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

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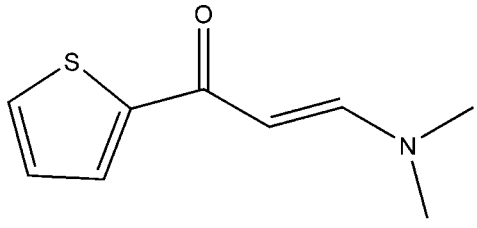
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.124; data-to-parameter ratio = 14.7.

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).

References

Amari, C., Ianelli, S., Pelizzi, C., Pelizzi, G. & Predieri, G. (1993). *Inorg. Chim. Acta*, **211**, 89–94.
Bi, J.-H. (2009). *Acta Cryst.* E**65**, m633.
Bruker (2000). *SADABS*, *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hu, T.-L. & Tian, J.-L. (2007). *Acta Cryst.* E**63**, m1092–m1093.
Li, G.-X., Li, J.-Q. & Kang, X.-Z. (2005). *Acta Cryst.* E**61**, m410–m411.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

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

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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.

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.

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.

Figures

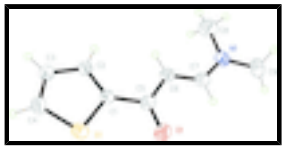

Fig. 1. Molecular structure of (I) showing the atomic numbering and 30% probabilty displacement ellipsoids.

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

Crystal data

$C_9H_{11}NOS$	F_{000} = 384
M_r = 181.26	D_x = 1.280 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 955 reflections

a = 5.9618 (12) Å	θ = 2.7–20.2º
b = 8.1241 (16) Å	μ = 0.30 mm^{-1}
c = 19.449 (4) Å	T = 291 K
β = 92.910 (3)º	Block, yellow
V = 940.8 (3) Å^3	0.45 × 0.30 × 0.15 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	1636 independent reflections
Radiation source: fine-focus sealed tube	1137 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 291 K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −7→6
T_{min} = 0.867, T_{max} = 0.964	k = −9→8
4740 measured reflections	l = −23→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.124	$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.2232P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
1636 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
111 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (Å^2)

	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, °)

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)		

Fig. 1