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

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Consideration of a previous unrecognized twinning of the original investigated crystal of the title compound [Kia *et al.* (2009). *Acta Cryst.* E**65**, 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

$C_7H_8N_2S$
$M_r = 152.21$
Monoclinic, $P2_1/c$
$a = 6.1321$ (2) Å
$b = 11.5663$ (3) Å
$c = 10.0098$ (3) Å
$\beta = 90.154$ (1)°

$V = 709.95$ (4) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.37$ mm^{-1}
$T = 100$ K
$0.54 \times 0.28 \times 0.22$ mm

Data collection

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

28316 measured reflections
3100 independent reflections
3040 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.080$
$S = 1.15$
3100 reflections
96 parameters

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$N2^i	0.857 (16)	2.130 (16)	2.9803 (10)	171.5 (16)
C3—H3$A\cdots$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: *SAINT* (Bruker, 2005); data reduction: *SAINT*; 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

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc. Madison, Wisconsin, USA.
Kia, R., Fun, H.-K. & Kargar, H. (2009). *Acta Cryst.* E**65**, o301.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

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supporting information

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

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

Crystal data

$C_7H_8N_2S$	$F(000) = 320$
$M_r = 152.21$	$D_x = 1.424$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 9869 reflections
$a = 6.1321$ (2) Å	$\theta = 2.5$–34.3°
$b = 11.5663$ (3) Å	$\mu = 0.37$ mm^{-1}
$c = 10.0098$ (3) Å	$T = 100$ K
$\beta = 90.154$ (1)°	Block, colourless
$V = 709.95$ (4) Å^3	$0.54 \times 0.28 \times 0.22$ mm
$Z = 4$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	28316 measured reflections
Radiation source: fine-focus sealed tube	3100 independent reflections
Graphite monochromator	3040 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.021$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$\theta_{max} = 35.0°$, $\theta_{min} = 1.8°$
$T_{min} = 0.825$, $T_{max} = 0.922$	$h = -9 \rightarrow 9$
	$k = -18 \rightarrow 17$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.027$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.080$	
$S = 1.15$	H atoms treated by a mixture of independent and constrained refinement
3100 reflections	
96 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 0.2148P]$ where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} = 0.001$
	$\Delta\rho_{max} = 0.52$ 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 (Å²)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
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 (Å²)

	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, º)

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, º)

D—H···A	D—H	H···A	D···A	D—H···A
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, $-y+1/2$, $z+1/2$.