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5,5′-Diphenyl-2,2′-[butane-1,4-diylbis(sulfanediyl)]bis(1,3,4-oxadiazole)

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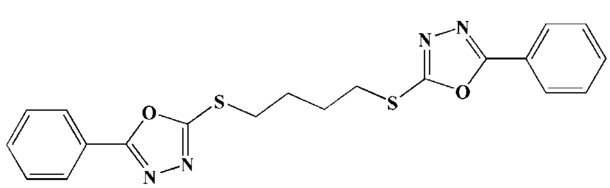
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.128; data-to-parameter ratio = 13.0.

The complete molecule of the title compound, $C_{20}H_{18}N_4O_2S_2$, is generated by crystallographic inversion symmetry. The benzene ring is almost coplanar with the oxadiazole ring [dihedral angle = 7.2 (2)°].

Related literature

Functionalized 1,3,4-oxadiazole derivatives are of interest because of their biological activity and their wide applications in medicine, coordination chemistry and their use as organic electroluminescent (EL) devices, since these compounds possess good electron-accepting properties, see: Bentiss *et al.* (2000); Hughes & Bryce (2005); Navidpour *et al.* (2006).



Experimental

Crystal data

$C_{20}H_{18}N_4O_2S_2$	V = 949.2 (3) Å^3
M_r = 410.50	Z = 2
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 12.202 (2) Å	μ = 0.31 mm^{-1}
b = 5.9317 (12) Å	T = 113 K
c = 13.518 (3) Å	0.20 × 0.18 × 0.12 mm
β = 104.04 (3)°	

Data collection

Rigaku Saturn CCD area-detector diffractometer	7030 measured reflections
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)	1661 independent reflections
T_{min} = 0.942, T_{max} = 0.964	1323 reflections with $I > 2\sigma(I)$
	R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040	128 parameters
$wR(F^2)$ = 0.128	H-atom parameters constrained
S = 1.10	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
1661 reflections	$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2072).

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supporting information

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S1. Comment

Functionalized 1,3,4-oxadiazole derivatives are of interest because of their biological activity and their wide applications in medicine, coordination chemistry and their use as organic electroluminescent (EL) devices, since these compounds possess good electron-accepting properties (Bentiss *et al.*, 2000; Navidpour *et al.*, 2006; Hughes & Bryce, 2005). We report here the synthesis and crystal structure of the title compound, $C_{20}H_{18}N_4O_2S_2$ (I). In the structure of the title compound the molecule has an inversion centre at the mid-point of the central C10—C10^{i} bond (symmetry code for (i): -*x* + 1,-*y* + 3, -*z* + 1), the asymmetric unit containing half a molecule (Fig. 1). The mean plane of the oxadiazole ring is almost coplanar with the mean plane of the attached benzene ring [dihedral angle 7.2 (2)°]. As a result of π-π conjugation, the C_{sp^2}-S bond [S1—C8 = 1.729 (2) Å] is significantly shorter than the C_{sp^3}-S bond [S1—C9 = 1.818 (2) Å].

S2. Experimental

A suspension of 5-phenyl-1,3,4-oxadiazole-2-thiol (2.0 mmol) and 1,4-dibromobutane (1.0 mmol) in ethanol (10 ml) was stirred at room temperature. The reaction progress was monitored *via* TLC. The resulting precipitate was filtered off, washed with cold ethanol, dried and purified to give the title compound as a light yellow solid in 93% yield. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform-ethanol (1:1).

S3. Refinement

All H atoms were positioned geometrically (C—H = 0.95–0.99 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

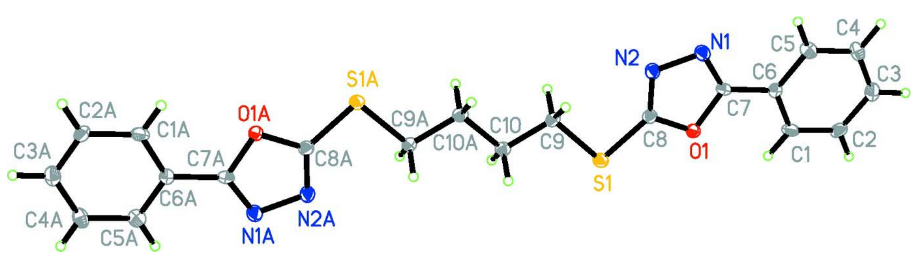

Figure 1

A view of the molecule of (I) showing the atom-labelling scheme. Atoms of the inversion-related atoms are indicated by symmetry code 'A' (-*x* + 1,-*y* + 3, -*z* + 1). Displacement ellipsoids are drawn at the 35% probability level.

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Crystal data

$C_{20}H_{18}N_4O_2S_2$
M_r = 410.50
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

a = 12.202 (2) Å
b = 5.9317 (12) Å
c = 13.518 (3) Å
β = 104.04 (3)°
V = 949.2 (3) Å^3
Z = 2
F(000) = 428
D_x = 1.436 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3017 reflections
θ = 1.7–27.9°
μ = 0.31 mm^{-1}
T = 113 K
Prism, colorless
0.20 × 0.18 × 0.12 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.942, T_{max} = 0.964

7030 measured reflections
1661 independent reflections
1323 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 25.0°, θ_{min} = 1.7°
h = −12→14
k = −7→6
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.128
S = 1.10
1661 reflections
128 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0778P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.067 (10)

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.

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 $F^2 > \sigma(F^2)$ 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}
S1	0.43518 (5)	1.09305 (10)	0.65529 (4)	0.0256 (3)
O1	0.30541 (12)	0.7504 (3)	0.68093 (12)	0.0210 (4)
N1	0.19647 (17)	0.6825 (3)	0.52644 (14)	0.0265 (5)
N2	0.26743 (17)	0.8685 (3)	0.51955 (14)	0.0242 (5)
C1	0.2073 (2)	0.3923 (4)	0.77192 (18)	0.0278 (6)
H1	0.2568	0.4939	0.8155	0.033*
C2	0.1655 (2)	0.2040 (4)	0.81204 (19)	0.0292 (6)

H2	0.1869	0.1762	0.8834	0.035*
C3	0.0925 (2)	0.0563 (4)	0.7481 (2)	0.0291 (6)
H3	0.0657	−0.0740	0.7757	0.035*
C4	0.0589 (2)	0.0987 (4)	0.64463 (19)	0.0278 (6)
H4	0.0071	−0.0001	0.6016	0.033*
C5	0.1004 (2)	0.2843 (4)	0.60345 (18)	0.0258 (6)
H5	0.0778	0.3123	0.5322	0.031*
C6	0.17557 (19)	0.4300 (4)	0.66720 (17)	0.0185 (6)
C7	0.22137 (19)	0.6207 (4)	0.62076 (17)	0.0193 (6)
C8	0.3285 (2)	0.8996 (4)	0.61119 (17)	0.0214 (6)
C9	0.4184 (2)	1.2482 (4)	0.53652 (18)	0.0235 (6)
H9A	0.4274	1.1445	0.4817	0.028*
H9B	0.3417	1.3145	0.5166	0.028*
C10	0.5064 (2)	1.4340 (4)	0.55008 (17)	0.0216 (6)
H10A	0.5829	1.3674	0.5705	0.026*
H10B	0.4970	1.5378	0.6048	0.026*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0253 (4)	0.0301 (5)	0.0194 (4)	−0.0069 (3)	0.0015 (3)	0.0035 (2)
O1	0.0202 (9)	0.0232 (9)	0.0192 (9)	−0.0025 (7)	0.0038 (7)	0.0028 (6)
N1	0.0304 (12)	0.0260 (12)	0.0215 (11)	−0.0067 (10)	0.0035 (9)	−0.0009 (9)
N2	0.0293 (12)	0.0238 (11)	0.0191 (11)	−0.0046 (9)	0.0056 (9)	0.0011 (8)
C1	0.0193 (14)	0.0368 (16)	0.0239 (14)	−0.0036 (11)	−0.0014 (11)	0.0017 (10)
C2	0.0258 (14)	0.0363 (16)	0.0244 (13)	−0.0007 (12)	0.0039 (11)	0.0127 (11)
C3	0.0250 (14)	0.0234 (13)	0.0418 (16)	0.0021 (11)	0.0138 (12)	0.0038 (11)
C4	0.0325 (16)	0.0220 (14)	0.0316 (15)	−0.0059 (11)	0.0129 (12)	−0.0073 (10)
C5	0.0288 (14)	0.0296 (15)	0.0207 (13)	−0.0018 (11)	0.0093 (11)	−0.0062 (10)
C6	0.0180 (13)	0.0179 (13)	0.0214 (12)	0.0033 (10)	0.0084 (10)	−0.0013 (9)
C7	0.0160 (13)	0.0238 (14)	0.0171 (12)	0.0010 (10)	0.0020 (10)	−0.0039 (9)
C8	0.0202 (13)	0.0241 (14)	0.0196 (12)	0.0000 (10)	0.0045 (10)	0.0019 (9)
C9	0.0249 (13)	0.0244 (13)	0.0199 (12)	−0.0010 (11)	0.0031 (10)	0.0054 (10)
C10	0.0225 (13)	0.0212 (13)	0.0199 (13)	0.0021 (10)	0.0031 (10)	−0.0018 (9)

Geometric parameters (Å, º)

S1—C8	1.729 (2)	C3—H3	0.9500
S1—C9	1.818 (2)	C4—C5	1.384 (3)
O1—C8	1.371 (3)	C4—H4	0.9500
O1—C7	1.378 (3)	C5—C6	1.396 (3)
N1—C7	1.290 (3)	C5—H5	0.9500
N1—N2	1.419 (3)	C6—C7	1.468 (3)
N2—C8	1.295 (3)	C9—C10	1.518 (3)
C1—C2	1.391 (3)	C9—H9A	0.9900
C1—C6	1.392 (3)	C9—H9B	0.9900
C1—H1	0.9500	C10—C10^{i}	1.539 (4)
C2—C3	1.390 (4)	C10—H10A	0.9900

C2—H2	0.9500	C10—H10B	0.9900
C3—C4	1.382 (3)		

C8—S1—C9	96.73 (11)	C1—C6—C7	121.2 (2)
C8—O1—C7	101.66 (17)	C5—C6—C7	118.3 (2)
C7—N1—N2	106.53 (18)	N1—C7—O1	112.81 (19)
C8—N2—N1	105.48 (18)	N1—C7—C6	128.2 (2)
C2—C1—C6	119.2 (2)	O1—C7—C6	118.9 (2)
C2—C1—H1	120.4	N2—C8—O1	113.5 (2)
C6—C1—H1	120.4	N2—C8—S1	129.42 (18)
C3—C2—C1	120.2 (2)	O1—C8—S1	117.02 (17)
C3—C2—H2	119.9	C10—C9—S1	109.62 (17)
C1—C2—H2	119.9	C10—C9—H9A	109.7
C4—C3—C2	120.2 (2)	S1—C9—H9A	109.7
C4—C3—H3	119.9	C10—C9—H9B	109.7
C2—C3—H3	119.9	S1—C9—H9B	109.7
C3—C4—C5	120.3 (2)	H9A—C9—H9B	108.2
C3—C4—H4	119.9	C9—C10—C10^{i}	110.2 (2)
C5—C4—H4	119.9	C9—C10—H10A	109.6
C4—C5—C6	119.6 (2)	C10^{i}—C10—H10A	109.6
C4—C5—H5	120.2	C9—C10—H10B	109.6
C6—C5—H5	120.2	C10^{i}—C10—H10B	109.6
C1—C6—C5	120.5 (2)	H10A—C10—H10B	108.1

C7—N1—N2—C8	0.1 (2)	C1—C6—C7—N1	−176.7 (2)
C6—C1—C2—C3	−0.4 (4)	C5—C6—C7—N1	4.3 (4)
C1—C2—C3—C4	−1.5 (4)	C1—C6—C7—O1	6.5 (3)
C2—C3—C4—C5	2.0 (4)	C5—C6—C7—O1	−172.54 (19)
C3—C4—C5—C6	−0.6 (4)	N1—N2—C8—O1	−0.1 (3)
C2—C1—C6—C5	1.8 (3)	N1—N2—C8—S1	177.74 (17)
C2—C1—C6—C7	−177.2 (2)	C7—O1—C8—N2	0.0 (2)
C4—C5—C6—C1	−1.3 (3)	C7—O1—C8—S1	−178.11 (15)
C4—C5—C6—C7	177.7 (2)	C9—S1—C8—N2	6.4 (2)
N2—N1—C7—O1	−0.1 (2)	C9—S1—C8—O1	−175.89 (17)
N2—N1—C7—C6	−177.1 (2)	C8—S1—C9—C10	−178.33 (17)
C8—O1—C7—N1	0.1 (2)	S1—C9—C10—C10^{i}	179.7 (2)
C8—O1—C7—C6	177.40 (19)		

Symmetry code: (i) $-x+1, -y+3, -z+1$.