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5,5′-(Disulfanediyl)bis(1-methyl-1*H*-tetrazole)

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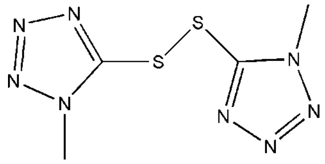
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(N–C) = 0.004 Å; R factor = 0.036; wR factor = 0.106; data-to-parameter ratio = 12.6.

In the title molecule, $C_4H_6N_8S_2$, two tetrazole rings linked by a disulfide bridge form a dihedral angle of 71.32 (7)° [C—S—S—C torsion angle = −80.51 (10)°]. In the crystal, strong intermolecular π–π interactions between the tetrazole rings [centroid–centroid distance = 3.285 (3) Å] link pairs of molecules into centrosymmetric dimers. Weak intermolecular C—H⋯N hydrogen bonds further link these dimers, related by translation in the [100] direction, into columns.

Related literature

For related structures, see: Kim *et al.* (2003); Brito *et al.* (2007); Tamilselvi & Mugesh (2010). For their use as ligands in transition-metal coordination chemistry, see: She *et al.* (2006); Carballo *et al.* (2009); Wang *et al.* (2010); Aromi *et al.* (2011).



Experimental

Crystal data

$C_4H_6N_8S_2$
M_r = 230.29
Monoclinic, $P2_1/n$
a = 6.3232 (3) Å
b = 8.1625 (3) Å
c = 18.3623 (7) Å
β = 98.906 (2)°
V = 936.31 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.54 mm^{-1}
T = 296 K
0.40 × 0.20 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.812, T_{max} = 0.899
8223 measured reflections
1606 independent reflections
1527 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.106
S = 1.09
1606 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C4—H4C⋯N6^i	0.96	2.61	3.518 (4)	158

Symmetry code: (i) $x - 1, y, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); 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: CV5132).

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supplementary materials

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5,5'-(Disulfanediyl)bis(1-methyl-1*H*-tetrazole)

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Comment

In recent years, the interesting coordination chemistry and increasingly biomedical properties of complexes derived from bis(1-methyl-1*H*-tetrazol) disulfide ligand have received much attention (Kim *et al.*, 2003; She *et al.*, 2006; Brito *et al.*, 2007; Carballo *et al.*, 2009; Tamilselvi & Mugesh, 2010; Wang *et al.*, 2010). Herein we report the synthesis and crystal structure of the title compound, (I).

In (I) (Fig. 1), the bond lengths and angles are normal and correspond to those observed in the related compounds (Kim *et al.*, 2003; Brito *et al.*, 2007; Tamilselvi & Mugesh, 2010) The dihedral angle between the two tetrazol rings is 71.32 (7) °. The S—S bond length is 2.0474 (8) Å. The C—S—S—C torsion angle of -80.51 (10) ° compares well with that of -79.71 (10) ° reported by Tamilselvi & Mugesh (2010). The C—S—S—C torsion angle in two bis-tetrazol disulfides reported by Kim *et al.* (2003) and Brito *et al.* (2007) are 81.54 (5) ° and 80.42 (6) °, respectively.

In the crystal structure, strong intermolecular π—π interaction between the tetrazole rings [centroid-centroid distance of 3.285 (3) Å] link two molecules into centrosymmetric dimer. Weak intermolecular C—H···N hydrogen bonds (Table 1) link further these dimers related by translation in [100] into columns.

Experimental

A water solution (5 ml) of $Fe(NO_3)_3$ (0.25 mmol) was added slowly to the water solution (15 ml) of 1-methyl-5-mercaptotetrazole (0.10 mmol). The reaction mixture was stirred at room temperature for 3 h. The solvent was removed and the solid product recrystallized from ethanol. After six days, the colourless crystals suitable for X-ray diffraction were obtained.

Refinement

All H atoms were placed in idealized positions and refined using a riding model (C—H = 0.96 Å) with $U_{iso}(H) = 1.5 U_{eq}(C)$.

Figures

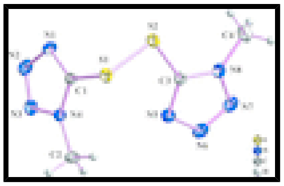

Fig. 1. View of (I) showing the atomic labeling and 30% probability displacement ellipsoids.

5,5'-(Disulfanediyl)bis(1-methyl-1*H*-tetrazole)

Crystal data

$C_4H_6N_8S_2$	$F(000) = 472$
$M_r = 230.29$	$D_x = 1.634$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 9988 reflections
$a = 6.3232$ (3) Å	$\theta = 2.5$–$40.5°$
$b = 8.1625$ (3) Å	$\mu = 0.54$ mm^{-1}
$c = 18.3623$ (7) Å	$T = 296$ K
$\beta = 98.906$ (2)°	Block, colourless
$V = 936.31$ (7) Å^3	0.40 × 0.20 × 0.20 mm
$Z = 4$	

Data collection

Bruker APEXII CCD area-detector diffractometer	1606 independent reflections
Radiation source: fine-focus sealed tube	1527 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.019$
phi and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$h = -7 \rightarrow 5$
$T_{min} = 0.812$, $T_{max} = 0.899$	$k = -9 \rightarrow 9$
8223 measured reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.036$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.106$	H-atom parameters constrained
$S = 1.09$	$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 0.6856P]$ where $P = (F_o^2 + 2F_c^2)/3$
1606 reflections	$(\Delta/\sigma)_{max} < 0.001$
127 parameters	$\Delta\rho_{max} = 0.38$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

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}
S1	0.21952 (9)	0.05034 (7)	0.39949 (3)	0.0367 (2)
S2	0.13427 (9)	0.20613 (8)	0.47738 (3)	0.0427 (2)
N2	0.2328 (4)	0.3565 (3)	0.24114 (12)	0.0461 (5)
N1	0.1217 (3)	0.2818 (2)	0.28933 (11)	0.0393 (5)
C1	0.2630 (3)	0.1878 (2)	0.32986 (11)	0.0296 (4)
N4	0.4531 (3)	0.2035 (2)	0.30732 (10)	0.0348 (4)
N6	0.7056 (3)	0.3555 (3)	0.55018 (13)	0.0484 (5)
N5	0.5698 (3)	0.2755 (3)	0.49736 (12)	0.0448 (5)
C3	0.3824 (4)	0.2790 (3)	0.52098 (12)	0.0351 (5)
N8	0.4035 (3)	0.3574 (2)	0.58550 (10)	0.0386 (4)
N3	0.4312 (3)	0.3089 (3)	0.25086 (11)	0.0430 (5)
C2	0.6534 (4)	0.1195 (4)	0.33142 (15)	0.0503 (6)
H2B	0.6382	0.0491	0.3722	0.075*
H2C	0.7640	0.1985	0.3465	0.075*
H2A	0.6908	0.0551	0.2915	0.075*
N7	0.6092 (3)	0.4054 (3)	0.60292 (12)	0.0485 (5)
C4	0.2441 (5)	0.3978 (4)	0.63164 (16)	0.0627 (8)
H4C	0.1080	0.3535	0.6101	0.094*
H4A	0.2330	0.5146	0.6355	0.094*
H4B	0.2858	0.3518	0.6799	0.094*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0401 (4)	0.0366 (3)	0.0343 (3)	−0.0056 (2)	0.0089 (2)	0.0033 (2)

S2	0.0329 (3)	0.0600 (4)	0.0367 (3)	−0.0085 (2)	0.0095 (2)	−0.0078 (2)
N2	0.0515 (12)	0.0450 (11)	0.0406 (11)	−0.0020 (9)	0.0028 (9)	0.0106 (9)
N1	0.0344 (10)	0.0417 (10)	0.0408 (11)	0.0010 (8)	0.0024 (8)	0.0035 (8)
C1	0.0268 (10)	0.0327 (10)	0.0293 (10)	−0.0033 (8)	0.0041 (8)	−0.0015 (8)
N4	0.0300 (9)	0.0411 (10)	0.0337 (10)	−0.0034 (7)	0.0065 (8)	0.0021 (7)
N6	0.0352 (11)	0.0539 (12)	0.0547 (13)	−0.0054 (9)	0.0024 (10)	0.0047 (10)
N5	0.0364 (11)	0.0549 (12)	0.0439 (11)	−0.0038 (9)	0.0088 (9)	0.0025 (9)
C3	0.0346 (12)	0.0382 (12)	0.0326 (11)	−0.0034 (9)	0.0051 (9)	0.0065 (9)
N8	0.0379 (10)	0.0422 (10)	0.0348 (10)	−0.0049 (8)	0.0028 (8)	0.0005 (8)
N3	0.0453 (12)	0.0498 (11)	0.0348 (10)	−0.0081 (9)	0.0090 (9)	0.0071 (8)
C2	0.0261 (11)	0.0749 (18)	0.0508 (14)	0.0049 (11)	0.0086 (10)	0.0060 (13)
N7	0.0397 (11)	0.0527 (12)	0.0503 (12)	−0.0071 (9)	−0.0023 (10)	0.0009 (10)
C4	0.0513 (16)	0.092 (2)	0.0472 (15)	−0.0110 (16)	0.0141 (13)	−0.0212 (15)

Geometric parameters (Å, °)

S1—C1	1.754 (2)	N5—C3	1.324 (3)
S1—S2	2.0474 (8)	C3—N8	1.335 (3)
S2—C3	1.752 (2)	N8—N7	1.349 (3)
N2—N3	1.299 (3)	N8—C4	1.452 (3)
N2—N1	1.357 (3)	C2—H2B	0.9600
N1—C1	1.317 (3)	C2—H2C	0.9600
C1—N4	1.337 (3)	C2—H2A	0.9600
N4—N3	1.338 (3)	C4—H4C	0.9600
N4—C2	1.448 (3)	C4—H4A	0.9600
N6—N7	1.287 (3)	C4—H4B	0.9600
N6—N5	1.359 (3)		
C1—S1—S2	101.53 (7)	C3—N8—C4	130.1 (2)
C3—S2—S1	102.49 (8)	N7—N8—C4	121.8 (2)
N3—N2—N1	111.26 (18)	N2—N3—N4	106.28 (18)
C1—N1—N2	104.84 (19)	N4—C2—H2B	109.5
N1—C1—N4	109.43 (19)	N4—C2—H2C	109.5
N1—C1—S1	127.98 (17)	H2B—C2—H2C	109.5
N4—C1—S1	122.48 (16)	N4—C2—H2A	109.5
C1—N4—N3	108.17 (18)	H2B—C2—H2A	109.5
C1—N4—C2	130.23 (19)	H2C—C2—H2A	109.5
N3—N4—C2	121.46 (19)	N6—N7—N8	106.3 (2)
N7—N6—N5	111.64 (19)	N8—C4—H4C	109.5
C3—N5—N6	104.7 (2)	N8—C4—H4A	109.5
N5—C3—N8	109.2 (2)	H4C—C4—H4A	109.5
N5—C3—S2	128.82 (19)	N8—C4—H4B	109.5
N8—C3—S2	121.87 (17)	H4C—C4—H4B	109.5
C3—N8—N7	108.06 (19)	H4A—C4—H4B	109.5
C1—S1—S2—C3	−80.51 (10)	S1—S2—C3—N5	17.9 (2)
N3—N2—N1—C1	0.9 (3)	S1—S2—C3—N8	−165.44 (17)
N2—N1—C1—N4	−0.2 (2)	N5—C3—N8—N7	0.3 (3)
N2—N1—C1—S1	−176.46 (16)	S2—C3—N8—N7	−176.89 (16)
S2—S1—C1—N1	−65.6 (2)	N5—C3—N8—C4	177.5 (3)
S2—S1—C1—N4	118.62 (17)	S2—C3—N8—C4	0.3 (4)

N1—C1—N4—N3	−0.5 (2)	N1—N2—N3—N4	−1.2 (3)
S1—C1—N4—N3	175.98 (15)	C1—N4—N3—N2	1.0 (2)
N1—C1—N4—C2	−176.1 (2)	C2—N4—N3—N2	177.1 (2)
S1—C1—N4—C2	0.4 (3)	N5—N6—N7—N8	0.3 (3)
N7—N6—N5—C3	−0.1 (3)	C3—N8—N7—N6	−0.4 (3)
N6—N5—C3—N8	−0.2 (3)	C4—N8—N7—N6	−177.8 (2)
N6—N5—C3—S2	176.80 (18)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4C···N6^{i}	0.96	2.61	3.518 (4)	158.

Symmetry codes: (i) $x-1, y, z$.

Fig. 1