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N′-[(5-Methyl-2-furyl)methylene]thiophene-2-carbohydrazide

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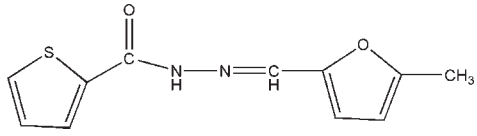
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.087; data-to-parameter ratio = 17.9.

In the title compound, $C_{11}H_{10}N_2O_2S$, the dihedral angle between the five-membered aromatic rings is 10.24 (12)°. In the crystal structure, molecules are linked by bifurcated N—H···(O,N) hydrogen bonds, generating [001] chains.

Related literature

For related structures, see: Jiang (2010*a*,*b*).



Experimental

Crystal data

$C_{11}H_{10}N_2O_2S$
M_r = 234.27
Tetragonal, $P4_3$
a = 8.8037 (12) Å
c = 14.670 (3) Å
V = 1137.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.19 mm

Data collection

Bruker SMART CCD diffractometer
10087 measured reflections
2597 independent reflections
2073 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.087
S = 0.96
2597 reflections
145 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: Flack (1983), 1241 Friedel pairs
Flack parameter: −0.11 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.86	2.30	3.064 (2)	149
N2—H2A···N1^{i}	0.86	2.51	3.218 (2)	140

Symmetry code: (i) $y, -x+1, z+\frac{1}{4}$.

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: HB5367).

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Jiang, J.-H. (2010*a*). Acta Cryst. E66, o922.
Jiang, J.-H. (2010*b*). Acta Cryst. E66, o923.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2010). E**66**, o924 [doi:10.1107/S1600536810010810]

N′-[(5-Methyl-2-furyl)methylene]thiophene-2-carbohydrazide

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S1. Comment

As part of our ongoing studies of Schiff bases (Jiang, 2010a,b), we have synthesized the title compound (I), and describe its structure here, which occurs in the unusual enantiomorphous space group of $P4_3$.

The molcular structure of (I) is shown in Fig. 1. In the crystal, the molecules are linked by bifurcated N—H···(O,N) hydrogen bonds (Table 1).

S2. Experimental

A mixture of thiophene-2-carbohydrazide (0.05 mol) and 5-methylfuran-2-carbaldehyde (0.05 mol) was stirred in refluxing ethanol (10 ml) for 4 h to afford the title compound (0.082 mol, yield 82%). Colourless blocks of (I) were obtained by recrystallization from ethanol at room temperature.

S3. Refinement

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}).

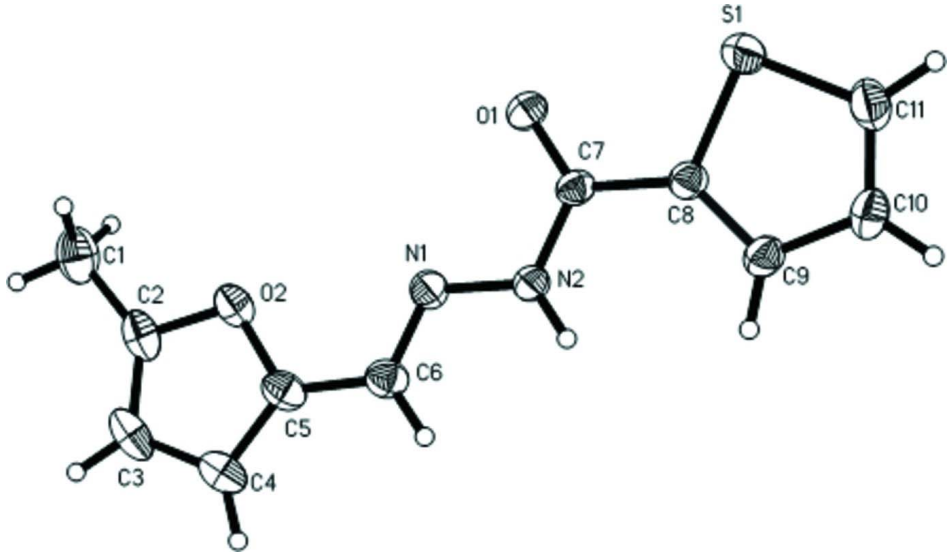

Figure 1

The molecular structure of (I) showing 30% probability displacement ellipsoids.

N′-[(5-Methyl-2-furyl)methylene]thiophene-2-carbohydrazide

Crystal data

$C_{11}H_{10}N_2O_2S$
$M_r = 234.27$
Tetragonal, $P4_3$
Hall symbol: P 4cw
$a = 8.8037$ (12) Å
$c = 14.670$ (3) Å
$V = 1137.0$ (3) Å^3
$Z = 4$
$F(000) = 488$
$D_x = 1.369$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2073 reflections
$\theta = 3.3$–27.5°
$\mu = 0.27$ mm^{-1}
$T = 293$ K
Block, colorless
0.25 × 0.20 × 0.19 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
10087 measured reflections
2597 independent reflections
2073 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.087$
$S = 0.96$
2597 reflections
145 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Absolute structure: Flack (1983), 1241 Friedel pairs
Absolute structure parameter: −0.11 (8)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
S1	0.12336 (7)	0.93062 (7)	0.06580 (4)	0.06358 (19)
N1	0.44476 (18)	0.45913 (18)	0.09498 (10)	0.0431 (4)
O2	0.51869 (17)	0.17921 (15)	0.03236 (10)	0.0504 (4)
N2	0.40630 (18)	0.59910 (17)	0.12954 (10)	0.0428 (4)

H2A	0.4438	0.6313	0.1801	0.051*
C7	0.3074 (2)	0.6842 (2)	0.08110 (12)	0.0403 (4)
O1	0.25704 (18)	0.64188 (17)	0.00679 (10)	0.0630 (4)
C8	0.2645 (2)	0.8314 (2)	0.12060 (13)	0.0407 (4)
C5	0.5748 (2)	0.2280 (2)	0.11433 (13)	0.0482 (5)
C6	0.5305 (2)	0.3756 (2)	0.14463 (14)	0.0477 (5)
H6A	0.5641	0.4113	0.2008	0.057*
C9	0.3203 (2)	0.9110 (2)	0.19201 (13)	0.0477 (4)
H9A	0.3977	0.8758	0.2296	0.057*
C11	0.1410 (3)	1.0764 (2)	0.14106 (17)	0.0620 (6)
H11A	0.0817	1.1638	0.1392	0.074*
C4	0.6643 (3)	0.1185 (3)	0.15086 (18)	0.0607 (6)
H4A	0.7162	0.1232	0.2060	0.073*
C2	0.5746 (2)	0.0350 (2)	0.01820 (16)	0.0545 (5)
C3	0.6633 (3)	−0.0049 (3)	0.08834 (18)	0.0658 (7)
H3A	0.7148	−0.0965	0.0950	0.079*
C10	0.2494 (3)	1.0520 (2)	0.20326 (15)	0.0561 (5)
H10A	0.2747	1.1209	0.2488	0.067*
C1	0.5204 (3)	−0.0399 (3)	−0.06593 (18)	0.0742 (7)
H1B	0.5641	−0.1396	−0.0703	0.111*
H1C	0.5501	0.0192	−0.1179	0.111*
H1D	0.4117	−0.0481	−0.0642	0.111*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0735 (4)	0.0617 (3)	0.0555 (3)	0.0211 (3)	−0.0203 (3)	−0.0078 (3)
N1	0.0509 (9)	0.0432 (9)	0.0352 (8)	0.0052 (7)	0.0015 (6)	−0.0014 (6)
O2	0.0607 (9)	0.0452 (8)	0.0451 (8)	0.0124 (6)	0.0076 (6)	0.0052 (6)
N2	0.0528 (9)	0.0439 (8)	0.0316 (8)	0.0086 (6)	−0.0065 (7)	−0.0071 (6)
C7	0.0423 (10)	0.0458 (10)	0.0328 (10)	0.0000 (7)	−0.0028 (7)	−0.0029 (7)
O1	0.0864 (11)	0.0568 (9)	0.0458 (8)	0.0139 (8)	−0.0277 (8)	−0.0164 (7)
C8	0.0430 (10)	0.0447 (10)	0.0344 (9)	0.0018 (8)	−0.0003 (7)	−0.0019 (8)
C5	0.0488 (11)	0.0557 (12)	0.0401 (11)	0.0075 (9)	0.0064 (8)	0.0099 (9)
C6	0.0494 (11)	0.0554 (12)	0.0384 (10)	0.0056 (9)	0.0010 (8)	0.0014 (8)
C9	0.0505 (11)	0.0524 (11)	0.0402 (10)	0.0018 (9)	−0.0021 (8)	−0.0080 (8)
C11	0.0805 (16)	0.0496 (13)	0.0559 (14)	0.0165 (11)	0.0038 (12)	−0.0033 (10)
C4	0.0579 (13)	0.0622 (14)	0.0622 (14)	0.0138 (10)	−0.0010 (11)	0.0177 (11)
C2	0.0635 (13)	0.0409 (11)	0.0591 (14)	0.0078 (9)	0.0238 (11)	0.0076 (9)
C3	0.0685 (14)	0.0488 (13)	0.0800 (18)	0.0203 (11)	0.0183 (12)	0.0207 (12)
C10	0.0690 (14)	0.0488 (12)	0.0506 (13)	−0.0005 (10)	0.0065 (11)	−0.0127 (9)
C1	0.0939 (19)	0.0570 (14)	0.0716 (18)	0.0044 (13)	0.0229 (14)	−0.0038 (12)

Geometric parameters (Å, º)

S1—C11	1.700 (2)	C9—C10	1.399 (3)
S1—C8	1.7187 (19)	C9—H9A	0.9300
N1—C6	1.281 (3)	C11—C10	1.338 (3)

N1—N2	1.375 (2)	C11—H11A	0.9300
O2—C5	1.369 (2)	C4—C3	1.422 (4)
O2—C2	1.377 (2)	C4—H4A	0.9300
N2—C7	1.350 (2)	C2—C3	1.339 (3)
N2—H2A	0.8600	C2—C1	1.479 (3)
C7—O1	1.234 (2)	C3—H3A	0.9300
C7—C8	1.469 (2)	C10—H10A	0.9300
C8—C9	1.353 (3)	C1—H1B	0.9600
C5—C4	1.356 (3)	C1—H1C	0.9600
C5—C6	1.428 (3)	C1—H1D	0.9600
C6—H6A	0.9300		

C11—S1—C8	90.80 (11)	C10—C11—S1	112.76 (17)
C6—N1—N2	116.74 (16)	C10—C11—H11A	123.6
C5—O2—C2	107.03 (16)	S1—C11—H11A	123.6
C7—N2—N1	117.51 (15)	C5—C4—C3	106.5 (2)
C7—N2—H2A	121.2	C5—C4—H4A	126.7
N1—N2—H2A	121.2	C3—C4—H4A	126.7
O1—C7—N2	121.93 (17)	C3—C2—O2	109.6 (2)
O1—C7—C8	121.47 (16)	C3—C2—C1	135.5 (2)
N2—C7—C8	116.59 (15)	O2—C2—C1	114.9 (2)
C9—C8—C7	132.01 (18)	C2—C3—C4	107.37 (19)
C9—C8—S1	111.17 (15)	C2—C3—H3A	126.3
C7—C8—S1	116.74 (13)	C4—C3—H3A	126.3
C4—C5—O2	109.5 (2)	C11—C10—C9	112.36 (19)
C4—C5—C6	133.1 (2)	C11—C10—H10A	123.8
O2—C5—C6	117.43 (17)	C9—C10—H10A	123.8
N1—C6—C5	120.43 (19)	C2—C1—H1B	109.5
N1—C6—H6A	119.8	C2—C1—H1C	109.5
C5—C6—H6A	119.8	H1B—C1—H1C	109.5
C8—C9—C10	112.89 (19)	C2—C1—H1D	109.5
C8—C9—H9A	123.6	H1B—C1—H1D	109.5
C10—C9—H9A	123.6	H1C—C1—H1D	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.86	2.30	3.064 (2)	149
N2—H2*A*···N1^{i}	0.86	2.51	3.218 (2)	140

Symmetry code: (i) $y, -x+1, z+1/4$.