	1.275 (4)
O4—C10	1.360 (4)	C6—O3	1.338 (4)
O4—C8	1.361 (4)	O3—C7	1.432 (5)
O6—C13	1.331 (4)	C5—C1	1.431 (4)
O6—C14	1.442 (4)	C5—H5A	0.9300
C8—C9	1.359 (4)	O1—C1	1.357 (4)
C8—C12	1.430 (4)	O1—C3	1.370 (5)
C12—H12A	0.9300	C1—C2	1.339 (5)
C9—C11	1.412 (6)	C2—C4	1.414 (6)
C9—H9A	0.9300	C2—H2B	0.9300
C14—H14A	0.9600	C7—H7A	0.9600
C14—H14B	0.9600	C7—H7B	0.9600
C14—H14C	0.9600	C7—H7C	0.9600
C11—C10	1.334 (6)	C4—C3	1.321 (6)
C11—H11A	0.9300	C4—H4B	0.9300
C10—H10A	0.9300	C3—H3B	0.9300
C12—N4—N3	115.1 (3)	C6—N1—N2	118.5 (3)
C13—N3—N4	118.1 (3)	C6—N1—H1A	120.7
C13—N3—H3A	121.0	N2—N1—H1A	120.7
N4—N3—H3A	121.0	C5—N2—N1	115.0 (3)
C10—O4—C8	105.9 (3)	O2—C6—O3	124.8 (3)
C13—O6—C14	114.4 (3)	O2—C6—N1	125.3 (3)
C9—C8—O4	110.1 (3)	O3—C6—N1	109.9 (3)
C9—C8—C12	131.0 (3)	C6—O3—C7	115.9 (3)
O4—C8—C12	118.9 (3)	N2—C5—C1	121.2 (3)
N4—C12—C8	120.8 (3)	N2—C5—H5A	119.4
N4—C12—H12A	119.6	C1—C5—H5A	119.4
C8—C12—H12A	119.6	C1—O1—C3	106.6 (3)
O5—C13—O6	124.2 (3)	C2—C1—O1	109.6 (3)
O5—C13—N3	125.2 (3)	C2—C1—C5	132.1 (3)

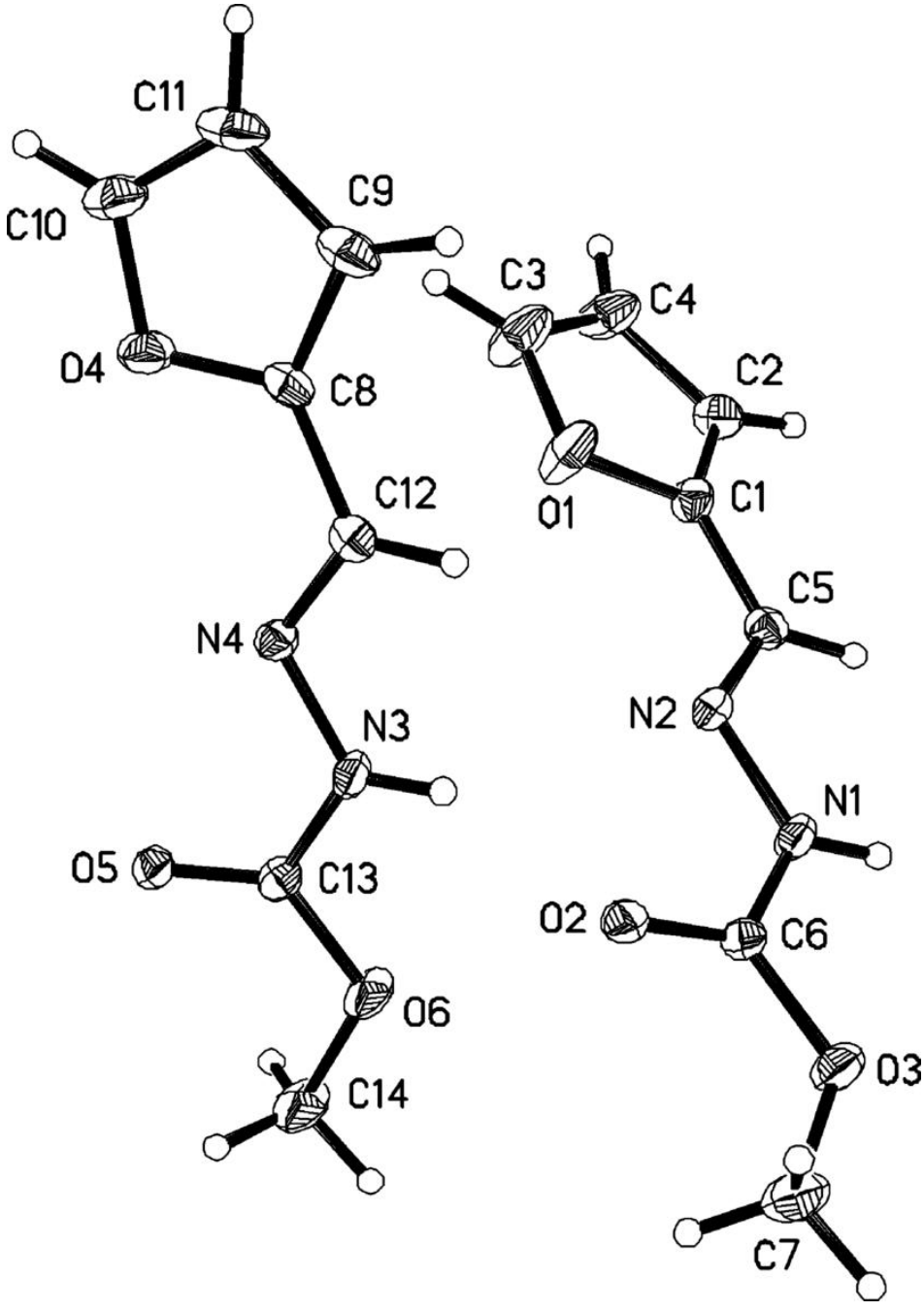
O6—C13—N3	110.6 (3)	O1—C1—C5	118.4 (3)
C8—C9—C11	106.2 (3)	C1—C2—C4	106.9 (3)
C8—C9—H9A	126.9	C1—C2—H2B	126.5
C11—C9—H9A	126.9	C4—C2—H2B	126.5
O6—C14—H14A	109.5	O3—C7—H7A	109.5
O6—C14—H14B	109.5	O3—C7—H7B	109.5
H14A—C14—H14B	109.5	H7A—C7—H7B	109.5
O6—C14—H14C	109.5	O3—C7—H7C	109.5
H14A—C14—H14C	109.5	H7A—C7—H7C	109.5
H14B—C14—H14C	109.5	H7B—C7—H7C	109.5
C10—C11—C9	106.6 (3)	C3—C4—C2	106.8 (3)
C10—C11—H11A	126.7	C3—C4—H4B	126.6
C9—C11—H11A	126.7	C2—C4—H4B	126.6
C11—C10—O4	111.1 (4)	C4—C3—O1	110.2 (4)
C11—C10—H10A	124.4	C4—C3—H3B	124.9
O4—C10—H10A	124.4	O1—C3—H3B	124.9

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O5^{i}	0.86	2.07	2.867 (4)	155
N3—H3A···O2	0.86	2.30	3.085 (4)	152
N3—H3A···N2	0.86	2.53	3.232 (3)	140

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1


C11
C10
C9
O4
C8
C12
N4
N3
O5
C13
O6
C14
C3
C4
C2
O1
C1
C5
N2
N1
O2
C6
O3
C7