Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Bis[1-(thiophen-2-yl)ethylidene]-ethane-1,2-diamine

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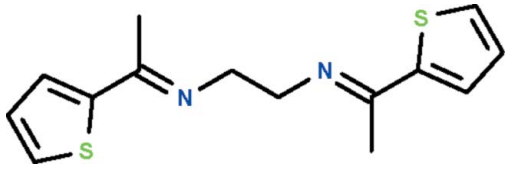
Received 17 August 2011; accepted 18 August 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.090; data-to-parameter ratio = 18.0.

Molecules of the title compound, $C_{14}H_{16}N_2S_2$, have a centre of inversion in the middle of the $–CH_2–CH_2–$ bond; the $(C_4H_3S)(CH_3)C{=}N–CH_2–$ moiety is almost planar (r.m.s. deviation for non-H atoms 0.027 Å).

Related literature

For a related transition metal adduct, see: Modder *et al.* (1995).



Experimental

Crystal data

$C_{14}H_{16}N_2S_2$
M_r = 276.41
Monoclinic, $P2_1/n$
a = 5.5831 (3) Å
b = 9.3939 (4) Å
c = 12.9202 (5) Å
β = 95.342 (4)°
V = 674.68 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 100 K
0.25 × 0.20 × 0.15 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.912, T_{max} = 0.946
3036 measured reflections
1495 independent reflections
1244 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 1.04
1495 reflections
83 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5618).

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supporting information

Acta Cryst. (2011). E**67**, o2465 [doi:10.1107/S1600536811033691]

N,*N*′-Bis[1-(thiophen-2-yl)ethylidene]ethane-1,2-diamine

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S1. Comment

A large number of transition metal adducts of Schiff bases derived by condensing ethylenediamine with a ketone have been reported; in these adducts, the ligand typically functions in a chelating mode. However, there are few studies on the title Schiff base (Scheme I), and only one crystal structure study has been reported (Modder *et al.*, 1995). The $C_{14}H_{16}N_2S_2$ molecule lies on a center-of-inversion (Fig. 1); the $(C_4H_3S)(CH_3)C{=}N–CH_2–$ moiety is planar, and the chain connecting the two aromatic rings adopts an extended zigzag conformation [C=N–C–C 88.1 (2)°].

S2. Experimental

Ethylenediamine (0.6 g, 10 mmol) and 2-acetylthiophene (0.7 g, 10 mmol) in dry benzene (50 ml) were refluxed in a Dean–Stark apparatus until no more water was collected (in about 2 h). The solvent was removed and the solid that separated was collected and recystallized from ethanol.

S3. Refinement

H-atoms were placed in calculated positions [C—H 0.95–0.98 Å, U_{iso}(H) = 1.2–1.5U_{eq}(C)] and were included in the refinement in the riding model approximation.

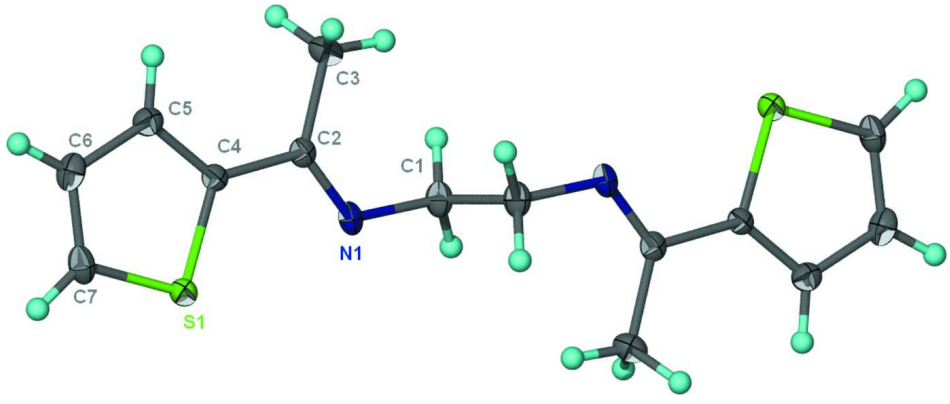

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{14}H_{16}N_2S_2$ at the 70% probability level; H atoms are drawn as spheres of arbitrary radius. The molecule lies on a center-of-inversion.

N,*N*′-Bis[1-(thiophen-2-yl)ethylidene]ethane-1,2-diamine

Crystal data

$C_{14}H_{16}N_2S_2$
$M_r = 276.41$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 5.5831$ (3) Å
$b = 9.3939$ (4) Å
$c = 12.9202$ (5) Å
$\beta = 95.342$ (4)°
$V = 674.68$ (5) Å^3
$Z = 2$
$F(000) = 292$
$D_x = 1.361$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1562 reflections
$\theta = 2.7$–$29.1°$
$\mu = 0.38$ mm^{-1}
$T = 100$ K
Prism, colourless
0.25 × 0.20 × 0.15 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min} = 0.912$, $T_{max} = 0.946$
3036 measured reflections
1495 independent reflections
1244 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.7°$
$h = -5 \rightarrow 7$
$k = -12 \rightarrow 9$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.090$
$S = 1.04$
1495 reflections
83 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
$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 0.5515P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.66665 (8)	0.89024 (5)	0.29153 (3)	0.01547 (15)
N1	0.5827 (3)	0.68042 (16)	0.45253 (11)	0.0141 (3)
C1	0.5756 (4)	0.56063 (19)	0.52477 (14)	0.0163 (4)
H1A	0.5065	0.5926	0.5887	0.020*
H1B	0.7412	0.5264	0.5446	0.020*
C2	0.4204 (3)	0.77676 (19)	0.44907 (13)	0.0122 (4)
C3	0.2062 (3)	0.7852 (2)	0.51239 (14)	0.0168 (4)
H3A	0.0574	0.7795	0.4659	0.025*
H3B	0.2102	0.8756	0.5503	0.025*
H3C	0.2120	0.7060	0.5619	0.025*
C4	0.4397 (3)	0.89283 (18)	0.37376 (13)	0.0113 (4)
C5	0.2995 (3)	1.0123 (2)	0.35677 (14)	0.0144 (4)
H5	0.1648	1.0330	0.3940	0.017*

C6	0.3775 (3)	1.1021 (2)	0.27724 (14)	0.0163 (4)
H6	0.3017	1.1893	0.2561	0.020*
C7	0.5731 (4)	1.0482 (2)	0.23535 (13)	0.0171 (4)
H7	0.6491	1.0930	0.1812	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0182 (3)	0.0134 (3)	0.0156 (2)	0.00002 (19)	0.00604 (18)	0.00080 (18)
N1	0.0170 (8)	0.0116 (7)	0.0135 (7)	−0.0028 (7)	0.0004 (6)	0.0025 (6)
C1	0.0195 (10)	0.0134 (9)	0.0154 (8)	−0.0006 (8)	−0.0007 (7)	0.0034 (8)
C2	0.0132 (9)	0.0120 (9)	0.0111 (8)	−0.0033 (7)	−0.0008 (7)	−0.0025 (7)
C3	0.0148 (9)	0.0213 (10)	0.0147 (8)	−0.0010 (8)	0.0030 (7)	0.0010 (8)
C4	0.0118 (8)	0.0118 (9)	0.0102 (8)	−0.0018 (7)	0.0006 (6)	−0.0013 (7)
C5	0.0131 (9)	0.0150 (9)	0.0151 (8)	0.0000 (8)	0.0007 (7)	−0.0015 (7)
C6	0.0185 (10)	0.0134 (9)	0.0156 (8)	0.0012 (8)	−0.0055 (7)	0.0013 (7)
C7	0.0239 (10)	0.0146 (9)	0.0123 (8)	−0.0052 (8)	−0.0006 (7)	0.0019 (7)

Geometric parameters (Å, º)

S1—C7	1.712 (2)	C3—H3A	0.9800
S1—C4	1.7278 (17)	C3—H3B	0.9800
N1—C2	1.279 (2)	C3—H3C	0.9800
N1—C1	1.465 (2)	C4—C5	1.375 (2)
C1—C1^{i}	1.523 (4)	C5—C6	1.428 (3)
C1—H1A	0.9900	C5—H5	0.9500
C1—H1B	0.9900	C6—C7	1.361 (3)
C2—C4	1.472 (2)	C6—H6	0.9500
C2—C3	1.513 (2)	C7—H7	0.9500
C7—S1—C4	92.09 (9)	H3A—C3—H3C	109.5
C2—N1—C1	120.31 (15)	H3B—C3—H3C	109.5
N1—C1—C1^{i}	110.72 (18)	C5—C4—C2	129.41 (16)
N1—C1—H1A	109.5	C5—C4—S1	110.65 (13)
C1^{i}—C1—H1A	109.5	C2—C4—S1	119.94 (13)
N1—C1—H1B	109.5	C4—C5—C6	112.95 (16)
C1^{i}—C1—H1B	109.5	C4—C5—H5	123.5
H1A—C1—H1B	108.1	C6—C5—H5	123.5
N1—C2—C4	116.88 (15)	C7—C6—C5	112.08 (17)
N1—C2—C3	127.72 (16)	C7—C6—H6	124.0
C4—C2—C3	115.39 (16)	C5—C6—H6	124.0
C2—C3—H3A	109.5	C6—C7—S1	112.24 (14)
C2—C3—H3B	109.5	C6—C7—H7	123.9
H3A—C3—H3B	109.5	S1—C7—H7	123.9
C2—C3—H3C	109.5		
C2—N1—C1—C1^{i}	88.1 (2)	C7—S1—C4—C5	0.05 (14)
C1—N1—C2—C4	−179.53 (15)	C7—S1—C4—C2	−179.44 (14)

C1—N1—C2—C3	−0.6 (3)	C2—C4—C5—C6	179.10 (17)
N1—C2—C4—C5	−176.62 (18)	S1—C4—C5—C6	−0.3 (2)
C3—C2—C4—C5	4.3 (3)	C4—C5—C6—C7	0.5 (2)
N1—C2—C4—S1	2.8 (2)	C5—C6—C7—S1	−0.5 (2)
C3—C2—C4—S1	−176.34 (13)	C4—S1—C7—C6	0.25 (15)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.