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(*E*)-*N*′-(4-Methoxybenzylidene)thiophene-2-carbohydrazide

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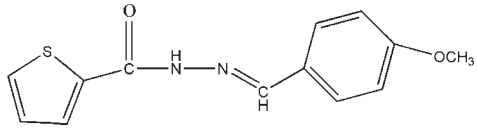
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.056; wR factor = 0.177; data-to-parameter ratio = 17.2.

In the title compound, $C_{13}H_{12}N_2O_2S$, the dihedral angle between the aromatic rings is 15.20 (11)°. In the crystal, inversion dimers linked by pairs of N—H···O hydrogen bonds generate $R_2^2(8)$ loops.

Related literature

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



Experimental

Crystal data

$C_{13}H_{12}N_2O_2S$
M_r = 260.31
Monoclinic, $P2_1/c$
a = 16.106 (3) Å
b = 5.3292 (11) Å
c = 14.812 (3) Å
β = 104.91 (3)°
V = 1228.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 293 K
0.25 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
11253 measured reflections
2807 independent reflections
2454 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.177
S = 1.00
2807 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.86	2.12	2.963 (2)	167

Symmetry code: (i) $-x, -y+2, -z+2$.

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: HB5449).

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS, Inc., Madison, Wisconsin, USA.
Li, Y.-F. & Jian, F.-F. (2010). Acta Cryst. E**66**, o1398.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2010). E**66**, o1400 [https://doi.org/10.1107/S1600536810017836]

(*E*)-*N*′-(4-Methoxybenzylidene)thiophene-2-carbohydrazide

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S1. Experimental

A mixture of thiophene-2-carbohydrazide (0.10 mol), and 4-methoxybenzaldehyde (0.10 mol) was stirred in refluxing ethanol (10 ml) for 4 h to afford the title compound (0.079 mol, yield 79%). Colourless blocks of (I) were obtained by recrystallization from ethanol at room temperature.

S2. 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}).

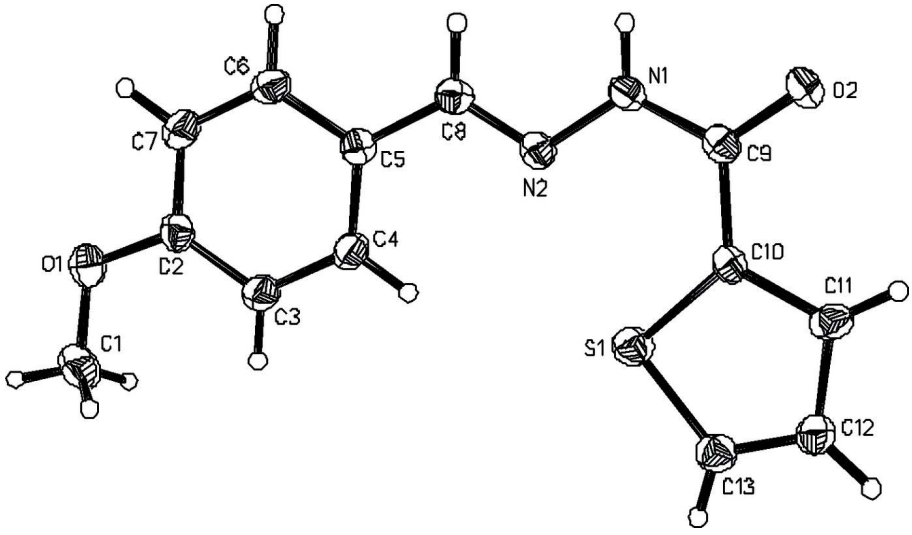

Figure 1

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

(*E*)-*N*′-(4-Methoxybenzylidene)thiophene-2-carbohydrazide

Crystal data

$C_{13}H_{12}N_2O_2S$
M_r = 260.31
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 16.106 (3) Å
b = 5.3292 (11) Å
c = 14.812 (3) Å
β = 104.91 (3)°
V = 1228.5 (4) Å^3
Z = 4
F(000) = 544
D_x = 1.407 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2454 reflections
θ = 2.7–25.3°
μ = 0.26 mm^{-1}

T = 293 K
Block, colorless

0.25 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
11253 measured reflections
2807 independent reflections

2454 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −20→20
k = −6→6
l = −19→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.177
S = 1.00
2807 reflections
163 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.1142P)^2 + 0.7797P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
S1	0.19516 (4)	0.31168 (11)	0.98996 (4)	0.0456 (2)
N2	0.17079 (11)	0.7123 (3)	1.09840 (12)	0.0364 (4)
N1	0.09320 (10)	0.7857 (3)	1.04270 (12)	0.0372 (4)
H1A	0.0643	0.9002	1.0620	0.045*
O2	−0.00677 (9)	0.7645 (3)	0.90675 (11)	0.0437 (4)
C9	0.06111 (12)	0.6815 (4)	0.95773 (14)	0.0347 (4)
C8	0.19896 (13)	0.8393 (4)	1.17289 (15)	0.0381 (4)
H8A	0.1659	0.9700	1.1865	0.046*
C5	0.28237 (13)	0.7838 (4)	1.23759 (14)	0.0366 (4)
O1	0.52295 (11)	0.6947 (4)	1.42184 (13)	0.0608 (5)
C11	0.07350 (14)	0.3690 (4)	0.83349 (18)	0.0449 (5)
H11A	0.0269	0.4297	0.7878	0.054*
C10	0.10555 (11)	0.4692 (4)	0.92598 (13)	0.0344 (4)
C2	0.44404 (14)	0.7112 (4)	1.35954 (15)	0.0428 (5)
C3	0.41450 (15)	0.5483 (5)	1.28526 (16)	0.0480 (5)

H3A	0.4485	0.4149	1.2758	0.058*
C6	0.31271 (15)	0.9418 (5)	1.31370 (16)	0.0473 (5)
H6A	0.2785	1.0739	1.3239	0.057*
C7	0.39260 (16)	0.9065 (5)	1.37430 (17)	0.0520 (6)
H7A	0.4118	1.0136	1.4249	0.062*
C4	0.33415 (15)	0.5854 (4)	1.22531 (16)	0.0454 (5)
H4A	0.3144	0.4752	1.1757	0.054*
C13	0.19081 (14)	0.1074 (4)	0.90128 (16)	0.0447 (5)
H13A	0.2289	−0.0259	0.9053	0.054*
C12	0.12683 (14)	0.1562 (5)	0.82410 (17)	0.0457 (5)
H12A	0.1178	0.0615	0.7697	0.055*
C1	0.57849 (17)	0.5001 (7)	1.4092 (2)	0.0675 (8)
H1B	0.6315	0.5105	1.4569	0.101*
H1C	0.5898	0.5168	1.3489	0.101*
H1D	0.5518	0.3407	1.4131	0.101*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0484 (4)	0.0437 (4)	0.0437 (3)	0.0088 (2)	0.0098 (2)	0.0038 (2)
N2	0.0340 (8)	0.0363 (9)	0.0375 (9)	0.0022 (6)	0.0069 (7)	0.0034 (7)
N1	0.0319 (8)	0.0382 (9)	0.0407 (9)	0.0047 (6)	0.0079 (7)	0.0012 (7)
O2	0.0310 (7)	0.0480 (9)	0.0477 (9)	0.0055 (6)	0.0019 (6)	0.0001 (7)
C9	0.0301 (9)	0.0343 (10)	0.0404 (10)	−0.0017 (7)	0.0103 (7)	0.0048 (7)
C8	0.0390 (10)	0.0389 (10)	0.0375 (10)	0.0040 (8)	0.0122 (8)	0.0011 (8)
C5	0.0389 (10)	0.0369 (10)	0.0343 (10)	0.0005 (8)	0.0099 (8)	0.0016 (7)
O1	0.0453 (9)	0.0744 (13)	0.0518 (10)	0.0062 (8)	−0.0072 (7)	−0.0129 (9)
C11	0.0408 (11)	0.0411 (11)	0.0596 (13)	−0.0091 (9)	0.0253 (10)	−0.0152 (10)
C10	0.0287 (8)	0.0361 (10)	0.0380 (9)	−0.0016 (7)	0.0079 (7)	0.0030 (8)
C2	0.0385 (10)	0.0487 (12)	0.0376 (10)	−0.0005 (9)	0.0033 (8)	−0.0016 (9)
C3	0.0462 (12)	0.0447 (12)	0.0479 (12)	0.0092 (9)	0.0030 (9)	−0.0065 (10)
C6	0.0508 (12)	0.0478 (12)	0.0417 (11)	0.0087 (10)	0.0091 (9)	−0.0097 (9)
C7	0.0542 (13)	0.0543 (14)	0.0423 (11)	0.0024 (11)	0.0029 (10)	−0.0153 (10)
C4	0.0477 (11)	0.0401 (11)	0.0422 (11)	0.0043 (9)	0.0005 (9)	−0.0084 (9)
C13	0.0442 (11)	0.0382 (11)	0.0525 (12)	0.0007 (9)	0.0142 (9)	−0.0021 (9)
C12	0.0386 (11)	0.0480 (12)	0.0505 (12)	−0.0069 (9)	0.0116 (9)	−0.0118 (10)
C1	0.0423 (13)	0.086 (2)	0.0669 (17)	0.0125 (13)	0.0002 (11)	−0.0018 (15)

Geometric parameters (Å, º)

S1—C13	1.694 (2)	C11—H11A	0.9300
S1—C10	1.727 (2)	C2—C7	1.382 (3)
N2—C8	1.274 (3)	C2—C3	1.386 (3)
N2—N1	1.366 (2)	C3—C4	1.382 (3)
N1—C9	1.351 (3)	C3—H3A	0.9300
N1—H1A	0.8600	C6—C7	1.379 (3)
O2—C9	1.239 (2)	C6—H6A	0.9300
C9—C10	1.479 (3)	C7—H7A	0.9300

C8—C5	1.466 (3)	C4—H4A	0.9300
C8—H8A	0.9300	C13—C12	1.353 (3)
C5—C4	1.387 (3)	C13—H13A	0.9300
C5—C6	1.391 (3)	C12—H12A	0.9300
O1—C2	1.368 (3)	C1—H1B	0.9600
O1—C1	1.413 (3)	C1—H1C	0.9600
C11—C10	1.437 (3)	C1—H1D	0.9600
C11—C12	1.451 (3)		

C13—S1—C10	91.43 (11)	C4—C3—C2	119.6 (2)
C8—N2—N1	115.96 (18)	C4—C3—H3A	120.2
C9—N1—N2	121.10 (17)	C2—C3—H3A	120.2
C9—N1—H1A	119.4	C7—C6—C5	121.3 (2)
N2—N1—H1A	119.4	C7—C6—H6A	119.4
O2—C9—N1	119.15 (19)	C5—C6—H6A	119.4
O2—C9—C10	120.17 (19)	C6—C7—C2	119.8 (2)
N1—C9—C10	120.68 (17)	C6—C7—H7A	120.1
N2—C8—C5	121.42 (19)	C2—C7—H7A	120.1
N2—C8—H8A	119.3	C3—C4—C5	121.3 (2)
C5—C8—H8A	119.3	C3—C4—H4A	119.3
C4—C5—C6	118.0 (2)	C5—C4—H4A	119.3
C4—C5—C8	123.29 (19)	C12—C13—S1	113.72 (18)
C6—C5—C8	118.65 (19)	C12—C13—H13A	123.1
C2—O1—C1	117.9 (2)	S1—C13—H13A	123.1
C10—C11—C12	107.8 (2)	C13—C12—C11	114.2 (2)
C10—C11—H11A	126.1	C13—C12—H12A	122.9
C12—C11—H11A	126.1	C11—C12—H12A	122.9
C11—C10—C9	120.20 (18)	O1—C1—H1B	109.5
C11—C10—S1	112.76 (16)	O1—C1—H1C	109.5
C9—C10—S1	127.02 (15)	H1B—C1—H1C	109.5
O1—C2—C7	115.6 (2)	O1—C1—H1D	109.5
O1—C2—C3	124.4 (2)	H1B—C1—H1D	109.5
C7—C2—C3	120.0 (2)	H1C—C1—H1D	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2^{i}	0.86	2.12	2.963 (2)	167

Symmetry code: (i) −*x*, −*y*+2, −*z*+2.