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4,4′-Diphenyl-2,2′-bi-1,3-thiazole

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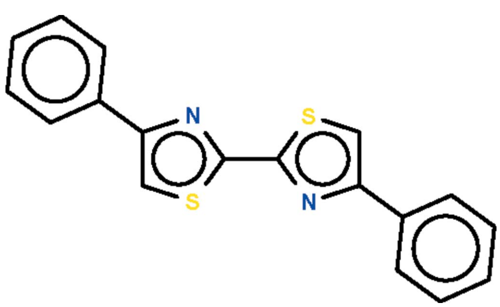
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.028; wR factor = 0.079; data-to-parameter ratio = 17.3.

In the centrosymmetric title compound, $C_{18}H_{12}N_2S_{24}$, the five- (r.m.s. deviation = 0.002 Å) and six-membered (r.m.s. deviation = 0.002 Å) rings are essentially coplanar [dihedral angle between rings = 1.9 (1)°].

Related literature

For the crystal structures of other 4,4′-disubstituted compounds, see: Bolognesi *et al.* (1987); Craig *et al.* (1988); Curtis *et al.* (2004).



Experimental

Crystal data

$C_{18}H_{12}N_2S_2$
M_r = 320.42
Monoclinic, $P2_1/c$
a = 5.7769 (4) Å
b = 7.6573 (5) Å
c = 17.1960 (12) Å
β = 99.614 (1)°
V = 749.99 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 100 K
0.30 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.902, T_{max} = 0.966
6993 measured reflections
1730 independent reflections
1575 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.079
S = 1.04
1730 reflections
100 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

I thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NK2046).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bolognesi, A., Catellani, M., Destri, S. & Porzio, W. (1987). *Acta Cryst.* C**43**, 1171–1173.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Craig, D. C., Goodwin, H. A., Onggo, D. & Rae, A. D. (1988). *Aust. J. Chem.* **41**, 1625–1644.
Curtis, D., Cao, J. & Kampf, J. F. (2004). *J. Am. Chem. Soc.* **126**, 4318–4328.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2010). E**66**, o2030 [**doi:10.1107/S1600536810027261**]

4,4'-Diphenyl-2,2'-bi-1,3-thiazole

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Comment

2,2'-Bithiazole and other 4,4'-disubstituted derivatives possess a pair of nitrogen-donor sites that renders such molecules capable of chelating metal atoms. The crystal structure of the parent compound as well as those of the methyl and ethyl substituted derivatives have been reported (Bolognesi *et al.*, 1987; Craig *et al.*, 1988, Curtis *et al.*, 2004). These molecules are centrosymmetric compounds having an inversion center midway along the C_{azolyl}–C_{azolyl} bond. In the parent compound, this bond is 1.468 (6) Å (Bolognesi *et al.*, 1987). The bond is somewhat shortened to 1.455 (2) Å in the phenyl analog (Scheme I, Fig. 1).

Experimental

The organic compound was returned unchanged in an attempted reaction of lead(II) nitrate (0.13 mmol, 0.04 g) with 4,4'-diphenyl-2,2'-bithiazole (0.25 mmol, 0.08 g) in the presence of potassium thiocyanate (0.25 mmol, 0.03 g) in a methanol/THF mixture. Crystals were obtained after one week of setting the mixture aside.

Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.95 Å) and included in the refinement in the riding model approximation, with *U*(H) set to $1.2U_{eq}$(C).

Figures

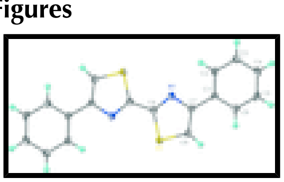

Fig. 1. Displacement ellipsoid plot (Barbour, 2001) of $C_{18}H_{12}N_2S_2$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. The molecule lies on an inversion center.

4,4'-Diphenyl-2,2'-bi-1,3-thiazole

Crystal data

$C_{18}H_{12}N_2S_2$	$F(000) = 332$
$M_r = 320.42$	$D_x = 1.419$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4091 reflections
$a = 5.7769$ (4) Å	θ = 2.4–28.3°
$b = 7.6573$ (5) Å	μ = 0.35 mm^{-1}
$c = 17.1960$ (12) Å	$T = 100$ K

$\beta = 99.614\ (1)°$	Prism, colorless
$V = 749.99\ (9)$ Å^3	0.30 × 0.10 × 0.10 mm
$Z = 2$	

Data collection

Bruker SMART APEX diffractometer	1730 independent reflections
Radiation source: fine-focus sealed tube	1575 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.026$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -7 \rightarrow 7$
$T_{min} = 0.902$, $T_{max} = 0.966$	$k = -9 \rightarrow 9$
6993 measured reflections	$l = -21 \rightarrow 22$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.028$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.079$	H-atom parameters constrained
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 0.350P]$ where $P = (F_o^2 + 2F_c^2)/3$
1730 reflections	$(\Delta/\sigma)_{max} = 0.001$
100 parameters	$\Delta\rho_{max} = 0.42$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.24$ e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.76174 (5)	0.35670 (4)	0.446214 (17)	0.01797 (12)
N1	0.35546 (18)	0.49301 (13)	0.39798 (6)	0.0151 (2)
C1	0.2750 (2)	0.43006 (15)	0.25545 (7)	0.0139 (2)
C2	0.0586 (2)	0.51551 (16)	0.24862 (7)	0.0156 (2)
H2	0.0132	0.5690	0.2936	0.019*
C3	−0.0906 (2)	0.52260 (16)	0.17611 (7)	0.0179 (3)
H3	−0.2377	0.5804	0.1719	0.022*
C4	−0.0255 (2)	0.44574 (17)	0.10999 (7)	0.0198 (3)
H4	−0.1278	0.4505	0.0607	0.024*
C5	0.1903 (2)	0.36157 (16)	0.11614 (7)	0.0193 (3)
H5	0.2355	0.3094	0.0708	0.023*
C6	0.3399 (2)	0.35345 (15)	0.18827 (7)	0.0165 (3)
H6	0.4868	0.2957	0.1921	0.020*
C7	0.4293 (2)	0.41960 (15)	0.33292 (7)	0.0140 (2)
C8	0.6444 (2)	0.34026 (16)	0.34867 (7)	0.0167 (3)

H8	0.7186	0.2835	0.3103	0.020*
C9	0.5133 (2)	0.46895 (15)	0.46100 (7)	0.0150 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01731 (17)	0.02092 (18)	0.01515 (17)	0.00472 (11)	0.00112 (12)	−0.00100 (11)
N1	0.0165 (5)	0.0146 (5)	0.0145 (5)	−0.0003 (4)	0.0035 (4)	0.0003 (4)
C1	0.0159 (6)	0.0113 (5)	0.0149 (6)	−0.0023 (4)	0.0038 (4)	0.0007 (4)
C2	0.0166 (6)	0.0142 (6)	0.0167 (6)	−0.0010 (4)	0.0046 (5)	−0.0004 (4)
C3	0.0156 (6)	0.0155 (6)	0.0221 (6)	−0.0006 (4)	0.0014 (5)	0.0004 (5)
C4	0.0229 (7)	0.0179 (6)	0.0167 (6)	−0.0023 (5)	−0.0020 (5)	−0.0003 (5)
C5	0.0256 (7)	0.0179 (6)	0.0147 (6)	−0.0011 (5)	0.0044 (5)	−0.0030 (4)
C6	0.0180 (6)	0.0149 (6)	0.0172 (6)	0.0006 (4)	0.0040 (5)	−0.0007 (4)
C7	0.0168 (6)	0.0115 (5)	0.0145 (5)	−0.0017 (4)	0.0043 (4)	−0.0004 (4)
C8	0.0187 (6)	0.0176 (6)	0.0141 (5)	0.0006 (4)	0.0034 (4)	−0.0013 (4)
C9	0.0164 (6)	0.0134 (5)	0.0157 (6)	0.0001 (4)	0.0041 (4)	0.0001 (4)

Geometric parameters (Å, °)

S1—C8	1.7056 (12)	C3—H3	0.9500
S1—C9	1.7278 (12)	C4—C5	1.3914 (18)
N1—C9	1.3076 (15)	C4—H4	0.9500
N1—C7	1.3817 (15)	C5—C6	1.3897 (17)
C1—C2	1.3981 (16)	C5—H5	0.9500
C1—C6	1.4013 (16)	C6—H6	0.9500
C1—C7	1.4762 (16)	C7—C8	1.3690 (17)
C2—C3	1.3934 (17)	C8—H8	0.9500
C2—H2	0.9500	C9—C9^{i}	1.455 (2)
C3—C4	1.3870 (18)		
C8—S1—C9	88.74 (6)	C6—C5—H5	119.9
C9—N1—C7	110.30 (10)	C4—C5—H5	119.9
C2—C1—C6	119.02 (11)	C5—C6—C1	120.33 (11)
C2—C1—C7	119.86 (11)	C5—C6—H6	119.8
C6—C1—C7	121.11 (11)	C1—C6—H6	119.8
C3—C2—C1	120.28 (11)	C8—C7—N1	114.40 (11)
C3—C2—H2	119.9	C8—C7—C1	126.45 (11)
C1—C2—H2	119.9	N1—C7—C1	119.14 (10)
C4—C3—C2	120.33 (11)	C7—C8—S1	111.12 (9)
C4—C3—H3	119.8	C7—C8—H8	124.4
C2—C3—H3	119.8	S1—C8—H8	124.4
C3—C4—C5	119.76 (11)	N1—C9—C9^{i}	123.47 (14)
C3—C4—H4	120.1	N1—C9—S1	115.44 (9)
C5—C4—H4	120.1	C9^{i}—C9—S1	121.09 (12)
C6—C5—C4	120.27 (11)		
C6—C1—C2—C3	0.60 (17)	C6—C1—C7—C8	0.67 (18)
C7—C1—C2—C3	−178.53 (11)	C2—C1—C7—N1	0.83 (16)
C1—C2—C3—C4	−0.32 (18)	C6—C1—C7—N1	−178.29 (11)

C2—C3—C4—C5	−0.17 (18)	N1—C7—C8—S1	−0.35 (13)
C3—C4—C5—C6	0.36 (19)	C1—C7—C8—S1	−179.35 (9)
C4—C5—C6—C1	−0.06 (18)	C9—S1—C8—C7	0.34 (10)
C2—C1—C6—C5	−0.41 (17)	C7—N1—C9—C9^{i}	−179.94 (14)
C7—C1—C6—C5	178.71 (11)	C7—N1—C9—S1	0.14 (13)
C9—N1—C7—C8	0.13 (15)	C8—S1—C9—N1	−0.28 (10)
C9—N1—C7—C1	179.22 (10)	C8—S1—C9—C9^{i}	179.80 (14)
C2—C1—C7—C8	179.79 (12)		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1