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O-Methyl *N*-phenylthiocarbamate

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The central CNC(═S)O entity in MeOC(═S)N(H)Ph, C_8H_9NOS, is effectively planar and shows that the molecule exists as a thione. In the crystal structure, molecules related by a centre of symmetry are associated *via* N—H···S interactions, forming thioamide dimers.

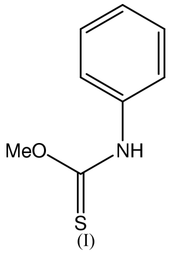
Key indicators

Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.108
Data-to-parameter ratio = 23.6

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

Comment

Neutral and deprotonated molecules related to the potentially polydentate title compound, MeOC(═S)N(H)Ph, (I), are known to coordinate metal centres in a variety of coordination modes involving combinations of the S, O and N atoms. The structure of MeOC(═S)N(H)Ph (Fig. 1 and Table 1) was determined in order to provide data to allow comparisons with the coordinated forms of the ligand. The deviation of the central atoms S, O, N and C1 from their least-squares plane are 0.0002 (3), 0.0019 (8), 0.0028 (10) and −0.0117 (12) Å, respectively. This planarity does not extend to include the phenyl group, as seen by the C1—N1—C2—C3 torsion angle of −60.13 (18)°. The C—S, C1—O and C1—N bond distances of 1.6708 (11), 1.3293 (13) and 1.3288 (15) Å, respectively, suggest some delocalization of π-electron density over the central atoms. The closest structure available for comparison is that of the *O*-ethyl analogue, *viz.* EtOC(═S)N(H)Ph (Taylor & Tiekink, 1994), with three independent molecules in the asymmetric unit. The average C—S, C1—O and C1—N distances were reported to be 1.650 (3), 1.302 (4) and 1.323 (4) Å, respectively.



(I)

In the crystal structure, symmetry-related molecules of MeOC(═S)N(H)Ph associate to form a centrosymmetric thioamide dimer (Fig. 1), having parameters N—H···S1^{i} = 2.51 Å and N1···S1^{i} = 3.3587 (12) Å with the angle subtended at H being 165° [symmetry code: (i) $-x$, $-y$, $1-z$].

Experimental

MeOC(═S)N(H)Ph was prepared according to the literature procedure (Hall *et al.*, 1993). Crystals suitable for structure analysis were grown by slow evaporation of a dichloromethane–hexane (3/1) solution of the compound (m.p. 365–367 K).

Crystal data

C_8H_9NOS
$M_r = 167.22$
Triclinic, $P\bar{1}$
$a = 5.8261\ (4)$ Å
$b = 8.3209\ (5)$ Å
$c = 9.6602\ (6)$ Å
$\alpha = 65.216\ (2)^\circ$
$\beta = 76.823\ (2)^\circ$
$\gamma = 84.066\ (3)^\circ$
$V = 413.97\ (5)$ Å^3
$Z = 2$
$D_x = 1.342$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2429 reflections
$\theta = 2.4$–30.0°
$\mu = 0.33$ mm^{-1}
$T = 223\ (2)$ K
Block, colourless
0.55 × 0.42 × 0.30 mm

Data collection

Bruker AXS SMART CCD diffractometer
ω scans
3446 measured reflections
2365 independent reflections
2128 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\rm max} = 30.0^\circ$
$h = -4 \rightarrow 8$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.108$
$S = 1.09$
2365 reflections
100 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.0605P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.22$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.33$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.6708 (11)	N1—C1	1.3288 (15)
O1—C1	1.3293 (13)	N1—C2	1.4314 (13)
O1—C8	1.4400 (15)		
C1—O1—C8	118.72 (9)	S1—C1—N1	122.98 (9)
C1—N1—C2	126.10 (10)	O1—C1—N1	112.51 (9)
S1—C1—O1	124.48 (8)		

The H atoms were introduced at calculated positions as riding atoms, with bond lengths of 0.87 (N—H), 0.94 (CH-aromatic), and 0.97 Å (CH_3). The displacement parameters were 1.2 (for CH and NH) or 1.5 (for CH_3) times $U_{\rm eq}$ of the parent atoms.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* and *SHELXTL* (Bruker, 2000); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHEXLTL*.

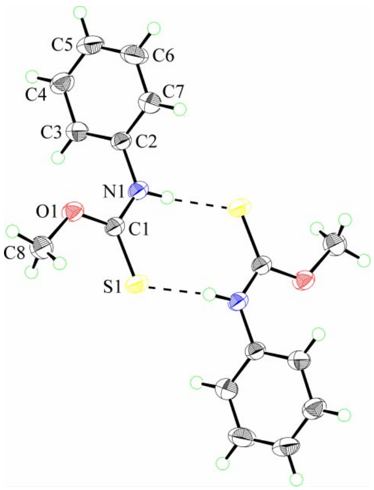


Figure 1
Hydrogen bonding and crystallographic numbering scheme for MeOC(=S)N(H)Ph. The second molecule is generated by the symmetry operation ($-x$, $-y$, $1 - z$). Displacement ellipsoids are shown at the 50% probability level (Johnson, 1976).

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