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1,4-Bis{*N*-[4-(ethoxycarbonyl)benzyl]-*N*-(4-tolylsulfonyl)aminomethyl}benzene

Martin Nieger,[a]* Holger Schwierz[b] and Fritz Vögtle[b]

[a]Institut für Anorganische Chemie, Universität Bonn, Gerhard-Domagk-Strasse 1, D-53121 Bonn, Germany, and [b]Kekulé-Institut für Organische Chemie, Universität Bonn, Gerhard-Domagk-Strasse 1, D-53121 Bonn, Germany

Correspondence e-mail: nieger@joyx.joensuu.fi

Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.002 Å
R factor = 0.033
wR factor = 0.093
Data-to-parameter ratio = 14.6

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

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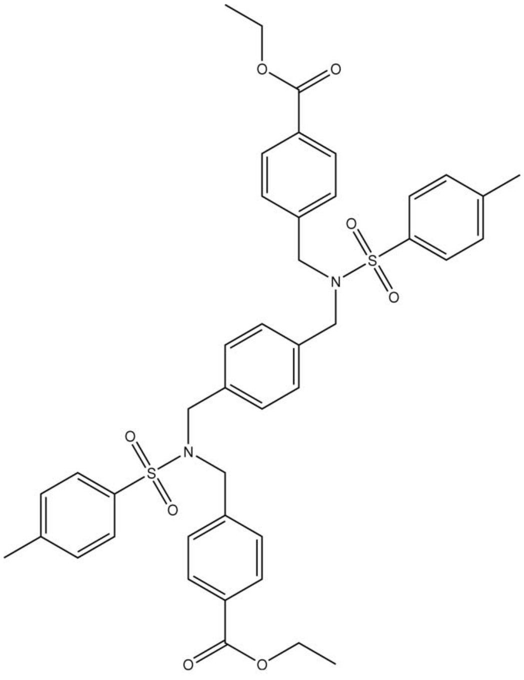
The title compound, $C_{42}H_{44}N_2O_8S_2$, features a molecular thread. The molecules have crystallographic C_i symmetry. The crystal packing shows staples stabilized by weak C—H···O interactions.

Comment

In supramolecular chemistry, and especially nanochemistry, macrocyclic and concave hydrocarbons play an important role. Nanometric scale molecules are facinating due to their often appealing architecture, high symmetry and host–guest interactions. Linear molecular threads play an important role in the synthesis of nanometer-scaled molecular ribbons and belts (Schwierz & Vögtle, 1999).



(I)

The title compound, (I), features a molecular thread. The backbone of the molecules (disregarding the tosyl residues) shows the form of the letter S. The molecules have crystallographic C_i symmetry (Fig. 1) and form, similar molecular ribbons (Breidenbach *et al.*, 1995), staples (Figs. 2 and 3) which are stabilized by weak C—H···O interactions (Table 1) (Steiner, 2002).

Experimental

The title compound was synthesized by the reaction of two equivalents of ethyl 4-(bromomethyl)benzoate and one equivalent of 1,4-

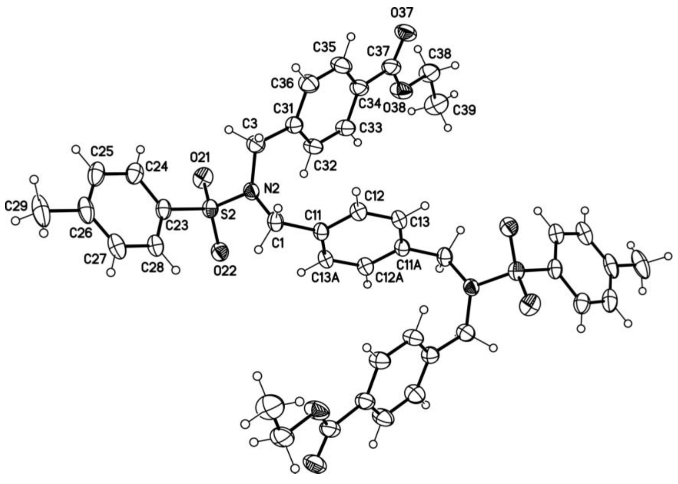


Figure 1
View of the molecule of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. [Symmetry code: (A, unlabelled atoms): $1 - x, 1 - y, 1 - z$.]

bis[*N*-(4-tolylsulfonyl)aminomethyl]benzene in *N*,*N*-dimethylformamide and K_2CO_3. The precipitate was recrystallized from CH_2Cl_2 (Schwierz, 1999).

Crystal data

$C_{42}H_{44}N_2O_8S_2$
$M_r = 768.91$
Triclinic, $P\bar{1}$
$a = 6.7007$ (2) Å
$b = 11.7108$ (5) Å
$c = 13.1888$ (5) Å
$\alpha = 78.912$ (2)°
$\beta = 80.801$ (2)°
$\gamma = 73.492$ (2)°
$V = 967.64$ (6) Å^3
$Z = 1$
$D_x = 1.320$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 15012 reflections
$\theta = 3.2$–28.3°
$\mu = 0.19$ mm^{-1}
$T = 123$ (2) K
Plates, colourless
0.35 × 0.30 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
φ scans
Absorption correction: none
15012 measured reflections
3582 independent reflections
3145 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 28.3°$
$h = -8 \rightarrow 8$
$k = -14 \rightarrow 14$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.093$
$S = 1.04$
3582 reflections
245 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.2922P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.24$ e Å^{-3}
$\Delta\rho_{\min} = -0.38$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C28—H28···O37$^{\rm i}$	0.95	2.53	3.3341 (19)	143

Symmetry code: (i) $x - 1, y + 1, z$.

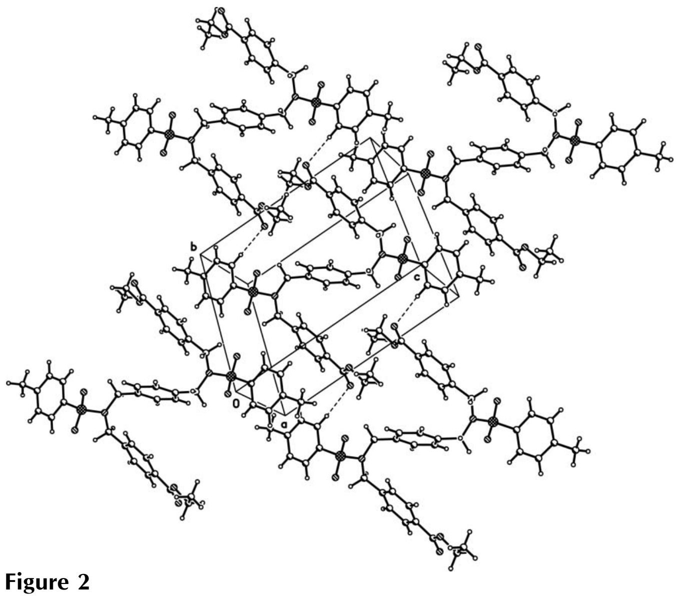


Figure 2
The crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

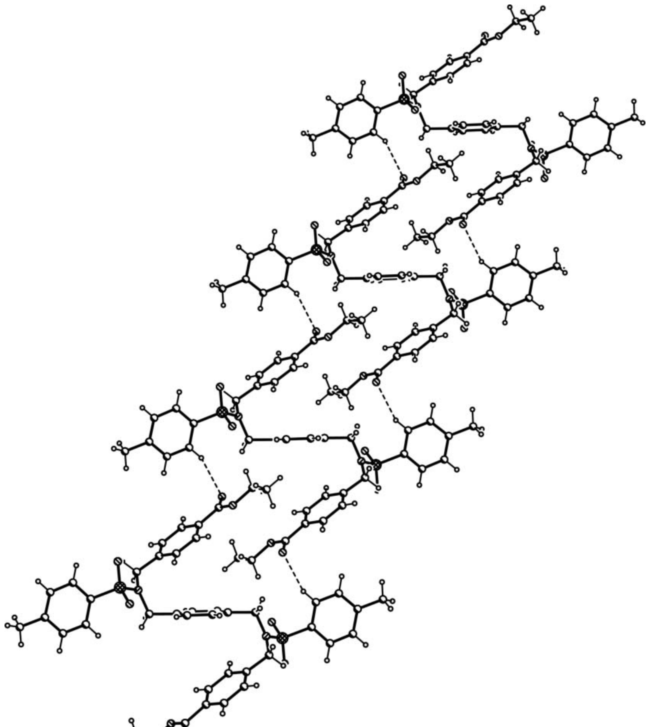


Figure 3
The staple formation of the title compound. Hydrogen bonds are shown as dashed lines.

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.98 Å and with $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–0.99 Å and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *COLLECT* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction:

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DENZO-SMN; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXL97*.

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