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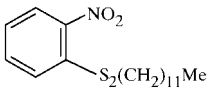
Dodecyl 2-nitrophenyl disulphide, $C_{18}H_{29}NO_2S_2$, contains an intramolecular S···O contact of 2.623 (3) Å. The angle between the planes of the NO_2 group and the attached phenyl ring is 4.2 (3)°. The thermal vibrations of the atoms increase along the paraffinic chain. The nitroso O atom not involved in the S···O intramolecular contact also has high thermal motion. Attempts to create disordered models to allow for the thermal motions were unsuccessful.

Comment

Examination of the title structure, (I), with *PLATON* (Spek, 1999) showed that there were no solvent-accessible voids in the crystal lattice.



(I)

Experimental

Dodecyl 2-nitrophenyl disulphide was obtained from $Bu_3SC_{12}H_{25}$ and 2-$O_2NC_6H_4SCl$ in $CHCl_3$ at room temperature. The solution was filtered, the filtrate was chromatographed on silica gel and the the product was recrystallized from ethanol (m.p. 314–316 K).

Crystal data

$C_{18}H_{29}NO_2S_2$
M_r = 355.54
Monoclinic, $P2_1/c$
a = 34.497 (7) Å
b = 7.796 (2) Å
c = 7.503 (2) Å
β = 95.12 (3)°
V = 2009.8 (8) Å^3
Z = 4
D_x = 1.175 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3701 reflections
θ = 2.37–26.01°
μ = 0.273 mm^{-1}
T = 150.0 (1) K
Plate, yellow
0.2 × 0.1 × 0.1 mm

Data collection

KappaCCD diffractometer
φ and ω scans with κ offset scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.947, T_{max} = 0.973
17 677 measured reflections
3701 independent reflections
2053 reflections with $I > 2\sigma(I)$
R_{int} = 0.081
θ_{max} = 26.01°
$h = -42 \rightarrow 42$
$k = -9 \rightarrow 9$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.210
S = 1.025
3701 reflections
208 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1121P)^2 + 0.0783P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Molecule (I) crystallized in the monoclinic system; space group $P2_1/c$ from the systematic absences. H atoms were treated as riding atoms with C—H 0.92–0.99 Å. An attempt to refine atoms O22 and C17 as disordered atoms, on two sites as indicated by *SHELXL*97 (Sheldrick, 1997), with the site occupancies for each atom pair tied by a free-variable resulted in a higher R factor. The high thermal motion of the atoms is not unexpected since this compound has a very low melting point.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97 and *WordPerfect* macro *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC, X-ray Crystallographic Service, University of Southampton, using an Enraf–Nonius KappaCCD diffractometer. The authors thank the staff for all there help and advice.

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