Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,4′-(4,4′-Thiodiphenoxy)diphthalonitrile

Hande Petek,[a]* Nesuhi Akdemir,[b] Musa Özil,[b] Erbil Ağar[b] and Ismet Şenel[a]

[a]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayís University, TR-55139 Kurupelit-Samsun, Turkey, and [b]Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139 Kurupelit-Samsun, Turkey

Correspondence e-mail: hpetek@omu.edu.tr

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.068
Data-to-parameter ratio = 12.6

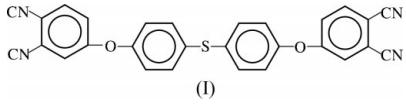
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{28}H_{14}N_4O_2S$, contains four aromatic rings, and the crystal structure is stabilized by π–π stacking.

Received 5 March 2004
Accepted 16 March 2004
Online 24 March 2004

Comment

4,4′-(4,4′-Thiodiphenoxy)diphthalonitrile, (I), is a starting material in the synthesis of network-polymeric phthalocyanines and high-performance aromatic polymers (McKeown, 1998; Takekoshi, 1987). In addition to their extensive use as dyes and pigments, phthalocyanines have found widespread application in catalysis, optical recording, photoconductive materials and photodynamic therapy, and as chemical sensors (Leznoff & Lever, 1989–1996). Polymeric phthalocyanines have been described for use as dyes and industrial high-technology materials and are also of additional interest because of their high thermostability (Leznoff & Lever, 1989–1996).



(I)

All four C≡N bonds in (I) (Table 1) show triple-bond character, and are also in good agreement with literature values (Ocak *et al.*, 2004).

The molecule of (I) is distorted from ideal C_{2v} symmetry, with dihedral angles between rings *A* (C5–C10) and *B* (C11–C16) of 50.14 (6)°, and between rings *C* (C17–C22) and *D* (C23–C28) of 67.12 (6)°. The S1—C14 and S1—C17 bond lengths and the C14—S1—C17 angle (Table 1) are in agreement with the values found for related structures (Ocak *et al.*, 2004).

The π–π stacking interaction in (I) involves ring *C* at (x, y, z) stacking with ring *C* at ($1-x$, $1-y$, $2-z$), with a distance of 3.5642 (11) Å between the centres of the two rings.

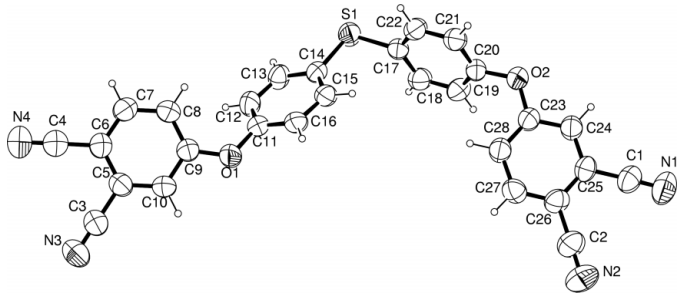


Figure 1
A view of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

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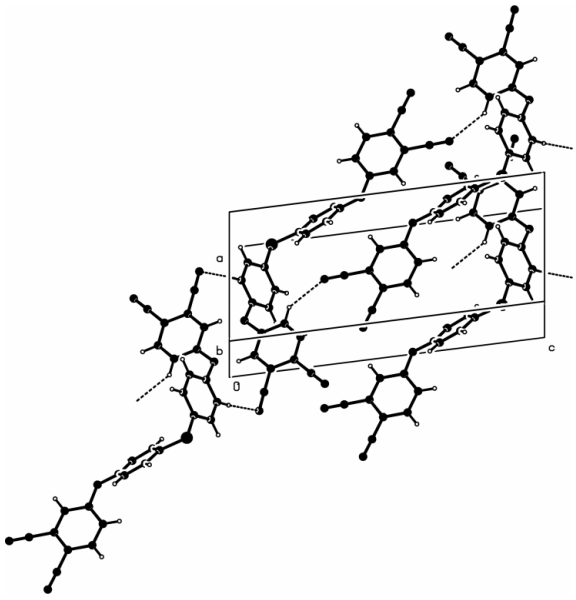

Figure 2
A packing diagram for (I), viewed on the *ac* plane.

Experimental

The title compound was synthesized according to the procedure of Takekoshi (1987). Single crystals of (I) were obtained from a solution in ethanol *via* slow evaporation at room temperature.

Crystal data

$C_{28}H_{14}N_4O_2S$
M_r = 470.49
Triclinic, $P\overline{1}$
a = 7.1028 (7) Å
b = 9.5705 (10) Å
c = 17.7700 (19) Å
α = 78.002 (2)°
β = 82.925 (8)°
γ = 78.016 (8)°
V = 1151.8 (2) Å^3
Z = 2
D_x = 1.357 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7205 reflections
θ = 1.2–26.9°
μ = 0.18 mm^{-1}
T = 293 (2) K
Plate, colourless
0.50 × 0.25 × 0.05 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: by integration (*X-RED*; Stoe & Cie, 2002)
T_{min} = 0.945, T_{max} = 0.991
15 492 measured reflections
4187 independent reflections
2287 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 25.3°
$h = -7 \rightarrow 8$
$k = -11 \rightarrow 11$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.068
S = 0.78
4187 reflections
332 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0346P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C14	1.7704 (16)	O2—C20	1.4018 (19)
S1—C17	1.7763 (16)	C3—N3	1.140 (2)
O1—C9	1.368 (2)	C1—N1	1.141 (2)
O1—C11	1.3998 (19)	C2—N2	1.134 (2)
O2—C23	1.3729 (18)	C4—N4	1.139 (2)
C9—O1—C11	121.34 (13)	C13—C14—S1	117.60 (12)
C23—O2—C20	118.40 (13)	C15—C14—S1	124.01 (13)

The H atoms were placed geometrically and refined using a riding model, fixing the aromatic C—H distance at 0.93 Å. U_{iso}(H) values were calculated as 1.2U_{eq}(aromatic C).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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