Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,4-Bis(benzothiazol-2-yl)benzene

Jairo Bordinhao,* Lorenzo do C. Visentin and Raquel B. Machado

Instituto de Química, Universidade Federal do Rio de Janeiro, Caixa Postal 68563, 21949-900 Rio de Janeiro, RJ, Brazil
Correspondence e-mail: jairobd@iq.ufrj.br

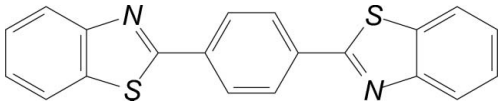
Received 11 May 2007; accepted 14 May 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.084; data-to-parameter ratio = 12.6.

The title compound, $C_{20}H_{12}N_2S_2$, was prepared by the reaction of aminothiophenol with 1,4-dicarboxyaldehyde. The molecule is centrosymmetric. The crystal structure is stabilized by an intramolecular C—H···S hydrogen-bonding interaction.

Related literature

For related literature, see: Allen *et al.* (1987); Jeffrey *et al.* (1985).



Experimental

Crystal data

$C_{20}H_{12}N_2S_2$
M_r = 344.44
Monoclinic, $C2/c$
a = 22.702 (5) Å
b = 6.4839 (13) Å
c = 11.626 (2) Å
β = 110.96 (3)°
V = 1598.1 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 295 K
0.4 × 0.04 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
8151 measured reflections
1475 independent reflections
1230 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.084
S = 1.03
1475 reflections
117 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···S1	0.91 (2)	2.75 (2)	3.139 (2)	106.7 (14)

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *PhiChi* (Duisenberg *et al.*, 2000); data reduction: *DIRAX* (Duisenberg, 1992); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank Professor Dr Renato Guimarães (LDRX), Universidade Federal Fluminense, Brazil, for use of the diffractometer facility.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2014).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L. L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.
Duisenberg, A. J. M., Hooft, R. W. W., Schreurs, A. M. M. & Kroon, J. (2000). *J. Appl. Cryst.* **33**, 893–898.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Jeffrey, G. A., Maluszynska, H. & Mitra, J. (1985). *Int. J. Biol. Macromol.* **7**, 336–348.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807023768

supplementary materials

Acta Cryst. (2007). E**63**, o3426 [**doi:10.1107/S1600536807023768**]

1,4-Bis(benzothiazol-2-yl)benzene

J. Bordinhao, L. do C. Visentin and R. B. Machado

Comment

In this work we communicate the synthesis and the structural characterization of the $C_{20}H_{12}N_2S_2$, molecule (I). Organic molecules with pairs of free electrons can be useful as ligand precursors in the synthesis of coordination complexes. The other very interesting aspect for this study are the intermolecular interactions driven by C—H··· π, directional forces, a feature with known influence to the development of supramolecular architectures. Even as weak interactions, is now clear that they play an important role in the tuning and prediction of important supramolecular precursors.

Compound (I) was synthesized considering the above statements, and his structural analysis showed a central phenyl ring environment hardwired with two phenylthiazole terminations, scheme 1. Figure 1 shows an *ORTEP* plot corresponding to 70% probability ellipsoids. Distance parameters of C—C, C—S and C—N bonds shown in table 1 are in good agreement with literature values (Allen *et al.*, 1987).

The crystal structure is stabilized by a single intramolecular C—H···S hydrogen bond (Jeffrey *et al.*, 1985) producing a five-membered ring. The corresponding geometric parameters are listed in table 2.

The C1/C2/S1/C7/N1 ring derives from the plane of C8/C9/C10/C10^{ii}/C9^{ii}/C8^{ii} [Symmetry code: (ii) = $-x$, $1-y$, $-z$)] ring from 18,3(1)°.

Experimental

1,4-dicarboxyaldehyde (0.1 mol, 0,134 g) was heated in ethanol to 313 K and the mixture stirred for 15 min. 2-amino-thiophenol (0.2 mol, 0,250 g) was added dropwise over 10 min. The temperature was maintained at this temperature for 2 h with efficient stirring before cooling to room temperature. The resulting yellow powder was filtered and dried overnight. The solid was recrystallized with methanol to yield 1,4-bis(benzothiazol-2-yl)benzene as yellow crystals. (yield: 0.28 g, 82%; m.p. 436 K).

Refinement

H10 and H8 atoms where located in a difference map and refined with distances of C10—H10 = 0.91 (2) Å and C8—H8 = 0.95 (2) and withU_{iso}(H) = 1.2U_{eq}(C). The others H atoms bonded to phenyl carbon atoms were obtained geometrically, the C—H distances fixed (0.93 Å for C_{sp2} H atoms),and the atoms refined as riding on their respective C atoms, with anisotropic displacement parameter 1.2 times the U_{eq} value for the attached C_{sp2} atom.

Figures

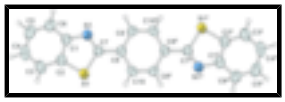


Fig. 1. - *ORTEP* of (I) with thermal parameters in a level of 70% probability.

1,4-Bis(benzothiazol-2-yl)benzene

Crystal data

$C_{20}H_{12}N_2S_2$	F_{000} = 712
M_r = 344.44	D_x = 1.432 Mg m^{-3}
Monoclinic, *C*2/*c*	Melting point: 436 K
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 22.702 (5) Å	θ = 1–27.5º
b = 6.4839 (13) Å	μ = 0.34 mm^{-1}
c = 11.626 (2) Å	*T* = 295 K
β = 110.96 (3)º	Block, yellow
V = 1598.1 (6) Å^3	0.4 × 0.04 × 0.04 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	1230 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.046
Monochromator: graphite	θ_{max} = 25.5º
T = 295 K	θ_{min} = 3.3º
φ scans, and ω scans with κ	*h* = −26→27
Absorption correction: none	*k* = −7→7
8151 measured reflections	*l* = −12→14
1475 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.031	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.084	$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 1.278P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
1475 reflections	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
117 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Distance BIND

3.1392 (0.0019) C10 - S1 2.7569 (0.0222) S1 - H10 3.4624 (0.0036) C10 - C10_$2 2.8586 (0.0226) H10 - C10_$2

Angle ANG

106.71 (1.61) C10 - H10 - S1 125.40 (1.70) C10 - H10 - C10_$2

Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)

17.7363 (0.0131) *x* + 3.6740 (0.0046) *y* − 0.4059 (0.0069) *z* = 1.9060 (0.0018)

* −0.0041 (0.0011) C1 * 0.0057 (0.0009) C2 * −0.0050 (0.0007) S1 * 0.0042 (0.0009) C7 * −0.0009 (0.0010) N1

Rms deviation of fitted atoms = 0.0043

19.8212 (0.0150) *x* + 3.1548 (0.0058) *y* − 3.9670 (0.0119) *z* = 1.5774 (0.0029)

Angle to previous plane (with approximate e.s.d.) = 18.25 (0.10)

* −0.0001 (0.0010) C8 * 0.0001 (0.0010) C9 * −0.0001 (0.0010) C10 * 0.0001 (0.0010) C10_$1 * −0.0001 (0.0010) C9_$1 * 0.0001 (0.0010) C8_$1

Rms deviation of fitted atoms = 0.0001

17.8471 (0.0109) *x* + 3.6414 (0.0027) *y* − 0.4678 (0.0063) *z* = 1.9056 (0.0016)

Angle to previous plane (with approximate e.s.d.) = 17.89 (0.09)

* 0.0065 (0.0015) C1 * −0.0071 (0.0015) C6 * −0.0082 (0.0015) C5 * 0.0023 (0.0016) C4 * 0.0064 (0.0014) C3 * 0.0082 (0.0015) C2 * −0.0150 (0.0009) S1 * 0.0008 (0.0012) C7 * 0.0061 (0.0012) N1

Rms deviation of fitted atoms = 0.0077

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C7	0.07816 (8)	0.1561 (3)	0.12153 (15)	0.0281 (4)
C8	0.01168 (9)	0.3397 (3)	−0.06910 (16)	0.0325 (4)

C9	0.03848 (8)	0.3333 (2)	0.05965 (14)	0.0267 (4)
C10	0.02618 (9)	0.4955 (3)	0.12723 (16)	0.0332 (4)
N1	0.10344 (7)	0.0265 (2)	0.06667 (13)	0.0312 (3)
C1	0.13679 (8)	−0.1263 (3)	0.14851 (15)	0.0299 (4)
C2	0.13663 (8)	−0.1094 (3)	0.26963 (15)	0.0304 (4)
C3	0.16811 (9)	−0.2525 (3)	0.36115 (17)	0.0390 (4)
H3	0.1678	−0.2405	0.4407	0.047*
C4	0.19969 (9)	−0.4124 (3)	0.32934 (19)	0.0434 (5)
H4	0.2212	−0.5090	0.3887	0.052*
C5	0.19989 (9)	−0.4317 (3)	0.20961 (19)	0.0430 (5)
H5	0.2213	−0.5413	0.1908	0.052*
C6	0.16897 (9)	−0.2915 (3)	0.11902 (18)	0.0383 (4)
H6	0.1694	−0.3059	0.0397	0.046*
S1	0.09188 (2)	0.10461 (7)	0.27816 (4)	0.03404 (17)
H8	0.0184 (9)	0.231 (3)	−0.1181 (18)	0.042 (5)*
H10	0.0433 (11)	0.494 (3)	0.211 (2)	0.055 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C7	0.0315 (9)	0.0276 (8)	0.0257 (8)	−0.0022 (7)	0.0109 (7)	0.0015 (7)
C8	0.0410 (10)	0.0297 (9)	0.0278 (9)	0.0033 (7)	0.0135 (8)	−0.0033 (7)
C9	0.0289 (9)	0.0258 (8)	0.0269 (8)	−0.0011 (7)	0.0119 (7)	0.0014 (7)
C10	0.0412 (10)	0.0352 (10)	0.0216 (9)	0.0034 (8)	0.0094 (8)	0.0008 (7)
N1	0.0364 (8)	0.0303 (8)	0.0285 (7)	0.0025 (6)	0.0134 (6)	0.0019 (6)
C1	0.0305 (9)	0.0291 (9)	0.0304 (8)	−0.0007 (7)	0.0113 (7)	0.0018 (7)
C2	0.0306 (9)	0.0294 (9)	0.0319 (9)	−0.0004 (7)	0.0119 (7)	0.0013 (7)
C3	0.0415 (11)	0.0413 (10)	0.0334 (9)	0.0049 (8)	0.0125 (8)	0.0087 (8)
C4	0.0409 (11)	0.0386 (10)	0.0478 (11)	0.0096 (9)	0.0123 (9)	0.0132 (9)
C5	0.0388 (11)	0.0360 (10)	0.0542 (12)	0.0087 (8)	0.0165 (9)	−0.0002 (9)
C6	0.0417 (11)	0.0374 (10)	0.0383 (10)	0.0044 (8)	0.0174 (8)	−0.0021 (8)
S1	0.0443 (3)	0.0340 (3)	0.0256 (2)	0.00824 (19)	0.01467 (19)	0.00382 (17)

Geometric parameters (Å, °)

C7—N1	1.305 (2)	C1—C2	1.414 (2)
C7—C9	1.478 (2)	C2—C3	1.400 (2)
C7—S1	1.7659 (17)	C2—S1	1.7435 (17)
C8—C10^{i}	1.386 (3)	C3—C4	1.384 (3)
C8—C9	1.400 (2)	C3—H3	0.9300
C8—H8	0.95 (2)	C4—C5	1.399 (3)
C9—C10	1.399 (2)	C4—H4	0.9300
C10—C8^{i}	1.386 (3)	C5—C6	1.378 (3)
C10—S1	3.1392 (19)	C5—H5	0.9300
C10—H10	0.91 (2)	C6—H6	0.9300
N1—C1	1.394 (2)	S1—H10	2.76 (2)
C1—C6	1.406 (2)		
N1—C7—C9	124.08 (15)	C6—C1—C2	119.22 (16)

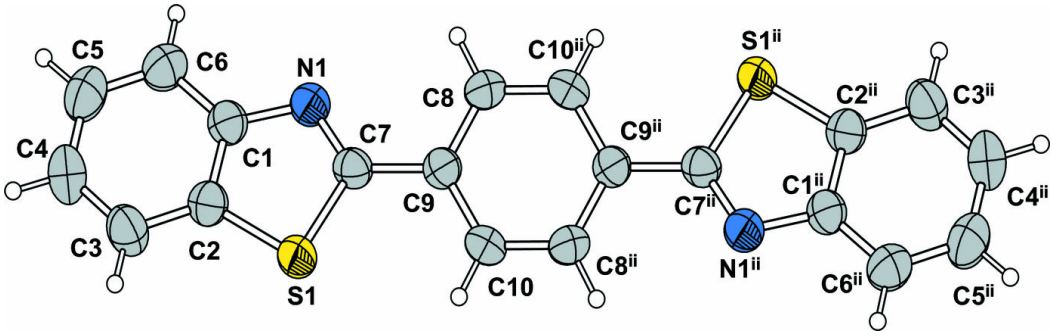
N1—C7—S1	115.85 (13)	C3—C2—C1	121.56 (16)
C9—C7—S1	120.04 (12)	C3—C2—S1	129.33 (14)
C10^{i}—C8—C9	120.04 (16)	C1—C2—S1	109.09 (12)
C10^{i}—C8—H8	118.8 (12)	C4—C3—C2	117.77 (17)
C9—C8—H8	121.1 (12)	C4—C3—H3	121.1
C10—C9—C8	118.70 (15)	C2—C3—H3	121.1
C10—C9—C7	121.34 (15)	C3—C4—C5	121.28 (17)
C8—C9—C7	119.95 (15)	C3—C4—H4	119.4
C8^{i}—C10—C9	121.26 (16)	C5—C4—H4	119.4
C8^{i}—C10—S1	169.30 (13)	C6—C5—C4	121.27 (17)
C9—C10—S1	63.69 (9)	C6—C5—H5	119.4
C8^{i}—C10—C10^{ii}	93.80 (11)	C4—C5—H5	119.4
C9—C10—C10^{ii}	131.24 (10)	C5—C6—C1	118.90 (17)
S1—C10—C10^{ii}	76.92 (5)	C5—C6—H6	120.5
C8^{i}—C10—H10	118.8 (14)	C1—C6—H6	120.5
C9—C10—H10	119.9 (14)	C2—S1—C7	89.04 (8)
S1—C10—H10	57.3 (14)	C2—S1—H10	153.5 (5)
C7—N1—C1	110.49 (14)	C7—S1—H10	68.1 (5)
N1—C1—C6	125.26 (16)	C2—S1—C10	141.34 (7)
N1—C1—C2	115.51 (15)	C7—S1—C10	52.97 (6)
C10^{i}—C8—C9—C10	0.0 (3)	C4—C5—C6—C1	0.1 (3)
C10^{i}—C8—C9—C7	179.20 (16)	N1—C1—C6—C5	−179.84 (17)
N1—C7—C9—C10	−163.27 (17)	C2—C1—C6—C5	−0.5 (3)
S1—C7—C9—C10	18.7 (2)	C3—C2—S1—C7	−179.78 (18)
N1—C7—C9—C8	17.6 (3)	C1—C2—S1—C7	−0.84 (13)
S1—C7—C9—C8	−160.46 (13)	C3—C2—S1—H10	150.6 (11)
C8—C9—C10—C8^{i}	0.0 (3)	C1—C2—S1—H10	−30.4 (11)
C7—C9—C10—C8^{i}	−179.19 (16)	C3—C2—S1—C10	170.32 (14)
C8—C9—C10—S1	169.13 (17)	C1—C2—S1—C10	−10.74 (19)
C7—C9—C10—S1	−10.02 (12)	N1—C7—S1—C2	0.74 (14)
C8—C9—C10—C10^{ii}	129.40 (17)	C9—C7—S1—C2	178.94 (14)
C7—C9—C10—C10^{ii}	−49.8 (3)	N1—C7—S1—H10	167.0 (5)
C9—C7—N1—C1	−178.50 (15)	C9—C7—S1—H10	−14.8 (5)
S1—C7—N1—C1	−0.38 (18)	N1—C7—S1—C10	173.01 (17)
C7—N1—C1—C6	179.07 (17)	C9—C7—S1—C10	−8.79 (11)
C7—N1—C1—C2	−0.3 (2)	C8^{i}—C10—S1—C2	141.5 (7)
N1—C1—C2—C3	179.88 (16)	C9—C10—S1—C2	21.41 (16)
C6—C1—C2—C3	0.5 (3)	C10^{ii}—C10—S1—C2	171.84 (10)
N1—C1—C2—S1	0.85 (19)	C8^{i}—C10—S1—C7	129.1 (7)
C6—C1—C2—S1	−178.58 (14)	C9—C10—S1—C7	8.97 (11)
C1—C2—C3—C4	0.0 (3)	C10^{ii}—C10—S1—C7	159.40 (10)
S1—C2—C3—C4	178.80 (15)	C8^{i}—C10—S1—H10	−71.5 (18)
C2—C3—C4—C5	−0.4 (3)	C9—C10—S1—H10	168.5 (17)
C3—C4—C5—C6	0.4 (3)	C10^{ii}—C10—S1—H10	−41.1 (17)

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···S1	0.91 (2)	2.75 (2)	3.139 (2)	106.7 (14)

Fig. 1


C5
C6
N1
C4
C1
C7
C8
C10ii
S1ii
C2ii
C3ii
C9ii
C1ii
C4ii
C9
C7ii
C3
C2
S1
C10
C8ii
N1ii
C6ii
C5ii