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#### Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.042  
 $wR$  factor = 0.132  
Data-to-parameter ratio = 16.0

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

## *N*-(4-Methoxybenzoyl)-*N'*-(4-methoxyphenyl)- thiourea

Molecules of the title compound,  $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_3\text{S}$ , are linked by  $\text{N}-\text{H}\cdots\text{S}$  hydrogen bonds to form centrosymmetric dimers [ $\text{N}\cdots\text{S} = 3.4501(13)$  Å]. The *N'*-phenyl and *N*-phenyl rings are twisted by  $52.7(1)$  and  $23.3(1)^\circ$ , respectively, from the essentially planar  $-\text{NHC}(=\text{S})\text{NC}(=\text{O})-$  moiety.

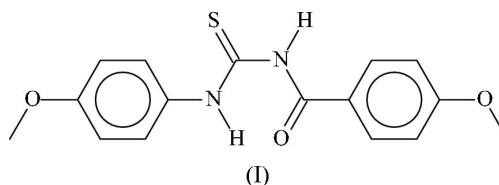
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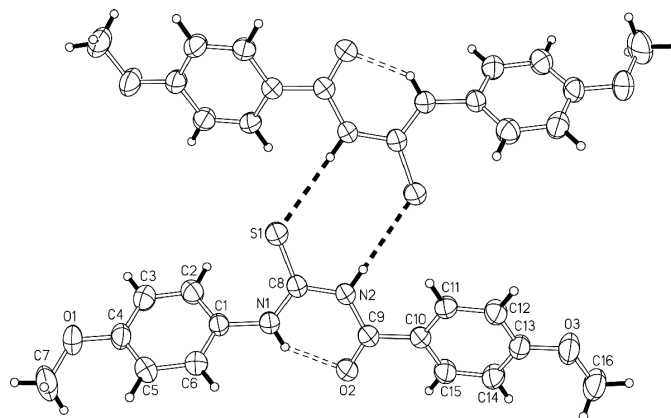
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#### Comment

The crystal structures of a number of aromatic thioureas have been determined; the parent compound *N*-benzoyl-*N'*-phenylthiourea exists as a weakly held dimer arising from  $\text{N}-\text{H}\cdots\text{S}$  interactions [ $\text{N}\cdots\text{S} = 3.654(1)$  Å; Yamin & Yusuf, 2003]. A non-planar conformation is adopted by the homolog having an electron-donating methoxy substituent in the *N'*-phenyl ring [ $\text{N}\cdots\text{S} = 3.507(3)$  Å; Cao *et al.*, 1996].



The title compound, (I), has a methoxy substituent in the 4-position of both aromatic rings (Fig. 1); the central  $-\text{NHC}(=\text{S})\text{NC}(=\text{O})-$  moiety is flat, being held in such a conformation owing to the strong intramolecular hydrogen bond [ $\text{N}1\cdots\text{O}2 = 2.626(2)$  Å,  $\text{H}1n\cdots\text{O}2 = 1.90(2)$  Å and  $\text{N}1-\text{H}1n\cdots\text{O}2 = 141(2)^\circ$ ]. The *N'*-phenyl group is twisted by  $52.7(1)^\circ$  with respect to this moiety, whereas the *N*-phenyl group is twisted by only  $23.3(1)^\circ$ . In the crystal structure,



**Figure 1**  
*ORTEP* plot (Johnson, 1976) of the title compound depicted as a centrosymmetric hydrogen-bonded dimer. Hydrogen bonds are shown as dashed lines, displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. Unlabeled atoms are related by the symmetry code  $(1-x, 1-y, 1-z)$ .

molecules are linked through N—H···S hydrogen bonds to form centrosymmetric dimers [N2···S1<sup>i</sup> = 3.4501 (13) Å, H2n···S1<sup>i</sup> = 2.629 (16) Å and N2—H2n···S1<sup>i</sup> = 164 (2)°; symmetry code: (i) 1 - x, 1 - y, 1 - z]. The bond distances in the title compound are similar to those found in related systems (Yamin & Yusuf, 2003).

### Experimental

An acetone solution of ammonium thiocyanate (0.50 g, 6.57 mmol) and 4-anisoyl chloride (1.12 g, 6.57 mmol) was vigorously stirred. To the solution was added 4-anisidine (0.80 g, 6.57 mmol) and the mixture was heated for 2 h. The solution when cooled yielded a brown precipitate; the crude compound was purified by recrystallization from ethyl acetate to give colorless crystals.

#### Crystal data

C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> S	$D_x = 1.369 \text{ Mg m}^{-3}$
$M_r = 316.37$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3590 reflections
$a = 11.4198 (7) \text{ \AA}$	$\theta = 2.5\text{--}26.8^\circ$
$b = 11.0121 (7) \text{ \AA}$	$\mu = 0.23 \text{ mm}^{-1}$
$c = 12.2262 (8) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\beta = 93.319 (1)^\circ$	Block, colorless
$V = 1534.94 (17) \text{ \AA}^3$	$0.44 \times 0.40 \times 0.24 \text{ mm}$
$Z = 4$	

#### Data collection

Bruker SMART area-detector diffractometer	2369 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.019$
Absorption correction: none	$\theta_{\text{max}} = 27.1^\circ$
9010 measured reflections	$h = -14 \rightarrow 14$
3338 independent reflections	$k = -14 \rightarrow 13$
	$l = -15 \rightarrow 7$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2 + 0.3087P]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.132$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$
3338 reflections	$\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$
209 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Selected geometric parameters (Å, °).

S1—C8	1.655 (2)	N2—C8	1.390 (2)
N1—C1	1.426 (2)	N2—C9	1.385 (2)
N1—C8	1.330 (2)		
C1—N1—C8	126.3 (2)	N1—C8—S1	124.8 (1)
C8—N2—C8	128.0 (2)	N2—C8—S1	119.4 (1)
N1—C8—N2	115.7 (2)		

Carbon-bound H atoms were placed at calculated positions (C—H = 0.93 Å for the aromatic H atoms and C—H = 0.96 Å for the methyl H atoms) and were included in the riding-model approximation, with  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$  for the aromatic H atoms and  $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$  for the methyl H atoms. The torsion angle of the methyl groups was refined. Nitrogen-bound H atoms were located in a difference Fourier map and were refined with an N—H = 0.86 (1) Å distance restraint.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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