

## 2,4,6-Trimethyl-1,3,5-tris(4-methylthiazol-2-ylsulfanylmethyl)benzene

Hui-Min Liu, Wei Zhang and Wen-Qin Zhang\*

Department of Chemistry, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail: wqzhang@tju.edu.cn

### Key indicators

Single-crystal X-ray study

$T = 293\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$

Disorder in main residue

$R$  factor = 0.059

$wR$  factor = 0.114

Data-to-parameter ratio = 13.3

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

The title compound,  $\text{C}_{24}\text{H}_{27}\text{N}_3\text{S}_6$ , crystallizes in the monoclinic space group  $P2_1/n$ . All of the 4-methylthiazol-2-ylsulfanyl groups point to the same side of the central benzene ring, resulting in a tripodal arrangement.

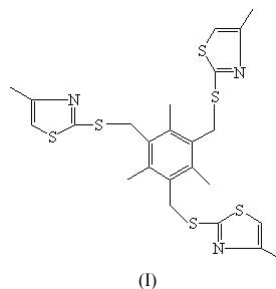
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### Comment

We are presently involved in the synthesis of multithiazoles, as thiazole and its derivatives are of considerable interest for their remarkable bioactivities (Tian *et al.*, 1996; Sasaki *et al.*, 1994, 1996) and their ability to act as potential donors to transition metals for the generation of one-, two- and three-dimensional coordination networks (Liu *et al.*, 2001; Sun *et al.*, 1997; Fisher *et al.*, 1985). Thus, we were prompted to explore new compounds containing two or more thiazolyl groups using different linkages. The selection of the linkages is crucial; the existing functions of linkages and the availability of the starting materials from commercial sources are two aspects of primary consideration. Here we report the synthesis and the structure of a new flexible ligand containing three thiazolyl groups, *viz.* 2,4,6-trimethyl-1,3,5-tris(4-methylthiazol-2-ylsulfanylmethyl)benzene, (I).



As shown in Fig. 1, the tripodal arrangement of all 4-methylthiazol-2-ylsulfanyl groups gives a conformation with all S atoms available for facile coordination to a metal ion. The methyl and methylene groups bonded to the benzene ring are nearly coplanar with the benzene ring plane, the largest deviation being 0.1504 (8) Å for atom C10. Similar arrangements are found between the methyl groups and the bonded thiazole rings of the 4-methylthiazol-2-yl groups. The three exocyclic S atoms (S1, S3 and S5) are approximately equidistant from the benzene ring; the angle between the S1/S3/S5 plane and the benzene plane is 2.2 (9)°.

### Experimental

2,4,6-Trimethyl-1,3,5-tris(bromomethyl)benzene was prepared according to a literature method (van der Made & van der Made,

1993). The title compound was synthesized according to a reported procedure (Zhang *et al.*, 2003) by the reaction of 2,4,6-trimethyl-1,3,5-tris(bromomethyl)benzene and potassium 4-methylthiazolylthiolate in EtOH at 323–333 K; yield 87.4%; m.p. 388–389 K; IR (KBr) 3111 (*w*), 2960 (*w*), 2916 (*w*), 1527 (*ms*), 1414 (*s*), 1414 (*s*), 1372 (*ms*), 1289 (*s*), 1032 (*vs*), 723 (*w*), 706 (*ms*)  $\text{cm}^{-1}$ ;  $^1\text{H NMR}$  ( $\text{CDCl}_3$ )  $\delta$  6.81 (3H, *s*), 4.49 (6H, *s*), 2.49 (9H, *s*), 2.45 (9H, *s*) p.p.m.; elemental analysis calculated for  $\text{C}_{24}\text{H}_{27}\text{N}_3\text{S}_6$  C 52.40, H 4.90, N 7.63%; found C 52.40, H 4.88, N 7.47%. Single crystals of (I) suitable for X-ray analysis were obtained by slow diffusion of acetone into a chloroform solution.

#### Crystal data

$\text{C}_{24}\text{H}_{27}\text{N}_3\text{S}_6$   
 $M_r = 549.91$   
 Monoclinic,  $P2_1/n$   
 $a = 12.216$  (4) Å  
 $b = 17.801$  (5) Å  
 $c = 12.528$  (4) Å  
 $\beta = 93.420$  (6)°  
 $V = 2719.4$  (15) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.343$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 992 reflections  
 $\theta = 2.5$ – $21.4$ °  
 $\mu = 0.52$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Prism, colorless  
 $0.25 \times 0.20 \times 0.15$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.880$ ,  $T_{\max} = 0.927$   
 12608 measured reflections

4772 independent reflections  
 2335 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.069$   
 $\theta_{\text{max}} = 25.0$ °  
 $h = -14 \rightarrow 13$   
 $k = -17 \rightarrow 21$   
 $l = -10 \rightarrow 14$

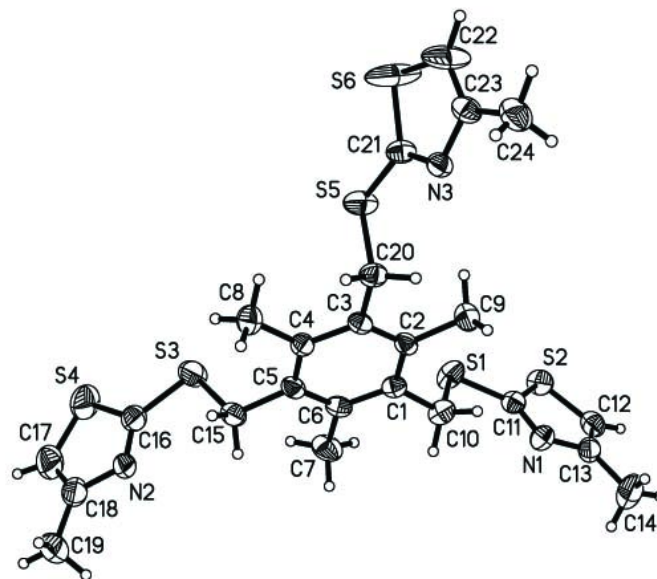
#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.059$   
 $wR(F^2) = 0.114$   
 $S = 1.00$   
 4772 reflections  
 360 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.7831P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.003$   
 $\Delta\rho_{\text{max}} = 0.25$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.19$  e Å<sup>-3</sup>

In the disordered thiazolyl ring, the bonds S6–C21, S6–C22, S6'–C21' and S6'–C22' were restrained to 1.71 (1) Å and the angles C21–S6–C22, C21'–S6'–C22' to 89 (1)°; other C–C and C–N bond parameters were restrained to appropriate values. Primed atoms have occupancy 0.53 (3) and unprimed 0.47 (3). The H atoms were included in calculated positions and refined with riding-model constraints.

Data collection: SMART (Bruker, 1997); cell refinement: SMART; data reduction: SAINT (Bruker, 1997) and SHELXTL (Bruker, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL; software used to prepare



**Figure 1**

The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Only the minor disorder component of the thiazolyl ring is shown.

material for publication: SHELXTL.

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