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4,4′,5,5′-Tetraphenyl-2,2′-dithiodi-1,3-oxazole

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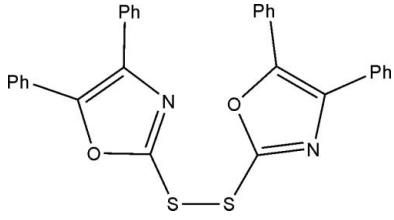
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.052; wR factor = 0.108; data-to-parameter ratio = 13.3.

The asymmetric unit of the title compound, $C_{30}H_{20}N_2O_2S_2$, contains one-half of the molecule; a twofold rotation axis passes through the mid-point of the S—S bond. In the molecule, the S—S bond length is 2.049 (2) Å.

Related literature

For normal values of S—S bond lengths in organic compounds, see: Schroth *et al.* (1998).



Experimental

Crystal data

$C_{30}H_{20}N_2O_2S_2$
M_r = 504.60
Orthorhombic, *Pbcn*
a = 30.60540 (12) Å
b = 10.1073 (4) Å
c = 8.1631 (3) Å
V = 2525.16 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 298 (2) K
0.20 × 0.16 × 0.08 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.953, T_{max} = 0.981
11778 measured reflections
2167 independent reflections
847 reflections with $I > 2\sigma(I)$
R_{int} = 0.127

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.108
S = 1.00
2167 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: CV2354).

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supplementary materials

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4,4',5,5'-Tetraphenyl-2,2'-dithiodi-1,3-oxazole

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Comment

In the title molecule (Fig. 1) the S—S bond length is 2.049 (2) Å, which is consistent with the literature data (Schroth *et al.*, 1998).

Experimental

To an ethanol (10 ml) solution of 4,5-diphenyl-2-mercaptooxazole (1 mmol) was added an ethanol (5 ml) solution of iodine (2 mmol). The mixture was stirring for 3 h at room temperature, an colorless solution was obtained, which was filtered. The filtrate was left undisturbed at room temperature for two weeks. Crystals of the title compound suitable for X-ray analysis were grown from an ethanol solution (yield 60%).

Refinement

All H atoms were placed in geometrically idealized positions (C—H 0.93 Å) and treated as riding on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

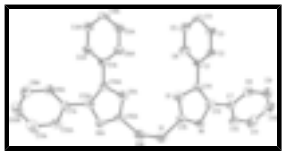


Fig. 1. The molecular structure of the title compound showing the atomic numbering and 30% probability displacement ellipsoids [symmetry code: (A) $-x + 2, y, -z + 1/2$].

4,4',5,5'-Tetraphenyl-2,2'-dithiodi-1,3-oxazole

Crystal data

$C_{30}H_{20}N_2O_2S_2$	$F_{000} = 1048$
$M_r = 504.60$	$D_x = 1.327$ Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n 2a b	Cell parameters from 1176 reflections
$a = 30.60540$ (12) Å	θ = 2.7–19.4º
$b = 10.1073$ (4) Å	μ = 0.24 mm^{-1}
$c = 8.1631$ (3) Å	$T = 298$ (2) K
$V = 2525.16$ (14) Å^3	Block, colourless
$Z = 4$	0.20 × 0.16 × 0.08 mm

Data collection

Siemens SMART CCD area-detector diffractometer	2167 independent reflections
Radiation source: fine-focus sealed tube	847 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.127$
$T = 298(2)$ K	$\theta_{max} = 25.0^{o}$
φ and ω scans	$\theta_{min} = 2.1^{o}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -36\rightarrow35$
$T_{min} = 0.953$, $T_{max} = 0.981$	$k = -10\rightarrow12$
11778 measured reflections	$l = -9\rightarrow9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.026P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
2167 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
163 parameters	$\Delta\rho_{min} = -0.20$ 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.

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 $F^2 > 2$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}
N1	0.90107 (11)	0.7419 (3)	0.2113 (4)	0.0480 (9)
O1	0.94457 (9)	0.5774 (3)	0.2838 (3)	0.0627 (9)
S1	0.97796 (4)	0.81655 (10)	0.34446 (15)	0.0691 (4)
C1	0.90583 (14)	0.3774 (4)	0.2110 (5)	0.0459 (11)
C2	0.87761 (12)	0.3110 (4)	0.1066 (5)	0.0553 (12)

H2	0.8582	0.3585	0.0414	0.066*
C3	0.87819 (13)	0.1759 (4)	0.0993 (5)	0.0591 (12)
H3	0.8593	0.1327	0.0280	0.071*
C4	0.90618 (16)	0.1022 (4)	0.1953 (6)	0.0667 (14)
H4	0.9056	0.0102	0.1915	0.080*
C5	0.93462 (16)	0.1664 (4)	0.2956 (6)	0.0711 (14)
H5	0.9540	0.1176	0.3593	0.085*
C6	0.93523 (14)	0.3028 (4)	0.3045 (6)	0.0661 (13)
H6	0.9552	0.3452	0.3727	0.079*
C7	0.83519 (13)	0.6307 (4)	0.1133 (5)	0.0445 (11)
C8	0.80258 (14)	0.5447 (4)	0.1608 (5)	0.0591 (12)
H8	0.8090	0.4778	0.2352	0.071*
C9	0.76072 (15)	0.5555 (5)	0.1006 (6)	0.0696 (14)
H9	0.7391	0.4969	0.1340	0.084*
C10	0.75143 (19)	0.6547 (6)	−0.0098 (7)	0.0871 (19)
H10	0.7234	0.6617	−0.0530	0.104*
C11	0.7829 (2)	0.7432 (6)	−0.0567 (6)	0.0845 (17)
H11	0.7760	0.8108	−0.1295	0.101*
C12	0.82454 (15)	0.7323 (4)	0.0034 (5)	0.0555 (12)
H12	0.8458	0.7925	−0.0288	0.067*
C13	0.87958 (14)	0.6239 (4)	0.1786 (4)	0.0447 (11)
C14	0.90666 (13)	0.5217 (4)	0.2202 (5)	0.0482 (11)
C15	0.93823 (15)	0.7093 (4)	0.2735 (5)	0.0504 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.046 (2)	0.0399 (19)	0.058 (2)	−0.0002 (18)	−0.0060 (19)	0.0021 (18)
O1	0.065 (2)	0.0476 (18)	0.075 (2)	0.0027 (16)	−0.0032 (17)	−0.0059 (16)
S1	0.0714 (8)	0.0506 (7)	0.0854 (10)	0.0046 (6)	−0.0135 (7)	−0.0172 (7)
C1	0.063 (3)	0.036 (2)	0.039 (3)	−0.003 (2)	0.006 (2)	0.003 (2)
C2	0.063 (3)	0.039 (3)	0.064 (3)	0.009 (2)	−0.007 (3)	0.005 (3)
C3	0.070 (3)	0.042 (3)	0.065 (3)	0.008 (2)	−0.002 (3)	−0.009 (3)
C4	0.079 (4)	0.025 (3)	0.097 (4)	0.008 (2)	−0.001 (3)	0.001 (3)
C5	0.086 (4)	0.044 (3)	0.083 (4)	0.015 (3)	−0.010 (3)	0.008 (3)
C6	0.076 (3)	0.042 (3)	0.080 (4)	0.009 (2)	−0.012 (3)	−0.002 (3)
C7	0.051 (3)	0.039 (2)	0.043 (3)	0.007 (2)	0.001 (2)	0.001 (2)
C8	0.057 (3)	0.051 (3)	0.069 (3)	0.001 (2)	0.006 (3)	−0.005 (3)
C9	0.058 (4)	0.079 (4)	0.072 (4)	−0.002 (3)	0.008 (3)	−0.026 (3)
C10	0.075 (5)	0.108 (5)	0.077 (5)	0.037 (4)	−0.010 (3)	−0.030 (4)
C11	0.084 (5)	0.100 (4)	0.070 (4)	0.032 (4)	−0.002 (3)	0.004 (3)
C12	0.067 (4)	0.044 (3)	0.056 (3)	0.012 (2)	0.008 (3)	0.003 (2)
C13	0.066 (3)	0.039 (2)	0.029 (3)	0.005 (2)	−0.004 (2)	0.001 (2)
C14	0.052 (3)	0.040 (3)	0.053 (3)	−0.011 (2)	−0.004 (2)	0.001 (2)
C15	0.065 (3)	0.034 (3)	0.053 (3)	−0.003 (2)	0.007 (2)	−0.002 (2)

Geometric parameters (Å, °)

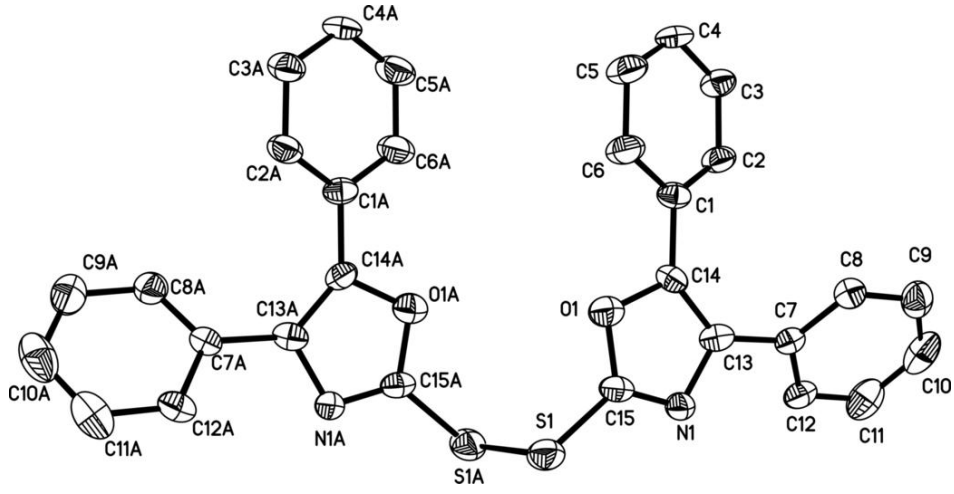
N1—C15	1.288 (4)	C5—H5	0.9300

N1—C13	1.388 (4)	C6—H6	0.9300
O1—C15	1.350 (4)	C7—C8	1.379 (5)
O1—C14	1.390 (4)	C7—C12	1.402 (5)
S1—C15	1.729 (4)	C7—C13	1.461 (5)
S1—S1^{i}	2.049 (2)	C8—C9	1.376 (5)
C1—C2	1.386 (5)	C8—H8	0.9300
C1—C6	1.400 (5)	C9—C10	1.377 (6)
C1—C14	1.461 (5)	C9—H9	0.9300
C2—C3	1.367 (4)	C10—C11	1.369 (6)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.380 (5)	C11—C12	1.369 (5)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.360 (5)	C12—H12	0.9300
C4—H4	0.9300	C13—C14	1.367 (5)
C5—C6	1.381 (5)		
C15—N1—C13	106.0 (3)	C9—C8—C7	121.6 (4)
C15—O1—C14	104.8 (3)	C9—C8—H8	119.2
C15—S1—S1^{i}	102.18 (14)	C7—C8—H8	119.2
C2—C1—C6	118.4 (4)	C8—C9—C10	118.9 (5)
C2—C1—C14	121.7 (4)	C8—C9—H9	120.5
C6—C1—C14	119.9 (4)	C10—C9—H9	120.5
C3—C2—C1	120.2 (4)	C11—C10—C9	120.8 (5)
C3—C2—H2	119.9	C11—C10—H10	119.6
C1—C2—H2	119.9	C9—C10—H10	119.6
C2—C3—C4	121.5 (4)	C10—C11—C12	120.2 (5)
C2—C3—H3	119.2	C10—C11—H11	119.9
C4—C3—H3	119.2	C12—C11—H11	119.9
C5—C4—C3	118.8 (4)	C11—C12—C7	120.3 (4)
C5—C4—H4	120.6	C11—C12—H12	119.9
C3—C4—H4	120.6	C7—C12—H12	119.9
C4—C5—C6	121.2 (4)	C14—C13—N1	108.3 (3)
C4—C5—H5	119.4	C14—C13—C7	133.6 (4)
C6—C5—H5	119.4	N1—C13—C7	118.1 (3)
C5—C6—C1	120.0 (4)	C13—C14—O1	107.1 (3)
C5—C6—H6	120.0	C13—C14—C1	137.0 (4)
C1—C6—H6	120.0	O1—C14—C1	115.9 (4)
C8—C7—C12	118.2 (4)	N1—C15—O1	113.8 (3)
C8—C7—C13	122.8 (4)	N1—C15—S1	126.4 (3)
C12—C7—C13	118.9 (4)	O1—C15—S1	119.8 (3)
C6—C1—C2—C3	1.4 (6)	C12—C7—C13—C14	−145.1 (4)
C14—C1—C2—C3	179.0 (4)	C8—C7—C13—N1	−140.9 (4)
C1—C2—C3—C4	0.6 (6)	C12—C7—C13—N1	36.1 (5)
C2—C3—C4—C5	−1.9 (6)	N1—C13—C14—O1	1.8 (4)
C3—C4—C5—C6	1.2 (7)	C7—C13—C14—O1	−177.0 (4)
C4—C5—C6—C1	0.9 (7)	N1—C13—C14—C1	−176.5 (4)
C2—C1—C6—C5	−2.2 (6)	C7—C13—C14—C1	4.7 (8)
C14—C1—C6—C5	−179.8 (4)	C15—O1—C14—C13	−1.1 (4)
C12—C7—C8—C9	1.2 (6)	C15—O1—C14—C1	177.6 (3)

C13—C7—C8—C9	178.2 (4)	C2—C1—C14—C13	18.9 (7)
C7—C8—C9—C10	0.1 (6)	C6—C1—C14—C13	−163.6 (5)
C8—C9—C10—C11	−1.4 (7)	C2—C1—C14—O1	−159.3 (3)
C9—C10—C11—C12	1.4 (7)	C6—C1—C14—O1	18.2 (5)
C10—C11—C12—C7	0.0 (7)	C13—N1—C15—O1	1.1 (4)
C8—C7—C12—C11	−1.2 (6)	C13—N1—C15—S1	−177.6 (3)
C13—C7—C12—C11	−178.4 (4)	C14—O1—C15—N1	0.0 (4)
C15—N1—C13—C14	−1.8 (4)	C14—O1—C15—S1	178.8 (3)
C15—N1—C13—C7	177.2 (3)	$S1^{i}$—S1—C15—N1	−101.7 (4)
C8—C7—C13—C14	37.9 (6)	$S1^{i}$—S1—C15—O1	79.6 (3)

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

Fig. 1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