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O-(3,5-Dimethoxyphenyl) *N*,*N*-dimethylthiocarbamate

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Molecules of the title compound, $C_{11}H_{15}NO_3S$, display a conformation where the aromatic group is almost orthogonal to the thiocarbamate moiety. The packing arrangement is such that two parallel thiocarbamate moieties are sandwiched between two phenyl rings, with molecules separated by normal van der Waals contacts.

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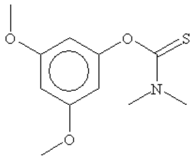
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.097
Data-to-parameter ratio = 12.1

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

Comment

The title compound, (I) (Fig. 1), was synthesized as a precursor material for an S-substituted PPV oligomer which is a possible candidate for a break-junction experiment (Weber *et al.*, 2001).



(I)

On cooling of a saturated hexane–ethyl acetate solution, (I) crystallized as large (up to 6 mm) prism-shaped crystals. The intramolecular distances and angles are as expected. The angle between the carbamate and benzene planes is 84.4 (1)°. A Cambridge Structural Database search (Allen, 2002) indicates that all compounds containing an aromatic ring substituted with an *N*,*N*-dimethylthiocarbamate moiety show the latter in an orientation nearly perpendicular to the aromatic ring. This is a steric effect, due to the large S atom interfering with the *ortho* substituents or H atoms. In the crystal structure, two parallel thiocarbamate moieties related by a centre of symmetry lie between two similarly related benzene rings, forming short stacks with different orientations, one example of which can be clearly seen in Fig. 2. The angle between one of these benzene rings and a thiocarbamate moiety is 16.9 (1)°.

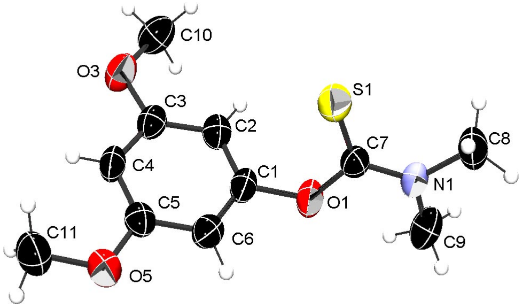


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme

There are no intermolecular contacts shorter than the sum of the van der Waals radii.

Experimental

The title compound was synthesized from 3,5-dimethoxyphenol, as reported by Wolfers *et al.* (1975) δ^1H (in p.p.m., relative to TMS, in $CDCl_3$): 6.36 (*t, J* = 2.13 Hz, 1H, H4); 6.25 (*d*, *J* = 2.13 Hz, 2H, H2 and H6), 3.75 (*s*, 6H, OCH_3), 3.45 (*s*, 3H, H8), 3.32 (*s*, 3H, H9); δ^{13}C (in p.p.m., relative to TMS, in $CDCl_3$): 187.55 (C7), 160.97 (C3 and C5), 155.57 (C1), 101.56 (C2 and C6), 98.45 (C4), 55.50 (C10 and C11), 43.24 (C8), 38.71 (C9).

Crystal data

$C_{11}H_{15}NO_3S$
$M_r = 241.30$
Orthorhombic, *Pbca*
$a = 13.113$ (3) Å
$b = 9.999$ (3) Å
$c = 18.474$ (3) Å
$V = 2422.2$ (10) Å^3
$Z = 8$
$D_x = 1.323$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 6$–18°
$\mu = 0.26$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.4 × 0.2 × 0.2 mm

Data collection

Enraf–Nonius MACH3 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
4457 measured reflections
2241 independent reflections
1159 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.059$

$\theta_{\rm max} = 25.5°$
$h = -15 \rightarrow 15$
$k = 0 \rightarrow 12$
$l = 0 \rightarrow 22$
3 standard reflections
frequency: 60 min
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.097$
$S = 0.95$
2241 reflections
185 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.20$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.21$ e Å^{-3}

The H atoms were placed in their calculated positions and allowed to refine freely, except for those on C8 and C9, which were constrained, allowing the methyl group to rotate and the distances to refine but keeping the H—C—H angles close to 109.5°.

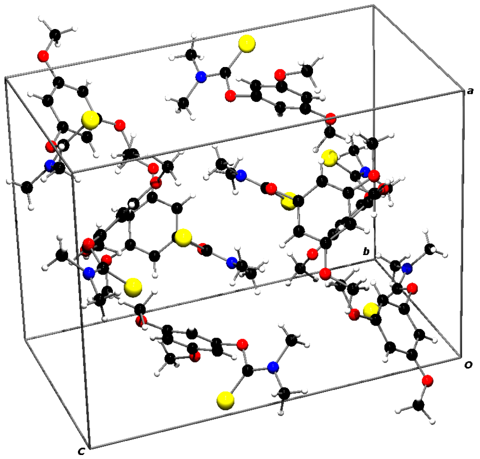


Figure 2
A view of the contents of the unit cell of (I), showing the parallel benzene and thiocarbamate moieties

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

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