

## 2,6-Bis(phenylthiomethyl)pyridine

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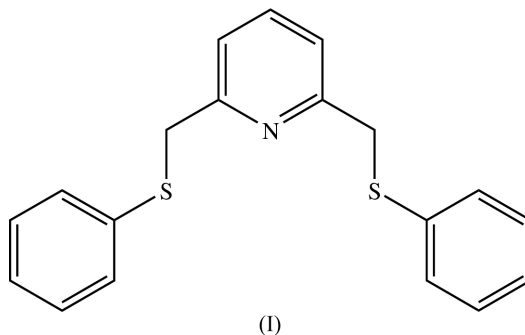
## Key indicators

Single-crystal X-ray study  
 $T = 150$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.034  
 $wR$  factor = 0.041  
Data-to-parameter ratio = 12.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The crystal structure of 2,6-bis(phenylthiomethyl)pyridine, 2,6-(C<sub>6</sub>H<sub>5</sub>SCH<sub>2</sub>)<sub>2</sub>C<sub>5</sub>H<sub>3</sub>N or C<sub>19</sub>H<sub>17</sub>NS<sub>2</sub>, shows the molecule to have *syn*-phenylthiol substituents with respect to the pyridyl ring.

## Comment

Compounds that have both nitrogen and sulfur centres available for coordination to metals are becoming topical with respect to their role in enzyme mimicry, where the N-donor fragments somewhat resemble the imidazole fragment of histidine and the S-donor fragments model the amino acid cysteine. Interest in the structure of such ligands comes from the desire to understand how the preferred conformation of the uncoordinated compound affects the coordination mode of the ligand when coordinated to a metal centre or metal centres, and how the ligand may best be modified to achieve a desired coordination mode. In the course of our work on transition metal halide complexes of mixed-donor N/S ligands (Ball *et al.*, 2001), we isolated the title compound, (I), as colourless blocks from methanol. This ligand has previously been complexed with inorganic metal compounds (Teixidor *et al.*, 1989, 1991; Vinãs *et al.*, 1998). Until now, it has not been possible to compare the structure of the uncoordinated ligand with the ligand incorporated into such complexes.



An *ORTEP* drawing of (I) is shown in Fig. 1. The bond distances and angles are comparable with those of 2,6-bis(*p*-nitrophenylthiomethyl)pyridine (Sillanpää *et al.*, 1994), which possesses deactivating nitro groups at the *para* position of the phenyl rings. The difference in structure between the two compounds arises in the position of the thiolate groups with respect to the plane of the pyridyl ring. Compound (I) has both phenyl thiolate moieties *syn* with respect to the pyridyl ring [ $\text{S}-\text{C}-\text{C}-\text{N}$  torsion angles  $-129.1$  (2) and  $77.4$  (2) $^\circ$ ], whereas the nitro-substituted compound has one thiolate S-centre almost in the plane of the pyridyl ring [ $\text{S}-\text{C}-\text{C}-\text{N}$  angle  $6.8$  (5) $^\circ$ ] with the other directed away from the pyridyl

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ring plane [S—C—C—N  $-112.0(4)^\circ$ ] (Sillanpää *et al.*, 1994). The lone pairs of electrons on the two sulfur centres in (I) are directed away from each other [C—C—S—C<sub>Ph</sub>  $71.1(3)$  and  $63.8(2)^\circ$ ]. We have observed, however, that the conformation of (I) can adjust so as to act as a bidentate or tridentate ligand toward metal centres (Ball *et al.*, 2001). The phenyl substituents are orientated in such a way that one is almost perpendicular to the plane of the pyridyl ring while the other tends towards the plane of the pyridyl ring.

## Experimental

The title compound was prepared according to literature procedures (Teixidor *et al.*, 1991). Crystals suitable for single-crystal X-ray diffraction studies were grown from a methanol solution at 269 K.

### Crystal data

C <sub>19</sub> H <sub>17</sub> NS <sub>2</sub>	Z = 2
<i>M<sub>r</sub></i> = 323.47	<i>D<sub>x</sub></i> = 1.307 Mg m <sup>-3</sup>
Triclinic, <i>P</i> $\bar{1}$	Mo <i>K</i> $\alpha$ radiation
<i>a</i> = 10.165 (2) Å	Cell parameters from 25 reflections
<i>b</i> = 10.365 (2) Å	$\theta$ = 45.2–49.9°
<i>c</i> = 9.053 (2) Å	$\mu$ = 0.32 mm <sup>-1</sup>
$\alpha$ = 112.93 (1)°	<i>T</i> = 150 K
$\beta$ = 100.12 (2)°	Block, colourless
$\gamma$ = 102.37 (1)°	0.3 × 0.3 × 0.2 mm
<i>V</i> = 821.6 (3) Å <sup>3</sup>	

### Data collection

Rigaku AFC-7S diffractometer	<i>R</i> <sub>int</sub> = 0.01
$\omega/2\theta$ scans	$\theta_{\max}$ = 25.0°
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968)	<i>h</i> = 0 → 12
<i>T</i> <sub>min</sub> = 0.883, <i>T</i> <sub>max</sub> = 0.938	<i>k</i> = -12 → 12
3073 measured reflections	<i>l</i> = -10 → 10
2894 independent reflections	3 standard reflections every 150 reflections
2487 reflections with <i>F</i> > 2 $\sigma$ ( <i>F</i> )	intensity decay: 1.3%

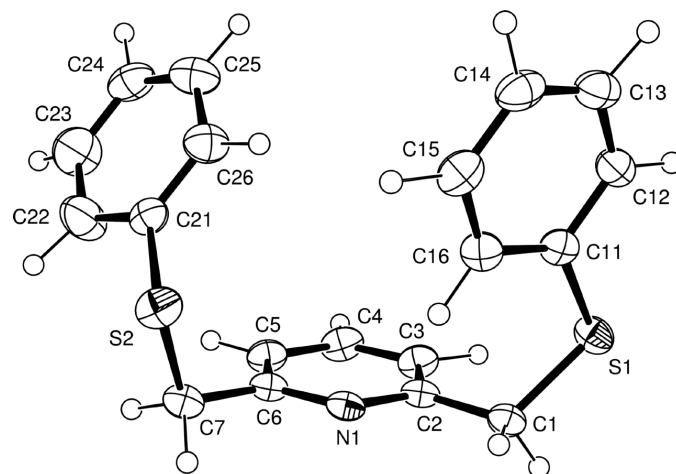
### Refinement

Refinement on <i>F</i>	H-atom parameters constrained
<i>R</i> = 0.034	$w = 1/[\sigma^2(F) + 0.008 F ^2]$
<i>wR</i> = 0.041	( $\Delta/\sigma$ ) <sub>max</sub> < 0.001
<i>S</i> = 3.02	$\Delta\rho_{\max} = 0.25 \text{ e } \text{Å}^{-3}$
2487 reflections	$\Delta\rho_{\min} = -0.31 \text{ e } \text{Å}^{-3}$
199 parameters	

**Table 1**

Selected geometric parameters (Å, °).

S1—C1	1.816 (2)	S2—C21	1.781 (2)
S1—C11	1.770 (2)	N1—C2	1.344 (3)
S2—C7	1.832 (2)	N1—C6	1.343 (3)
C1—S1—C11	104.13 (10)	N1—C2—C1	115.6 (2)
C7—S2—C21	100.90 (10)	N1—C2—C3	122.3 (2)
C2—N1—C6	118.5 (2)	S2—C7—C6	112.3 (1)
S1—C1—C2	115.1 (1)		
S1—C1—C2—N1	-129.1 (2)	C1—S1—C11—C16	5.5 (4)
S1—C1—C2—C3	52.3 (2)	C1—C2—N1—C6	-177.5 (1)
S1—C11—C12—C13	-176.9 (2)	C1—C2—C3—C4	177.5 (1)
S1—C11—C12—C13	-176.9 (2)	C2—N1—C6—C7	-179.6 (1)
S2—C7—C6—N1	77.4 (2)	C4—C5—C6—C7	178.7 (2)
S2—C7—C6—C5	-101.9 (2)	C6—C7—S2—C21	63.8 (2)
S2—C21—C22—C23	178.5 (2)	C7—S2—C21—C22	63.3 (2)
S2—C21—C26—C25	-176.9 (2)	C7—S2—C21—C26	-119.5 (2)
C1—S1—C11—C12	-176.5 (2)		



**Figure 1**

A view of the title molecule showing the atom-labelling scheme. Ellipsoids are at the 50% probability level (Johnson, 1976).

No reflections had unacceptable values for  $\Delta(F_o - F_c)/\sigma(F_o)$  although 140 reflections had values of  $\Delta(F_o - F_c)/\sigma(F_o)$  between 5 and 10, and 20 reflections had values of  $\Delta(F_o - F_c)/\sigma(F_o)$  greater than 10. The large number of these reflections most probably accounts for the large goodness-of-fit value (3.02) for the refined structure.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1992); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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