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Crystal structure of 1,3-bis(1-methyl-1*H*-tetrazol-5-ylthio)propane, $C_3H_6(SCN_4CH_3)_2$

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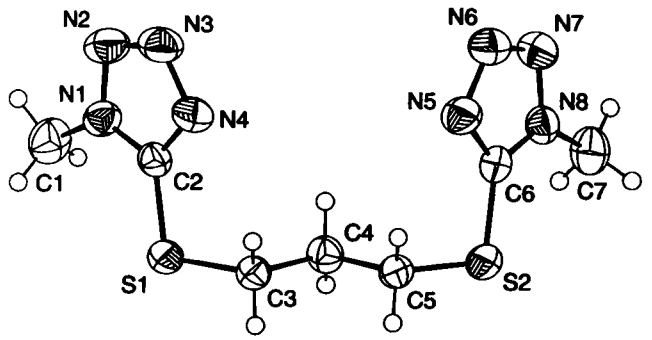

Abstract

$C_7H_{12}N_8S_2$, orthorhombic, *Pcab* (no. 61), $a = 9.146(2)$ Å, $b = 14.113(3)$ Å, $c = 18.998(4)$ Å, $V = 2452.1$ Å^3, $Z = 8$, $R_{gt}(F) = 0.037$, $wR_{ref}(F^2) = 0.111$, $T = 293$ K.

Source of material

Sodium hydroxide (2 g, 0.05 mol) was added slowly to 5-mercapto-1-methyltetrazole (5.8 g, 0.05 mol) in 20 ml of dry DMSO. The reaction mixture was stirred at 60 °C for 1 h. Then 2.4 ml (0.025 mol) of 1,3-dichloropropane was added in portions to the suspension which became grey. The solution was stirred for 4 h, cooled to room temperature and filtered. The solvent was removed under reduced pressure. 1.58 g (62 %) of a white solid were obtained. Single crystals suitable for X-ray diffraction were isolated after a week from acetone (m.p. 139-140 °C).

Discussion

Tetrazole compounds have a wide range of pharmaceutical applications [1], where they act as stimulants or sedatives on the central nervous system. These compounds have anti-inflammatory, antilipemic, antimicrobial, and antiallergic activities [2]. Moreover, such compounds are useful as oxidizers and effective agents for regulating plant growth and as explosives and rocket propellants [3]. In addition, tetrazole compounds have a significant role in medicinal chemical research [4]. The title compound was investigated as part of our endeavor to prepare and study a series of tetrazole compounds.

1,3-bis(1-methyl-1*H*-tetrazol-5-ylthio)propane crystallizes centrosymmetrically with one independent molecule in the asymmetric unit. In the molecule the rings are mainly planar, the tetrazole N—C distances are 1.334(2) Å for N1—C2, 1.329(2) Å for N4—C2, 1.336(2) Å for N5—C6, and 1.332(2) Å for N8—C6. The larger C—S bond lengths are for 1.738(2) Å for S1—C2, 1.817(2) Å for S1—C3, 1.730(2) Å for S2—C6, and 1.813(2) Å for S2—C5. Intermolecular N5···H1C′ interactions (2.591 Å, 155°) link the molecules into loops running along the *a* axis. The nitrogen function acts as donor and hydrogen acts as acceptor. A similar ligand molecule was studied in [5].

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.2 × 0.3 × 0.4 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	4.27 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	55.22°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8795, 2823
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1850
$N(param)_{refined}$:	156
Programs:	SHELXS-97 [6], SHELXL-97 [7]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1A)	8*c*	0.5059	0.3654	−0.0978	0.092
H(1B)	8*c*	0.3880	0.3806	−0.1565	0.092
H(1C)	8*c*	0.4154	0.4596	−0.1001	0.092
H(3A)	8*c*	0.8687	0.3351	−0.3024	0.045
H(3B)	8*c*	0.8457	0.2252	−0.3062	0.045
H(4A)	8*c*	0.6367	0.2492	−0.3773	0.051
H(3B)	8*c*	0.6653	0.3589	−0.3751	0.051
H(5A)	8*c*	0.8705	0.2303	−0.4316	0.048
H(5B)	8*c*	0.8832	0.3409	−0.4355	0.048
H(7A)	8*c*	0.5472	0.3670	−0.6600	0.087
H(7B)	8*c*	0.4299	0.4448	−0.6433	0.087
H(7C)	8*c*	0.4383	0.3529	−0.5972	0.087

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	8*c*	0.67780(6)	0.29112(3)	−0.22876(2)	0.0559(3)	0.0348(3)	0.0412(3)	−0.0027(2)	0.0089(2)	0.0028(2)
S(2)	8*c*	0.71960(7)	0.28767(3)	−0.51998(2)	0.0665(4)	0.0399(3)	0.0391(3)	0.0019(2)	−0.0101(2)	−0.0064(2)
N(1)	8*c*	0.5707(2)	0.4536(1)	−0.17319(7)	0.044(1)	0.0430(8)	0.0454(8)	0.0077(7)	−0.0035(8)	−0.0041(7)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(2)	8*c*	0.5905(2)	0.5486(1)	−0.17673(9)	0.060(1)	0.0427(9)	0.065(1)	0.0108(8)	−0.015(1)	−0.0070(8)
N(3)	8*c*	0.6911(2)	0.5627(1)	−0.22251(9)	0.072(1)	0.0369(9)	0.064(1)	−0.0042(9)	−0.014(1)	0.0018(8)
N(4)	8*c*	0.7405(2)	0.4802(1)	−0.25047(9)	0.061(1)	0.0375(8)	0.0542(9)	−0.0043(8)	0.0007(9)	0.0047(8)
N(5)	8*c*	0.7585(2)	0.4788(1)	−0.49687(9)	0.057(1)	0.0437(9)	0.0503(9)	−0.0024(8)	−0.0093(8)	−0.0054(8)
N(6)	8*c*	0.7002(2)	0.5589(1)	−0.52411(9)	0.067(1)	0.0424(9)	0.057(1)	−0.0006(9)	−0.003(1)	0.0003(8)
N(7)	8*c*	0.6042(2)	0.5408(1)	−0.57122(8)	0.061(1)	0.047(1)	0.0534(9)	0.0065(8)	0.001(1)	0.0059(7)
N(8)	8*c*	0.5969(2)	0.4452(1)	−0.57622(7)	0.0431(9)	0.0487(9)	0.0353(7)	0.0029(7)	−0.0024(7)	0.0012(6)
C(1)	8*c*	0.4607(3)	0.4112(2)	−0.1281(1)	0.052(1)	0.072(2)	0.060(1)	0.007(1)	0.012(1)	−0.003(1)
C(2)	8*c*	0.6633(2)	0.4131(1)	−0.21840(9)	0.043(1)	0.0387(9)	0.0351(8)	0.0009(8)	−0.0053(9)	0.0027(7)
C(3)	8*c*	0.7953(2)	0.2857(1)	−0.30576(8)	0.039(1)	0.0368(9)	0.0379(9)	−0.0004(8)	0.0012(8)	0.0005(7)
C(4)	8*c*	0.7123(2)	0.2973(1)	−0.37415(8)	0.040(1)	0.047(1)	0.041(1)	0.0039(9)	−0.0023(9)	0.0017(7)
C(5)	8*c*	0.8147(2)	0.2884(1)	−0.43623(9)	0.045(1)	0.038(1)	0.0364(8)	0.0055(8)	−0.0065(8)	−0.0023(7)
C(6)	8*c*	0.6913(2)	0.4080(1)	−0.53054(8)	0.041(1)	0.043(1)	0.0319(8)	−0.0011(8)	−0.0003(8)	−0.0036(7)
C(7)	8*c*	0.4944(2)	0.3985(2)	−0.62317(9)	0.053(1)	0.075(2)	0.046(1)	−0.002(1)	−0.013(1)	−0.003(1)

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