

2-(2-Thienyl)-4,5-dihydro-1H-imidazole. Corrigendum

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Received 5 May 2009; accepted 18 May 2009

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.001$ Å; R factor = 0.027; wR factor = 0.080; data-to-parameter ratio = 32.3.

Consideration of a previous unrecognized twinning of the original investigated crystal of the title compound [Kia *et al.* (2009). *Acta Cryst.* **E65**, o301] led to improved reliability factors and to a slightly higher precision for all geometric parameters. The crystal under investigation was twinned by pseudo-merohedry with $[100, 0\bar{1}0, 00\bar{1}]$ as the twin matrix and a refined twin domain fraction of 0.9610 (5):0.0390 (5). The results of the new crystal structure refinement are given here.

Experimental

Crystal data

| | |
|--|-----------------------------------|
| $\text{C}_7\text{H}_8\text{N}_2\text{S}$ | $V = 709.95$ (4) Å ³ |
| $M_r = 152.21$ | $Z = 4$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 6.1321$ (2) Å | $\mu = 0.37$ mm ⁻¹ |
| $b = 11.5663$ (3) Å | $T = 100$ K |
| $c = 10.0098$ (3) Å | $0.54 \times 0.28 \times 0.22$ mm |
| $\beta = 90.154$ (1)° | |

Data collection

| | |
|--|--|
| Bruker SMART APEXII CCD area-detector diffractometer | 28316 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2005) | 3100 independent reflections |
| $T_{\min} = 0.825$, $T_{\max} = 0.922$ | 3040 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.021$ |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.027$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.080$ | |
| $S = 1.15$ | $\Delta\rho_{\text{max}} = 0.52$ e Å ⁻³ |
| 3100 reflections | $\Delta\rho_{\text{min}} = -0.24$ e Å ⁻³ |
| 96 parameters | |

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|------------|-------------|-------------|---------------|
| $\text{N1}-\text{H1}\cdots\text{N2}^i$ | 0.857 (16) | 2.130 (16) | 2.9803 (10) | 171.5 (16) |
| $\text{C3}-\text{H3A}\cdots\text{N2}^i$ | 0.95 | 2.59 | 3.4815 (11) | 156 |

 Symmetry code: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINTE* (Bruker, 2005); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2233).

References

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Kia, R., Fun, H.-K. & Kargar, H. (2009). *Acta Cryst.* **E65**, o301.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
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[‡] Thomson Reuters ResearcherID: A-5471-2009.

[§] Thomson Reuters ResearcherID: A-3561-2009.

supporting information

Acta Cryst. (2009). E65, e15 [https://doi.org/10.1107/S1600536809018790]

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2-(2-Thienyl)-4,5-dihydro-1H-imidazole

Crystal data

$C_7H_8N_2S$

$M_r = 152.21$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 6.1321$ (2) Å

$b = 11.5663$ (3) Å

$c = 10.0098$ (3) Å

$\beta = 90.154$ (1)°

$V = 709.95$ (4) Å³

$Z = 4$

$F(000) = 320$

$D_x = 1.424$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9869 reflections

$\theta = 2.5$ – 34.3 °

$\mu = 0.37$ mm⁻¹

$T = 100$ K

Block, colourless

$0.54 \times 0.28 \times 0.22$ mm

Data collection

Bruker SMART APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

$T_{\min} = 0.825$, $T_{\max} = 0.922$

28316 measured reflections

3100 independent reflections

3040 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 35.0$ °, $\theta_{\min} = 1.8$ °

$h = -9 \rightarrow 9$

$k = -18 \rightarrow 17$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.080$

$S = 1.15$

3100 reflections

96 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 atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 0.2148P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.52$ e Å⁻³

$\Delta\rho_{\min} = -0.24$ e Å⁻³

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|---------------|-------------|----------------------------------|
| S1 | 0.46976 (3) | 0.141639 (18) | 0.59512 (2) | 0.01527 (6) |
| N2 | 0.06708 (11) | 0.29657 (6) | 0.61145 (7) | 0.01355 (11) |
| N1 | 0.04589 (11) | 0.30384 (6) | 0.83752 (7) | 0.01323 (11) |
| C1 | 0.63940 (14) | 0.05379 (8) | 0.68566 (9) | 0.01780 (15) |
| H1A | 0.7552 | 0.0101 | 0.6480 | 0.021* |
| C2 | 0.58842 (14) | 0.05399 (7) | 0.81867 (9) | 0.01659 (14) |
| H2A | 0.6646 | 0.0100 | 0.8839 | 0.020* |
| C3 | 0.40890 (13) | 0.12729 (7) | 0.84861 (8) | 0.01337 (13) |
| H3A | 0.3524 | 0.1382 | 0.9360 | 0.016* |
| C4 | 0.32621 (12) | 0.18073 (6) | 0.73587 (7) | 0.01149 (12) |
| C5 | 0.14267 (12) | 0.26046 (6) | 0.72548 (7) | 0.01079 (11) |
| C6 | -0.15422 (13) | 0.36275 (7) | 0.79460 (8) | 0.01479 (14) |
| H6A | -0.1723 | 0.4380 | 0.8404 | 0.018* |
| H6B | -0.2848 | 0.3144 | 0.8103 | 0.018* |
| C7 | -0.11001 (13) | 0.37870 (7) | 0.64400 (8) | 0.01491 (13) |
| H7A | -0.2425 | 0.3611 | 0.5911 | 0.018* |
| H7B | -0.0643 | 0.4591 | 0.6248 | 0.018* |
| H1 | 0.058 (3) | 0.2686 (14) | 0.9125 (16) | 0.025 (4)* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|-------------|--------------|-------------|-------------|-------------|--------------|
| S1 | 0.01701 (9) | 0.01822 (10) | 0.01059 (9) | 0.00444 (6) | 0.00195 (6) | -0.00027 (6) |
| N2 | 0.0150 (3) | 0.0168 (3) | 0.0088 (2) | 0.0027 (2) | -0.0001 (2) | 0.0007 (2) |
| N1 | 0.0146 (3) | 0.0166 (3) | 0.0084 (2) | 0.0032 (2) | 0.0013 (2) | 0.0004 (2) |
| C1 | 0.0174 (3) | 0.0179 (3) | 0.0181 (4) | 0.0052 (3) | 0.0000 (3) | -0.0017 (3) |
| C2 | 0.0188 (3) | 0.0151 (3) | 0.0159 (3) | 0.0033 (3) | -0.0028 (3) | 0.0004 (2) |
| C3 | 0.0164 (3) | 0.0128 (3) | 0.0109 (3) | 0.0005 (2) | -0.0005 (2) | 0.0004 (2) |
| C4 | 0.0132 (3) | 0.0117 (3) | 0.0096 (3) | 0.0006 (2) | 0.0003 (2) | -0.0002 (2) |
| C5 | 0.0119 (3) | 0.0114 (3) | 0.0090 (3) | -0.0006 (2) | 0.0006 (2) | -0.0005 (2) |
| C6 | 0.0138 (3) | 0.0178 (3) | 0.0127 (3) | 0.0027 (2) | 0.0021 (2) | 0.0005 (2) |
| C7 | 0.0147 (3) | 0.0179 (3) | 0.0121 (3) | 0.0035 (2) | 0.0001 (2) | 0.0020 (2) |

Geometric parameters (Å, °)

| | | | |
|-------------|-------------|-------------|-------------|
| S1—C1 | 1.7120 (9) | C2—H2A | 0.9500 |
| S1—C4 | 1.7236 (8) | C3—C4 | 1.3819 (11) |
| N2—C5 | 1.2996 (10) | C3—H3A | 0.9500 |
| N2—C7 | 1.4798 (11) | C4—C5 | 1.4586 (10) |
| N1—C5 | 1.3657 (10) | C6—C7 | 1.5435 (12) |
| N1—C6 | 1.4669 (11) | C6—H6A | 0.9900 |
| N1—H1 | 0.858 (16) | C6—H6B | 0.9900 |
| C1—C2 | 1.3684 (13) | C7—H7A | 0.9900 |
| C1—H1A | 0.9500 | C7—H7B | 0.9900 |
| C2—C3 | 1.4221 (12) | | |
| C1—S1—C4 | 91.94 (4) | C5—C4—S1 | 120.21 (5) |
| C5—N2—C7 | 105.85 (6) | N2—C5—N1 | 116.64 (7) |
| C5—N1—C6 | 107.17 (6) | N2—C5—C4 | 122.62 (7) |
| C5—N1—H1 | 120.4 (11) | N1—C5—C4 | 120.71 (6) |
| C6—N1—H1 | 123.3 (11) | N1—C6—C7 | 101.10 (6) |
| C2—C1—S1 | 111.96 (6) | N1—C6—H6A | 111.6 |
| C2—C1—H1A | 124.0 | C7—C6—H6A | 111.6 |
| S1—C1—H1A | 124.0 | N1—C6—H6B | 111.6 |
| C1—C2—C3 | 112.65 (7) | C7—C6—H6B | 111.6 |
| C1—C2—H2A | 123.7 | H6A—C6—H6B | 109.4 |
| C3—C2—H2A | 123.7 | N2—C7—C6 | 105.62 (6) |
| C4—C3—C2 | 112.15 (7) | N2—C7—H7A | 110.6 |
| C4—C3—H3A | 123.9 | C6—C7—H7A | 110.6 |
| C2—C3—H3A | 123.9 | N2—C7—H7B | 110.6 |
| C3—C4—C5 | 128.49 (7) | C6—C7—H7B | 110.6 |
| C3—C4—S1 | 111.29 (6) | H7A—C7—H7B | 108.7 |
| C4—S1—C1—C2 | 0.09 (7) | C6—N1—C5—N2 | 12.15 (9) |
| S1—C1—C2—C3 | -0.35 (10) | C6—N1—C5—C4 | -169.84 (7) |
| C1—C2—C3—C4 | 0.50 (11) | C3—C4—C5—N2 | -173.20 (8) |
| C2—C3—C4—C5 | 179.29 (8) | S1—C4—C5—N2 | 6.50 (10) |
| C2—C3—C4—S1 | -0.43 (9) | C3—C4—C5—N1 | 8.92 (12) |
| C1—S1—C4—C3 | 0.20 (7) | S1—C4—C5—N1 | -171.38 (6) |
| C1—S1—C4—C5 | -179.55 (7) | C5—N1—C6—C7 | -17.77 (8) |
| C7—N2—C5—N1 | 0.30 (9) | C5—N2—C7—C6 | -11.91 (9) |
| C7—N2—C5—C4 | -177.67 (7) | N1—C6—C7—N2 | 17.89 (8) |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|--------------------------|-------------|---------------|-----------------------|-------------------------|
| N1—H1...N2 ⁱ | 0.857 (16) | 2.130 (16) | 2.9803 (10) | 171.5 (16) |
| C3—H3A...N2 ⁱ | 0.95 | 2.59 | 3.4815 (11) | 156 |

Symmetry code: (i) *x*, -*y*+1/2, *z*+1/2.

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

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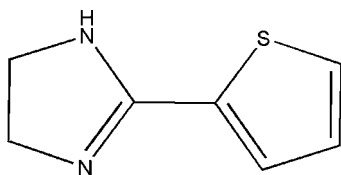
Received 8 January 2009; accepted 9 January 2009

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.050; wR factor = 0.128; data-to-parameter ratio = 34.1.

In title compound, $\text{C}_7\text{H}_8\text{N}_2\text{S}$, the five-membered rings are twisted by a dihedral angle of $5.17(10)^\circ$. Two intermolecular $\text{N}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds to the same acceptor N atom form seven-membered rings, producing $R_2^1(7)$ ring motifs. These interactions link neighbouring molecules into one-dimensional chains extended along the c axis. The crystal structure is further stabilized by weak intermolecular $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For reference geometrical data, see: Allen *et al.* (1987). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995). For a related structure and the synthesis, see: Kia *et al.* (2008); Stibrany *et al.* (2004). For the applications of imidazoline derivatives, see, for example: Blancafort (1978); Chan (1993); Vizi (1986); Li *et al.* (1996); Ueno *et al.* (1995); Corey & Grogan (1999).



Experimental

Crystal data

$\text{C}_7\text{H}_8\text{N}_2\text{S}$
 $M_r = 152.21$
Monoclinic, $P2_1/c$
 $a = 6.1321(2)$ Å
 $b = 11.5663(3)$ Å
 $c = 10.0098(3)$ Å
 $\beta = 90.154(1)^\circ$

$V = 709.95(4)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.37$ mm⁻¹
 $T = 100.0(1)$ K
 $0.54 \times 0.28 \times 0.22$ mm

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Bruker SMART APEXII CCD
area-detector diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2005)
 $T_{\min} = 0.825$, $T_{\max} = 0.922$

27675 measured reflections
3100 independent reflections
3040 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.128$
 $S = 1.24$
3100 reflections

91 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.62$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.39$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{N1}-\text{H1N1}\cdots\text{N2}^i$ | 0.75 | 2.23 | 2.977 (2) | 171 |
| $\text{C3}-\text{H3A}\cdots\text{N2}^i$ | 0.95 | 2.60 | 3.482 (2) | 155 |
| $\text{C6}-\text{H6A}\cdots\text{Cg1}^{ii}$ | 0.99 | 2.89 | 3.539 (2) | 124 |
| $\text{C6}-\text{H6B}\cdots\text{Cg1}^{iii}$ | 0.99 | 2.83 | 3.691 (2) | 146 |

Symmetry codes: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $-x, y + \frac{1}{2}, -z + \frac{3}{2}$; (iii) $x - 1, y, z$. Cg1 is the centroid of the S1/C1-C4 (thiophen) ring.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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* and *PLATON* (Spek, 2003).

HKF and RK thanks the Malaysian Government and Universiti Sains Malaysia for the Science Fund grant No. 305/PFIZIK/613312. RK thanks Universiti Sains Malaysia for a post-doctoral research fellowship. HK thanks PNU for the financial support. HKF also thanks Universiti Sains Malaysia for the Research University Golden Goose grant No. 1001/PFIZIK/811012.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2706).

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supporting information

Acta Cryst. (2009). E65, o301 [doi:10.1107/S1600536809001068]

2-(2-Thienyl)-4,5-dihydro-1*H*-imidazole

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S1. Comment

Imidazoline derivatives are of great importance because they exhibit significant biological and pharmacological activities including antihypertensive (Blancafort 1978), antihyperglycemic (Chan 1993), antidepressive (Vizi 1986), antihypercholesterolemic (Li *et al.*, 1996) and antiinflammatory properties (Ueno *et al.*, 1995). These compounds are also used as catalysts and synthetic intermediates in some organic reactions (Corey & Grogan 1999). Due to these important applications of imidazolines, here we report the crystal structure of the title compound (I).

In the title compound (I) (Fig. 1), bond lengths (Allen *et al.* 1987) and angles are within the normal ranges and are comparable with the related structures (Stibrany *et al.* 2004; Kia *et al.*, 2008). The two five-membered rings are not coplanar to each other and twisted by a dihedral angle of 5.17 (10)°. Two intermolecular N—H···N and C—H···N hydrogen bonds involving a nitrogen atom as an acceptor form seven-membered rings, producing, $R^2_2(7)$ ring motifs (Table 1). These interactions link neighbouring molecules into 1-D extended chains along the *c* axis (, Fig. 2). The crystal structure is further stabilized by weak intermolecular C—H··· π interactions [C6—H6A···Cg1ⁱ and C6—H6B···Cg1ⁱⁱ: (i) -*x*, 1/2 + *y*, 3/2 - *z*, (ii) -1 + *x*, *y*, *z*; Cg1 is the centroid of the S1/C1–C4 thiophene ring.

S2. Experimental

The synthetic method was based on the previous work (Stibrany *et al.* 2004), except that 10 mmol of 2-cyano-thiophene and 40 mmol of ethylenediamine was used. Single crystals suitable for *X*-ray diffraction were obtained by evaporation of a toluene solution at room temperature.

S3. Refinement

The hydrogen atom bound to N1 was located from the difference Fourier map and constrained to refine with the respective parent atom, see Table 1. The rest of the hydrogen atoms were positioned geometrically and refined in a riding model approximation with C—H = 0.95–0.99 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

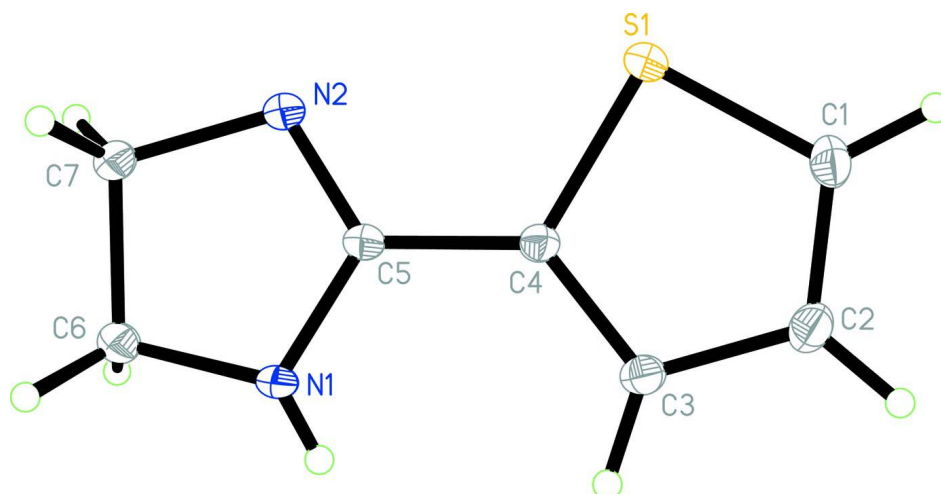


Figure 1

The molecular structure of (I) with atom labels and 50% probability ellipsoids for non-H atoms.

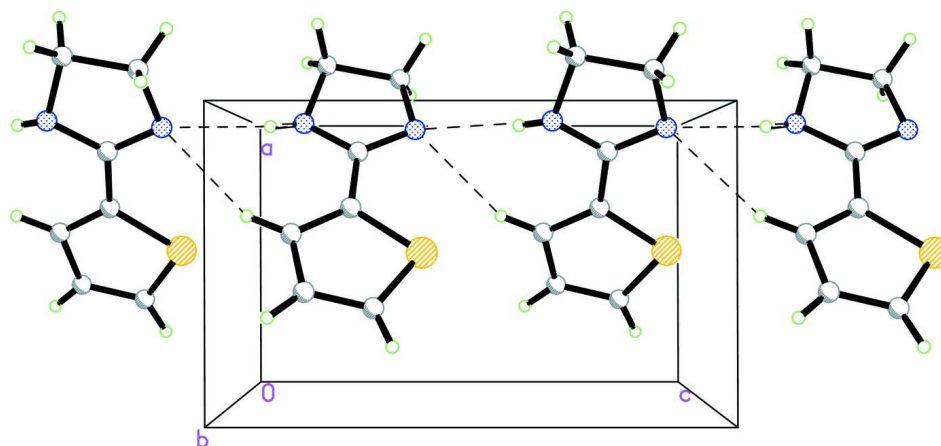


Figure 2

The crystal packing of (I), viewed down the *b*-axis showing 1-D infinite chain along the *c*-axis by intermolecular N—H...N and C—H...N interactions. The intermolecular interactions are shown as dashed lines.

2-(2-Thienyl)-4,5-dihydro-1H-imidazole

Crystal data

$C_7H_8N_2S$

$M_r = 152.21$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 6.1321(2)\ \text{\AA}$

$b = 11.5663(3)\ \text{\AA}$

$c = 10.0098(3)\ \text{\AA}$

$\beta = 90.154(1)^\circ$

$V = 709.95(4)\ \text{\AA}^3$

$Z = 4$

$F(000) = 320$

$D_x = 1.424\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 9869 reflections

$\theta = 2.5\text{--}34.3^\circ$

$\mu = 0.37\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Block, colourless

$0.54 \times 0.28 \times 0.22\ \text{mm}$

Data collection

Bruker SMART APEXII CCD area-detector
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 2005)
 $T_{\min} = 0.825$, $T_{\max} = 0.922$

27675 measured reflections
3100 independent reflections
3040 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$
 $\theta_{\max} = 35.0^\circ$, $\theta_{\min} = 2.7^\circ$
 $h = -9 \rightarrow 9$
 $k = -18 \rightarrow 17$
 $l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.128$
 $S = 1.24$
3100 reflections
91 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
 $w = 1/[\sigma^2(F_o^2) + 1.7551P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.62 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.39 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. The low-temperature data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|--------------|--------------|----------------------------------|
| S1 | 0.46967 (8) | 0.14161 (4) | 0.59514 (4) | 0.01548 (10) |
| N2 | 0.0669 (2) | 0.29635 (14) | 0.61122 (15) | 0.0137 (2) |
| N1 | 0.0460 (2) | 0.30376 (14) | 0.83746 (14) | 0.0133 (2) |
| H1N1 | 0.0584 | 0.2724 | 0.9026 | 0.016* |
| C1 | 0.6387 (3) | 0.05389 (17) | 0.6858 (2) | 0.0180 (3) |
| H1A | 0.7542 | 0.0100 | 0.6482 | 0.022* |
| C2 | 0.5888 (3) | 0.05418 (16) | 0.81838 (19) | 0.0169 (3) |
| H2A | 0.6655 | 0.0103 | 0.8835 | 0.020* |
| C3 | 0.4092 (3) | 0.12742 (15) | 0.84860 (17) | 0.0136 (3) |
| H3A | 0.3530 | 0.1385 | 0.9360 | 0.016* |
| C4 | 0.3260 (3) | 0.18060 (14) | 0.73589 (16) | 0.0117 (3) |
| C5 | 0.1427 (3) | 0.26052 (14) | 0.72556 (16) | 0.0109 (3) |
| C6 | -0.1543 (3) | 0.36276 (17) | 0.79447 (17) | 0.0154 (3) |
| H6A | -0.1724 | 0.4380 | 0.8403 | 0.018* |
| H6B | -0.2849 | 0.3144 | 0.8101 | 0.018* |

| | | | | |
|-----|-------------|--------------|--------------|------------|
| C7 | -0.1097 (3) | 0.37874 (16) | 0.64419 (17) | 0.0151 (3) |
| H7A | -0.2423 | 0.3615 | 0.5912 | 0.018* |
| H7B | -0.0634 | 0.4591 | 0.6252 | 0.018* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|--------------|--------------|--------------|--------------|--------------|---------------|
| S1 | 0.01727 (19) | 0.01847 (19) | 0.01071 (17) | 0.00446 (15) | 0.00185 (13) | -0.00026 (14) |
| N2 | 0.0153 (6) | 0.0161 (6) | 0.0098 (6) | 0.0027 (5) | 0.0003 (4) | 0.0009 (5) |
| N1 | 0.0148 (6) | 0.0170 (6) | 0.0080 (5) | 0.0029 (5) | 0.0016 (4) | 0.0004 (5) |
| C1 | 0.0166 (7) | 0.0181 (8) | 0.0192 (8) | 0.0057 (6) | -0.0001 (6) | -0.0015 (6) |
| C2 | 0.0186 (7) | 0.0155 (7) | 0.0167 (7) | 0.0029 (6) | -0.0034 (6) | 0.0009 (6) |
| C3 | 0.0164 (7) | 0.0129 (7) | 0.0113 (6) | -0.0001 (5) | -0.0002 (5) | 0.0004 (5) |
| C4 | 0.0131 (6) | 0.0120 (6) | 0.0100 (6) | 0.0005 (5) | -0.0003 (5) | -0.0005 (5) |
| C5 | 0.0120 (6) | 0.0113 (6) | 0.0094 (6) | -0.0011 (5) | 0.0005 (5) | -0.0004 (5) |
| C6 | 0.0143 (7) | 0.0186 (7) | 0.0132 (7) | 0.0030 (6) | 0.0019 (5) | 0.0007 (6) |
| C7 | 0.0152 (7) | 0.0181 (7) | 0.0120 (7) | 0.0035 (6) | 0.0000 (5) | 0.0018 (5) |

Geometric parameters (Å, °)

| | | | |
|------------|-------------|------------|-------------|
| S1—C1 | 1.7099 (19) | C2—H2A | 0.9500 |
| S1—C4 | 1.7239 (17) | C3—C4 | 1.381 (2) |
| N2—C5 | 1.302 (2) | C3—H3A | 0.9500 |
| N2—C7 | 1.480 (2) | C4—C5 | 1.459 (2) |
| N1—C5 | 1.364 (2) | C6—C7 | 1.541 (2) |
| N1—C6 | 1.468 (2) | C6—H6A | 0.9900 |
| N1—H1N1 | 0.7501 | C6—H6B | 0.9900 |
| C1—C2 | 1.362 (3) | C7—H7A | 0.9900 |
| C1—H1A | 0.9500 | C7—H7B | 0.9900 |
| C2—C3 | 1.423 (3) | | |
| C1—S1—C4 | 91.82 (9) | C5—C4—S1 | 120.22 (12) |
| C5—N2—C7 | 105.57 (14) | N2—C5—N1 | 116.78 (15) |
| C5—N1—C6 | 107.14 (14) | N2—C5—C4 | 122.49 (15) |
| C5—N1—H1N1 | 119.6 | N1—C5—C4 | 120.71 (14) |
| C6—N1—H1N1 | 124.2 | N1—C6—C7 | 101.03 (13) |
| C2—C1—S1 | 112.21 (14) | N1—C6—H6A | 111.6 |
| C2—C1—H1A | 123.9 | C7—C6—H6A | 111.6 |
| S1—C1—H1A | 123.9 | N1—C6—H6B | 111.6 |
| C1—C2—C3 | 112.63 (16) | C7—C6—H6B | 111.6 |
| C1—C2—H2A | 123.7 | H6A—C6—H6B | 109.4 |
| C3—C2—H2A | 123.7 | N2—C7—C6 | 105.80 (14) |
| C4—C3—C2 | 112.08 (15) | N2—C7—H7A | 110.6 |
| C4—C3—H3A | 124.0 | C6—C7—H7A | 110.6 |
| C2—C3—H3A | 124.0 | N2—C7—H7B | 110.6 |
| C3—C4—C5 | 128.52 (15) | C6—C7—H7B | 110.6 |
| C3—C4—S1 | 111.26 (13) | H7A—C7—H7B | 108.7 |

| | | | |
|-------------|--------------|-------------|--------------|
| C4—S1—C1—C2 | -0.16 (16) | C6—N1—C5—N2 | 11.9 (2) |
| S1—C1—C2—C3 | -0.2 (2) | C6—N1—C5—C4 | -169.73 (15) |
| C1—C2—C3—C4 | 0.5 (2) | C3—C4—C5—N2 | -173.27 (18) |
| C2—C3—C4—C5 | 179.52 (17) | S1—C4—C5—N2 | 6.9 (2) |
| C2—C3—C4—S1 | -0.60 (19) | C3—C4—C5—N1 | 8.5 (3) |
| C1—S1—C4—C3 | 0.44 (14) | S1—C4—C5—N1 | -171.36 (13) |
| C1—S1—C4—C5 | -179.67 (15) | C5—N1—C6—C7 | -17.79 (18) |
| C7—N2—C5—N1 | 0.6 (2) | C5—N2—C7—C6 | -12.26 (19) |
| C7—N2—C5—C4 | -177.67 (15) | N1—C6—C7—N2 | 18.12 (18) |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|---|-------------|---------------|-----------------------|-------------------------|
| N1—H1 <i>M</i> 1...N2 ⁱ | 0.75 | 2.23 | 2.977 (2) | 171 |
| C3—H3 <i>A</i> ...N2 ⁱ | 0.95 | 2.60 | 3.482 (2) | 155 |
| C6—H6 <i>A</i> ...C <i>g</i> 1 ⁱⁱ | 0.99 | 2.89 | 3.539 (2) | 124 |
| C6—H6 <i>B</i> ...C <i>g</i> 1 ⁱⁱⁱ | 0.99 | 2.83 | 3.691 (2) | 146 |

Symmetry codes: (i) $x, -y+1/2, z+1/2$; (ii) $-x, y+1/2, -z+3/2$; (iii) $x-1, y, z$.