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(*E*)-3-Dimethylamino-1-(2-thienyl)prop-2-en-1-one

Jian-Hong Bi

Deparment of Chemistry and Chemical Engineering, Hefei Teachers College, Hefei 230061, People's Republic of China
Correspondence e-mail: bi010101@126.com

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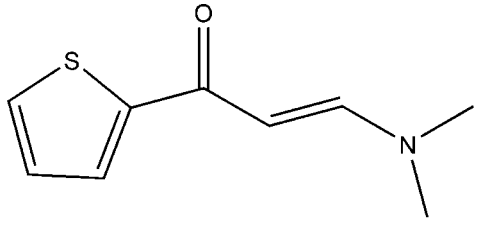
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.124; data-to-parameter ratio = 14.7.

The molecular skeleton of the title molecule, $C_9H_{11}NOS$, is essentially planar: the thiophene ring is inclined to the mean plane of the rest non-H atoms by 2.92 (3)°. The crystal packing exhibits no significantly short intermolecular contacts.

Related literature

For general backgroud, see Amari *et al.* (1993). For the crystal structures of related compounds, see: Li *et al.* (2005); Hu *et al.* (2007); Bi (2009).



Experimental

Crystal data

$C_9H_{11}NOS$
M_r = 181.26
Monoclinic, $P2_1/n$
a = 5.9618 (12) Å
b = 8.1241 (16) Å
c = 19.449 (4) Å
β = 92.910 (3)°
V = 940.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 291 K
0.45 × 0.30 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.867, T_{max} = 0.964
4740 measured reflections
1636 independent reflections
1137 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.124
S = 1.05
1636 reflections
111 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2582).

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supporting information

Acta Cryst. (2009). E**65**, o1847 [doi:10.1107/S1600536809025331]

(*E*)-3-Dimethylamino-1-(2-thienyl)prop-2-en-1-one

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S1. Comment

Many coordinated complexes derived from 2-[3-(dimethylamino)prop-2-enoyl] pyridine or thiophene have been reported recently in chemical research (Amari *et al.*, 1993; Bi, 2009; Hu & Tian, 2007; Li *et al.*, 2005). In continuation of our ongoing program directed to the development of similar compounds (Bi, 2009), herein we report the molecular structure of the title compound (I) - the newly synthesized ligand derived from 2-acetylthiophene.

In (I) (Fig. 1), the dihedral angle between the thiophene ring and the mean plane of the restnon-hydrogen atoms is 2.92 (3)°. The crystal packing exhibits no significantly short intermolecular contacts.

S2. Experimental

All solvents and chemicals were of analytical grade and were used without further purification. A solution of 2-acetyl-thiophene (0.2 mmol) and dimethoxy-*N*,*N*-dimethylmethanamine(0.2 mmol) in 150 ml DMF was refluxed for 8 h, and then concentrated to give the title compound. Single crystals suitable for X-ray analysis were grown from the methanol solution by slow evaporation at room temperature in air. Anal. Calcd.for $C_9H_{11}NOS$: C, 59.64; H, 6.12; N, 7.73. Found: C, 39.65; H,6.16; N, 7.71.

S3. Refinement

All hydrogen atoms were geometrically positioned (C—H 0.93–0.97 Å) and refined as riding, with U_{iso}(H)=1.2–1.5 U_{eq} of the parent atom.

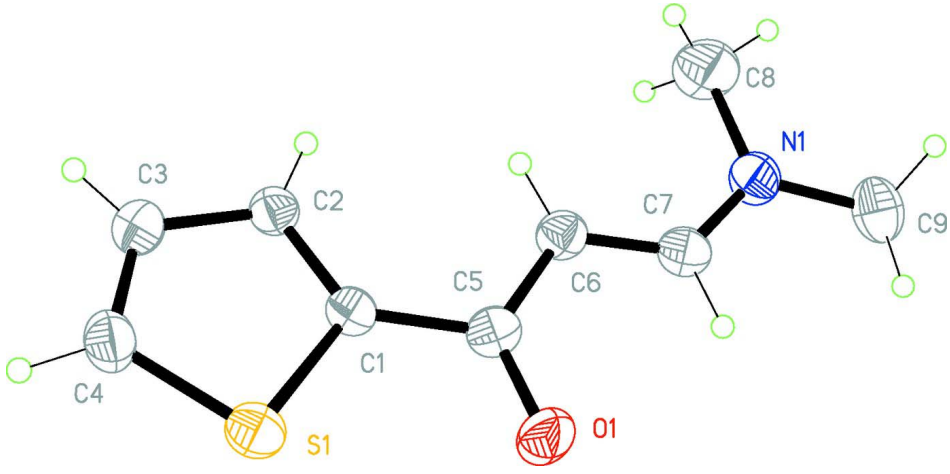

Figure 1

Molecular structure of (I) showing the atomic numbering and 30% probabilty displacement ellipsoids.

(*E*)-3-Dimethylamino-1-(2-thienyl)prop-2-en-1-one

Crystal data

$C_9H_{11}NOS$
$M_r = 181.26$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 5.9618\ (12)$ Å
$b = 8.1241\ (16)$ Å
$c = 19.449\ (4)$ Å
$\beta = 92.910\ (3)°$
$V = 940.8\ (3)$ Å^3
$Z = 4$
$F(000) = 384$
$D_x = 1.280$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 955 reflections
$\theta = 2.7–20.2°$
$\mu = 0.30$ mm^{-1}
$T = 291$ K
Block, yellow
0.45 × 0.30 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.867$, $T_{max} = 0.964$
4740 measured reflections
1636 independent reflections
1137 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -7\rightarrow6$
$k = -9\rightarrow8$
$l = -23\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.124$
$S = 1.05$
1636 reflections
111 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
$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.2232P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

Experimental. The structure was solved by direct methods (Bruker, 2000) and successive difference Fourier syntheses.
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}
C1	0.0234 (4)	0.4667 (3)	0.16370 (13)	0.0425 (6)
C2	0.2349 (4)	0.5260 (3)	0.18109 (14)	0.0462 (7)
H2	0.3586	0.5108	0.1545	0.055*

C3	0.2416 (5)	0.6127 (3)	0.24415 (16)	0.0581 (8)
H3	0.3707	0.6620	0.2635	0.070*
C4	0.0404 (5)	0.6165 (4)	0.27337 (15)	0.0594 (8)
H4	0.0155	0.6685	0.3149	0.071*
C5	−0.0592 (4)	0.3689 (3)	0.10366 (14)	0.0479 (7)
C6	0.0996 (4)	0.3228 (3)	0.05454 (14)	0.0481 (7)
H6	0.2501	0.3510	0.0618	0.058*
C7	0.0307 (4)	0.2381 (3)	−0.00247 (14)	0.0499 (7)
H7	−0.1220	0.2142	−0.0066	0.060*
C8	0.3912 (5)	0.2183 (5)	−0.05347 (19)	0.0906 (12)
H8A	0.4146	0.3350	−0.0566	0.136*
H8B	0.4532	0.1650	−0.0922	0.136*
H8C	0.4638	0.1775	−0.0117	0.136*
C9	0.0524 (6)	0.0980 (4)	−0.11220 (15)	0.0691 (9)
H9A	−0.1052	0.0830	−0.1064	0.104*
H9B	0.1233	−0.0074	−0.1162	0.104*
H9C	0.0732	0.1611	−0.1531	0.104*
N1	0.1517 (4)	0.1844 (3)	−0.05331 (12)	0.0566 (6)
O1	−0.2623 (3)	0.3317 (3)	0.09894 (10)	0.0688 (6)
S1	−0.15994 (12)	0.51590 (10)	0.22552 (4)	0.0598 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0437 (14)	0.0414 (15)	0.0427 (15)	0.0011 (11)	0.0066 (12)	0.0028 (12)
C2	0.0414 (14)	0.0467 (16)	0.0509 (17)	−0.0023 (11)	0.0057 (12)	−0.0032 (13)
C3	0.0515 (16)	0.0588 (19)	0.0636 (19)	−0.0033 (14)	−0.0019 (14)	−0.0104 (16)
C4	0.0681 (19)	0.0601 (19)	0.0499 (18)	0.0025 (15)	0.0019 (15)	−0.0097 (15)
C5	0.0451 (15)	0.0498 (17)	0.0489 (17)	−0.0032 (12)	0.0040 (13)	0.0067 (14)
C6	0.0435 (14)	0.0520 (17)	0.0492 (17)	−0.0036 (12)	0.0065 (13)	0.0014 (14)
C7	0.0480 (16)	0.0532 (17)	0.0492 (17)	0.0003 (12)	0.0093 (14)	0.0046 (14)
C8	0.062 (2)	0.128 (3)	0.084 (3)	−0.002 (2)	0.0275 (19)	−0.016 (2)
C9	0.091 (2)	0.064 (2)	0.0531 (19)	−0.0050 (18)	0.0129 (17)	−0.0053 (17)
N1	0.0547 (14)	0.0666 (16)	0.0494 (14)	−0.0018 (12)	0.0109 (11)	−0.0068 (13)
O1	0.0444 (11)	0.0969 (16)	0.0658 (14)	−0.0154 (10)	0.0100 (10)	−0.0200 (12)
S1	0.0495 (5)	0.0741 (6)	0.0571 (5)	−0.0014 (4)	0.0145 (4)	−0.0052 (4)

Geometric parameters (Å, º)

C1—C2	1.376 (3)	C6—H6	0.9300
C1—C5	1.476 (4)	C7—N1	1.327 (3)
C1—S1	1.713 (2)	C7—H7	0.9300
C2—C3	1.413 (4)	C8—N1	1.455 (4)
C2—H2	0.9300	C8—H8A	0.9600
C3—C4	1.353 (4)	C8—H8B	0.9600
C3—H3	0.9300	C8—H8C	0.9600
C4—S1	1.688 (3)	C9—N1	1.444 (4)
C4—H4	0.9300	C9—H9A	0.9600

C5—O1	1.247 (3)	C9—H9B	0.9600
C5—C6	1.429 (3)	C9—H9C	0.9600
C6—C7	1.351 (4)		
C2—C1—C5	130.4 (2)	N1—C7—H7	115.7
C2—C1—S1	110.8 (2)	C6—C7—H7	115.7
C5—C1—S1	118.81 (18)	N1—C8—H8A	109.5
C1—C2—C3	111.9 (2)	N1—C8—H8B	109.5
C1—C2—H2	124.0	H8A—C8—H8B	109.5
C3—C2—H2	124.0	N1—C8—H8C	109.5
C4—C3—C2	112.9 (3)	H8A—C8—H8C	109.5
C4—C3—H3	123.5	H8B—C8—H8C	109.5
C2—C3—H3	123.5	N1—C9—H9A	109.5
C3—C4—S1	112.0 (2)	N1—C9—H9B	109.5
C3—C4—H4	124.0	H9A—C9—H9B	109.5
S1—C4—H4	124.0	N1—C9—H9C	109.5
O1—C5—C6	124.1 (3)	H9A—C9—H9C	109.5
O1—C5—C1	118.2 (2)	H9B—C9—H9C	109.5
C6—C5—C1	117.7 (2)	C7—N1—C9	122.3 (2)
C7—C6—C5	119.9 (2)	C7—N1—C8	120.7 (3)
C7—C6—H6	120.1	C9—N1—C8	116.9 (2)
C5—C6—H6	120.1	C4—S1—C1	92.36 (13)
N1—C7—C6	128.7 (3)		