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S-Phenyl 4-cyanothiobenzoate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.077
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.

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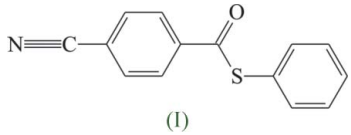
Molecules of the title compound, $C_{14}H_9NOS$, exhibit a chiral non-planar structure in which the 4-cyanophenyl and *S*-phenyl rings are tilted at dihedral angles of 1.81 (2) and 72.49 (1)° with respect to the central thiocarbonate unit.

Comment

In previous papers on the vibrational spectra and theoretical analysis of *S*-phenyl 4-substituted-thiobenzoates, we have assigned and interpreted the characteristic IR bands and predicted their molecular structures using possibilities of linear-dichroic infrared spectroscopy (Arnaudov *et al.*, 2003; Ivanova & Arnaudov, 2003). With the goal of comparing an experimental structure with the predictions of IR–LD spectroscopic analysis and *ab initio* calculations, we have now determined the single-crystal X-ray structure of the title compound, (I).



(I)

Molecules of (I) are chiral owing to the fact that the *S*-phenyl ring is twisted by 72.49 (1)° out of the plane of the thiocarbonate function to minimize the O1···C16 contact. In contrast, the 4-cyanophenyl ring (C2–C7) is almost coplanar with the central thiocarbonate unit and exhibits an interplanar angle of only 1.81 (2)°. Our IR–LD spectroscopic analysis and *ab initio* calculations predicted interplanar angles of 90.8 (6) and 0.0 (1)°, respectively. The experimental and theoretical metrical parameters obtained for (I) are closely similar.

(I) crystallizes in the non-centrosymmetric monoclinic space group $P2_1$ and participates in very weak intermolecular hydrogen bonds (Table 1). The observed structure of (I) is in good agreement with those determined for other *S*-phenyl thiobenzoates (Allouchi *et al.*, 1995; Chrusciel *et al.*, 1995; Ganesh *et al.*, 2005; Jovanovski *et al.*, 1993; Karczmarzyk *et al.*, 2001; Low *et al.*, 2000; Sakamoto *et al.*, 1996; Takahashi, Sekine *et al.*, 1998; Takahashi, Fujita *et al.*, 1998).

Experimental

The title compound was purchased as a white powder from Merck. 0.532 g were dissolved in 5 ml of methanol and the solution left (2.22 mmol) to stand to afford white crystals of (I) within 5 days. Elemental analysis for $C_{14}H_9NOS$ found: C 70.2, H 2.8, N 5.9%; calculated: C 70.3, H 3.8, N 5.9%; FAB–MS (Fisons VG Autospec) *m*/*z* 238.3 (100%).

Crystal data

$C_{14}H_9NOS$
M_r = 239.28
Monoclinic, $P2_1$
a = 7.499 (5) Å
b = 7.835 (3) Å
c = 10.624 (7) Å
β = 107.37 (8)°
V = 595.8 (6) Å^3
Z = 2
D_x = 1.334 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 15 reflections
θ = 7.6–15.8°
μ = 0.25 mm^{-1}
T = 294 (2) K
Needle, colourless
0.59 × 0.26 × 0.21 mm

Data collection

Siemens P4 four-circle diffractometer
ω scans
Absorption correction: ψ-scan (*XPREP* in *SHELXTL-Plus*; Sheldrick, 1995)
T_{min} = 0.928, T_{max} = 0.947
2572 measured reflections
2068 independent reflections
1816 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 25.1°
$h = -1 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -12 \rightarrow 12$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.077
S = 1.02
2068 reflections
155 parameters
H-atom parameters constrained.
$w = 1/[\sigma^2(F_o^2) + (0.0284P)^2 + 0.1314P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.016 (3)
Absolute structure: Flack (1983), 942 Friedel pairs
Flack parameter: −0.05 (8)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O1^{i}	0.93	2.75	3.359 (3)	124
C15—H15···O1^{i}	0.93	2.96	3.472 (4)	116
C6—H6···O1^{ii}	0.93	2.64	3.333 (4)	132
C6—H6···N5^{iii}	0.93	2.88	3.626 (4)	138
C13—H13···N5^{iv}	0.93	2.99	3.599 (4)	125

Symmetry codes: (i) $-x-1, y+\frac{1}{2}, -z+2$; (ii) $x+1, y, z$; (iii) $-x+1, y+\frac{1}{2}, -z+1$; (iv) $x-1, y, z+1$.

The H atoms were refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{iso}(C).

Data collection: *R3m/V User's Guide* (Siemens, 1989); cell refinement: *R3m/V User's Guide*; data reduction: *XDISK* (Siemens, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1995); software used to prepare material for publication: *SHELXL97*.

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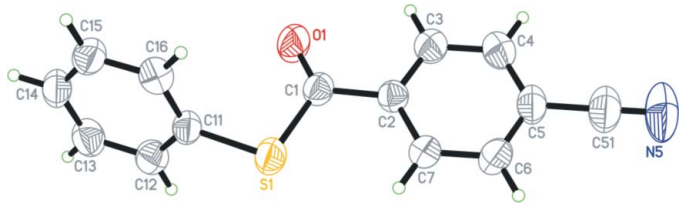

Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% propability level.

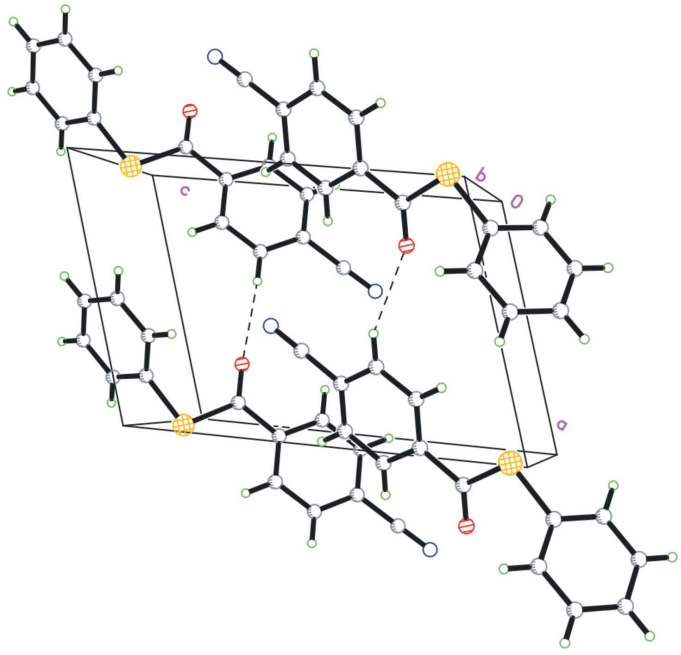

Figure 2
The packing of (I), with hydrogen bonds shown as dashed lines.

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