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1,1′-(1,2-Ethanediyl)bis(2,3-dihydro-3-methyl-1*H*-imidazole-2-thione)

Qingjian Liu,[a]*† Daqing Shi,[b] Kaibei Yu[c] and Jianhua Xu[d]

[a]Department of Chemistry, Shandong Normal University, Jinan 250014, Shandong, People's Republic of China, [b]Department of Chemistry, Xuzhou Normal University, Xuzhou 221009, People's Republic of China, [c]Chengdu Institute of Organic Chemistry, Chinese Academy of Sciences, Chengdu 610041, People's Republic of China, and [d]Department of Chemistry, Nanjing University, Nanjing 210093, People's Republic of China

† Current address: Department of Chemistry, Nanjing University, Nanjing 210093, People's Republic of China

Correspondence e-mail: qjnliu@yahoo.com

Key indicators

Single-crystal X-ray study
T = 288 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.104
Data-to-parameter ratio = 14.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{10}H_{14}N_4S_2$, obtained from the alkylation of methimazole with ethylene dibromide, is centrosymmetric and the two imidazole-2-thione ring moieties are anti-parallel to one another.

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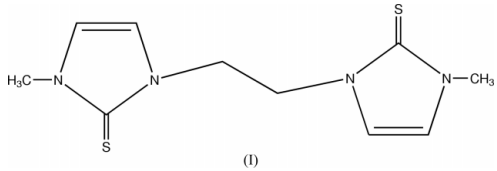
This paper is dedicated to Professor Mingli Shi on the occasion of his 70 th birthday.

Comment

Acyclic crown ethers with nitrogen heterocycles as the end groups, which can coordinate and transport metals, continue to receive attention (Vögtle & Weber, 1979; Meth-Cohn & Smith, 1982; Liu & Shi, 1992; Liu *et al.*, 1992, 2001; Matthews *et al.*, 1996). We have reported the syntheses, characterization and coordination properties of non-cyclic crown ethers with methimazole end groups (Liu & Shi, 1992; Liu *et al.*, 1992). We report here the X-ray crystal structure of the title compound, (I).



(I)

The whole molecule possesses a centre of symmetry (Fig. 1). The two imidazole-2-thione ring moieties are anti-parallel to one another. The perpendicular distance between the two rings is 1.504 (2) Å. The bridging chain moiety, $-CH_2CH_2-$, adopts an antiperiplanar conformation. The bond lengths and angles in (I) have normal values (Table 1). There is no intermolecular S···S short contact in the crystal packing (Fig. 2).

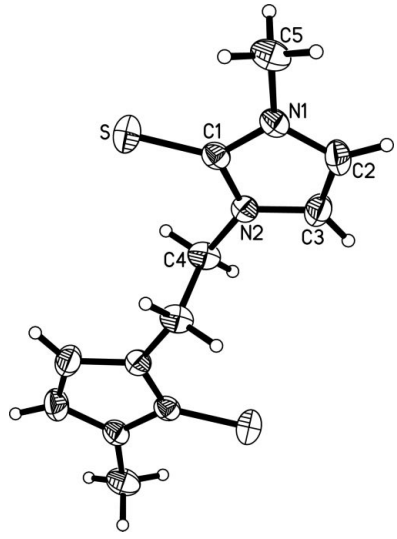


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids, and the numbering scheme for non-H atoms.

Experimental

The title compound, (I), was prepared *via* alkylation of methimazole with ethylene dibromide under phase-transfer catalytic conditions (m.p. 467–468.5 K). Single crystals of (I) suitable for X-ray diffraction analysis were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{10}H_{14}N_4S_2$
M_r = 254.37
Monoclinic, $P2_1/c$
a = 4.667 (1) Å
b = 19.720 (3) Å
c = 7.037 (1) Å
β = 107.08 (1)°
V = 619.0 (2) Å^3
Z = 2
D_x = 1.365 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 27 reflections
θ = 4.8–13.6°
μ = 0.41 mm^{-1}
T = 288 (2) K
Block, colourless
0.40 × 0.28 × 0.20 mm

Data collection

Siemens $P4$ diffractometer
ω scans
Absorption correction: refined from ΔF (*SHELXA*; Sheldrick, 1997)
T_{min} = 0.860, T_{max} = 0.921
1339 measured reflections
1097 independent reflections
804 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.0°
$h = 0 \rightarrow 5$
$k = 0 \rightarrow 23$
$l = -8 \rightarrow 8$
3 standard reflections
every 97 reflections
intensity decay: 2.9%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.104
S = 1.01
1097 reflections
74 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S—C1	1.679 (2)	N2—C3	1.381 (3)
N1—C1	1.358 (3)	N2—C4	1.451 (3)
N1—C2	1.374 (3)	C2—C3	1.329 (4)
N2—C1	1.364 (3)		
C1—N1—C5	124.6 (2)	N1—C1—S	127.63 (19)
C1—N2—C4	124.4 (2)	N2—C1—S	127.16 (18)
C3—N2—C4	125.9 (2)		
C5—N1—C1—N2	177.4 (2)	C3—N2—C1—S	−178.99 (19)
C2—N1—C1—S	179.3 (2)	C4—N2—C1—S	−1.1 (3)
C5—N1—C1—S	−3.6 (3)	C1—N1—C2—C3	−0.4 (3)
C4—N2—C1—N1	177.93 (19)	C4—N2—C3—C2	−178.2 (2)

All H atoms were positioned geometrically and treated as riding atoms, with C—H distances of 0.93 or 0.97 Å.

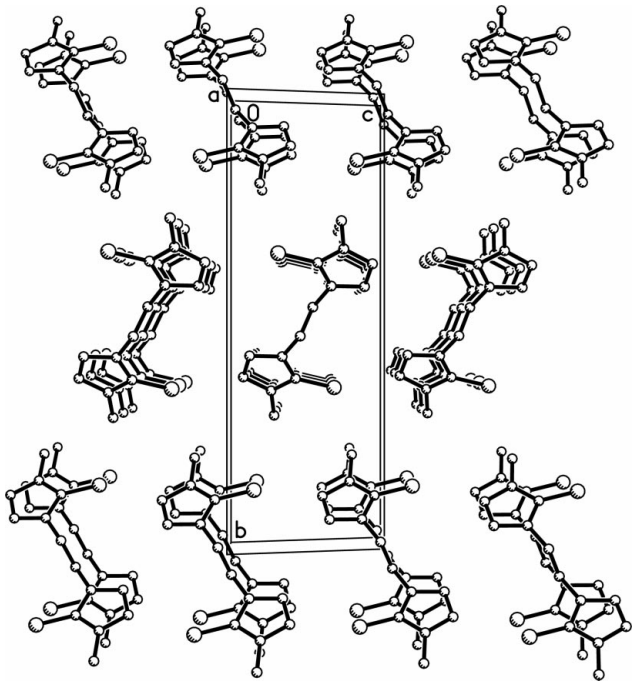


Figure 2
The molecular packing diagram of (I); H atoms are omitted.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Sheldrick, 1997); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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