Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,5-Bis(benzoylsulfanyl)-1,3-dithiol-2-one

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.025
wR factor = 0.065
Data-to-parameter ratio = 16.8

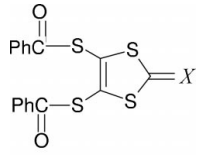
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 2 November 2004
Accepted 4 November 2004
Online 13 November 2004

The title compound [systematic name: *S*,*S*′-2-oxo-1,3-dithiol-4,5-diyl bis(thiobenzoate)], $C_{17}H_{10}O_3S_4$, obtained from 4,5-bis(benzoylsulfanyl)-1,3-dithiole-2-thione and mercury(II) acetate in acetic acid/chloroform, exists as isolated molecules with no significant intermolecular S···S, S···O or O···O interactions.

Comment

The title compound, 4,5-bis(benzoylsulfanyl)-1,3-dithiol-2-one, (I), and the zincate salts $[Q]_2[Zn(dmio)_2]$ (Q is the onium cation and dmio is 2-oxo-1,3-dithiole-4,5-dithiolate) are very useful stable sources of the dmio dianion and have found extended use as precursors of both organic dmio compounds and metal–dmio complexes. Additionally, dmio compounds, such as the title compound, are good sources of tetrathiafulvalenes on reaction with phosphites (Svenstrup & Becher, 1995).



(I) *X* = O
(II) *X* = S

While the crystal structure of a $Zn(dmio)_2$ salt has been reported (Candiota *et al.*, 2003), no previous study of the structure of (I) has been reported.

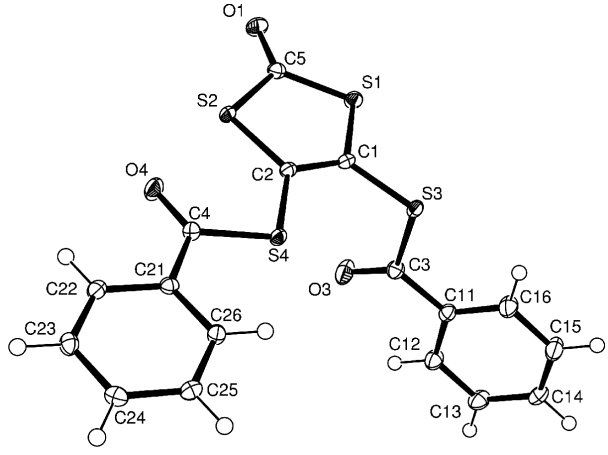


Figure 1
The molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as circles of arbitrary radii.

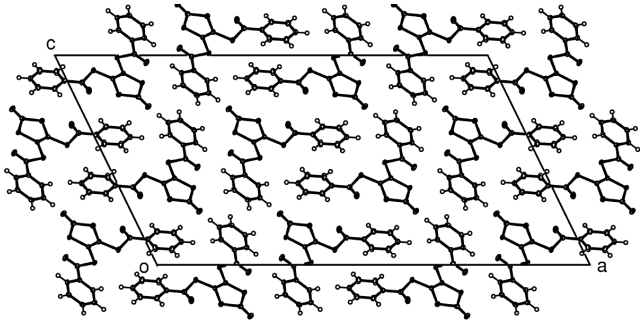


Figure 2
The unit cell contents of (I), projected on to the (101) plane.

Bond lengths and angles within the five-membered dmio ring in (I) are within the ranges found for other dmio compounds, such as [Q][Sn(dmio)$_3$] and [Q][Zn(dmio)$_2$] (Candiota *et al.*, 2003; Chohan *et al.*, 2003; Aupers *et al.*, 2002; de Assis *et al.*, 1999).

The dmio ring, together with the attached carbonyl O atom, is essentially planar, with S1 showing the largest deviation [0.0158 (6) Å] from the mean plane. The two phenyl rings are inclined at angles of 78.60 (4) (C11–C16) and 6.94 (8)° (C21–C26) to the dmio ring. Molecules of (I) show no strong association with each other, the closest intermolecular S···S, S···O and O···O separations being 3.6561 (5), 3.4524 (12) and 3.1479 (17) Å, respectively, all just outside the van der Waals radii sum for the appropriate atoms; van der Waals radii for S and O are taken as 1.80 and 1.52 Å, respectively (*PLATON*; Spek, 2004).

The structure of the analogous 4,5-bis(benzoylsulfanyl)-1,3-dithiole-2-thione compound, (II), has been reported at both 120 (Cox & Doidge-Harrison, 1996) and 288 K (Solans *et al.*, 1987). There are weak C—H···O and S···S intermolecular interactions in (II).

Experimental

The title compound was prepared using a modification of a published method (Hartke *et al.*, 1980). A solution of mercury(II) acetate (4.78 g, 15.0 mmol) in glacial acetic acid (120 ml) was added with vigorous agitation to a solution of 4,5-bis(benzoylsulfanyl)-1,3-dithiole-2-thione [(II); 6.09 g, 15.0 mmol] (Steimecke, 1979) in chloroform (120 ml). After refluxing for 5 h, the reaction mixture was filtered, and the filtrate was successively washed with water, saturated aqueous sodium bicarbonate solution and more water, dried over $MgSO_4$ and evaporated to leave a yellow solid, which was recrystallized from chloroform/methanol (yield 54%, m.p. 388–389 K). IR (CsI, cm^{-1}): 3083 (ν C—H), 1701, 1697, 1668, 1621 (ν C═O), 1467 (ν C═C), 896 (ν C—S).

Crystal data

$C_{17}H_{10}O_3S_4$
M_r = 390.49
Monoclinic, $C2/c$
a = 35.6460 (6) Å
b = 5.20360 (10) Å
c = 19.1402 (3) Å
β = 116.0945 (8)°
V = 3188.39 (10) Å^3
Z = 8
D_x = 1.627 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4041 reflections
θ = 2.7–27.5°
μ = 0.61 mm^{-1}
T = 120 (2) K
Block, colourless
0.60 × 0.30 × 0.20 mm

Data collection

Bruker–Nonius KappaCCD diffractometer with rotating-anode source
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.787, T_{max} = 0.883
25 707 measured reflections
3656 independent reflections
3191 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 27.5°
$h = -46 \rightarrow 46$
$k = -6 \rightarrow 6$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.065
S = 1.06
3656 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.031P)^2 + 3.4602P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···S3	0.95	2.59	3.0392 (15)	109
C26—H26···S4	0.95	2.58	3.0146 (14)	108

All H atoms were first identified in a difference map and then placed in geometrical positions and refined using a riding model with C–H distances of 0.95 Å. Analysis of molecular interactions was carried out using *PLATON* (Spek, 2004).

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

We thank the EPSRC's X-ray Crystallographic Service, University of Southampton, for the collection of the data. The Brazil-based authors thank CNPq, CAPES and FUJB for support.

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supporting information

Acta Cryst. (2004). E**60**, o2284–o2286 [https://doi.org/10.1107/S1600536804028387]

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Monoclinic, $C2/c$
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$a = 35.6460\ (6)$ Å
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Cell parameters from 4041 reflections
$\theta = 2.7–27.5°$
$\mu = 0.61$ mm^{-1}
$T = 120$ K
Block, colourless
0.60 × 0.30 × 0.20 mm

Data collection

Bruker-Nonius FR591 rotating anode diffractometer
Radiation source: Bruker-Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.787$, $T_{max} = 0.883$
25707 measured reflections
3656 independent reflections
3191 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -46\rightarrow46$
$k = -6\rightarrow6$
$l = -24\rightarrow24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.065$
$S = 1.06$
3656 reflections
217 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
$w = 1/[\sigma^2(F_o^2) + (0.031P)^2 + 3.4602P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

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.
All H atoms were located from the difference map then refined using a riding model and the appropriate AFIX commands in *SHELXL*.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.103610 (11)	−0.37285 (7)	0.31289 (2)	0.01562 (9)
S2	0.170596 (10)	0.02062 (6)	0.36723 (2)	0.01379 (9)
C1	0.10785 (4)	−0.1736 (3)	0.38918 (8)	0.0128 (3)
C2	0.13792 (4)	0.0093 (3)	0.41389 (7)	0.0117 (3)
S3	0.072238 (10)	−0.22872 (7)	0.42787 (2)	0.01456 (9)
S4	0.141682 (10)	0.21377 (6)	0.489622 (19)	0.01325 (8)
C5	0.14634 (4)	−0.2398 (3)	0.30231 (8)	0.0144 (3)
O1	0.15830 (3)	−0.3129 (2)	0.25555 (6)	0.0210 (2)
C3	0.03248 (4)	0.0064 (3)	0.37048 (8)	0.0156 (3)
O3	0.03936 (3)	0.1632 (2)	0.33152 (7)	0.0258 (3)
C11	−0.00718 (4)	−0.0137 (3)	0.37810 (8)	0.0148 (3)
C12	−0.03761 (5)	0.1718 (3)	0.34099 (9)	0.0197 (3)
H12	−0.0328	0.3035	0.3115	0.024*
C13	−0.07498 (5)	0.1644 (3)	0.34707 (9)	0.0217 (3)
H13	−0.0957	0.2919	0.3220	0.026*
C14	−0.08222 (4)	−0.0285 (3)	0.38965 (8)	0.0181 (3)
H14	−0.1078	−0.0331	0.3937	0.022*
C15	−0.05214 (5)	−0.2143 (3)	0.42622 (10)	0.0241 (3)
H15	−0.0571	−0.3465	0.4553	0.029*
C16	−0.01465 (5)	−0.2077 (3)	0.42043 (10)	0.0231 (3)
H16	0.0059	−0.3359	0.4454	0.028*
C4	0.18540 (4)	0.4181 (3)	0.50620 (8)	0.0138 (3)
O4	0.20356 (3)	0.4106 (2)	0.46565 (6)	0.0222 (2)
C21	0.19594 (4)	0.6008 (3)	0.57182 (8)	0.0125 (3)
C22	0.22677 (4)	0.7850 (3)	0.58349 (8)	0.0142 (3)
H22	0.2406	0.7867	0.5508	0.017*
C23	0.23726 (4)	0.9649 (3)	0.64249 (8)	0.0157 (3)
H23	0.2583	1.0888	0.6505	0.019*
C24	0.21686 (4)	0.9640 (3)	0.69012 (8)	0.0154 (3)
H24	0.2235	1.0900	0.7297	0.019*
C25	0.18678 (4)	0.7790 (3)	0.67965 (8)	0.0150 (3)
H25	0.1733	0.7769	0.7128	0.018*
C26	0.17627 (4)	0.5969 (3)	0.62096 (8)	0.0144 (3)
H26	0.1558	0.4701	0.6142	0.017*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01629 (17)	0.01632 (18)	0.01618 (17)	−0.00254 (13)	0.00890 (14)	−0.00503 (13)

S2	0.01553 (17)	0.01420 (17)	0.01608 (17)	−0.00109 (12)	0.01102 (13)	−0.00182 (12)
C1	0.0123 (6)	0.0145 (6)	0.0136 (6)	0.0017 (5)	0.0074 (5)	−0.0004 (5)
C2	0.0122 (6)	0.0127 (6)	0.0116 (6)	0.0021 (5)	0.0065 (5)	0.0016 (5)
S3	0.01304 (16)	0.01559 (17)	0.01811 (17)	0.00110 (12)	0.00967 (14)	0.00230 (13)
S4	0.01409 (16)	0.01429 (17)	0.01468 (17)	−0.00234 (12)	0.00937 (13)	−0.00326 (12)
C5	0.0162 (6)	0.0135 (7)	0.0145 (7)	0.0023 (5)	0.0075 (6)	0.0011 (5)
O1	0.0259 (6)	0.0229 (5)	0.0204 (5)	0.0003 (4)	0.0159 (5)	−0.0048 (4)
C3	0.0144 (6)	0.0167 (7)	0.0155 (7)	−0.0003 (5)	0.0064 (5)	0.0003 (5)
O3	0.0187 (5)	0.0303 (6)	0.0316 (6)	0.0044 (5)	0.0140 (5)	0.0144 (5)
C11	0.0127 (6)	0.0169 (7)	0.0153 (7)	−0.0014 (5)	0.0066 (5)	−0.0015 (5)
C12	0.0186 (7)	0.0222 (7)	0.0207 (7)	0.0025 (6)	0.0106 (6)	0.0053 (6)
C13	0.0175 (7)	0.0258 (8)	0.0225 (8)	0.0068 (6)	0.0095 (6)	0.0052 (6)
C14	0.0127 (6)	0.0251 (8)	0.0180 (7)	−0.0011 (6)	0.0082 (5)	−0.0023 (6)
C15	0.0200 (7)	0.0257 (8)	0.0309 (9)	0.0013 (6)	0.0151 (7)	0.0088 (7)
C16	0.0164 (7)	0.0220 (8)	0.0331 (9)	0.0049 (6)	0.0130 (7)	0.0099 (7)
C4	0.0141 (6)	0.0132 (6)	0.0151 (6)	−0.0005 (5)	0.0073 (5)	0.0006 (5)
O4	0.0251 (5)	0.0246 (6)	0.0258 (6)	−0.0091 (4)	0.0193 (5)	−0.0088 (5)
C21	0.0128 (6)	0.0119 (6)	0.0128 (6)	0.0020 (5)	0.0056 (5)	0.0010 (5)
C22	0.0127 (6)	0.0157 (7)	0.0154 (7)	0.0011 (5)	0.0072 (5)	0.0014 (5)
C23	0.0124 (6)	0.0159 (7)	0.0168 (7)	−0.0020 (5)	0.0045 (5)	0.0003 (5)
C24	0.0148 (6)	0.0144 (7)	0.0140 (6)	0.0018 (5)	0.0035 (5)	−0.0016 (5)
C25	0.0148 (6)	0.0180 (7)	0.0134 (6)	0.0021 (5)	0.0073 (5)	0.0003 (5)
C26	0.0134 (6)	0.0141 (7)	0.0164 (7)	−0.0011 (5)	0.0073 (5)	0.0005 (5)

Geometric parameters (Å, º)

S1—C1	1.7424 (14)	C14—C15	1.383 (2)
S1—C5	1.7640 (14)	C14—H14	0.9500
S2—C2	1.7529 (13)	C15—C16	1.389 (2)
S2—C5	1.7839 (14)	C15—H15	0.9500
C1—C2	1.3539 (19)	C16—H16	0.9500
C1—S3	1.7518 (13)	C4—O4	1.2102 (17)
C2—S4	1.7551 (13)	C4—C21	1.4856 (19)
S3—C3	1.8281 (14)	C21—C26	1.3988 (18)
S4—C4	1.7960 (14)	C21—C22	1.4003 (19)
C5—O1	1.2098 (17)	C22—C23	1.386 (2)
C3—O3	1.2013 (18)	C22—H22	0.9500
C3—C11	1.4872 (19)	C23—C24	1.394 (2)
C11—C16	1.391 (2)	C23—H23	0.9500
C11—C12	1.391 (2)	C24—C25	1.389 (2)
C12—C13	1.388 (2)	C24—H24	0.9500
C12—H12	0.9500	C25—C26	1.3891 (19)
C13—C14	1.387 (2)	C25—H25	0.9500
C13—H13	0.9500	C26—H26	0.9500
C1—S1—C5	95.83 (6)	C14—C15—C16	120.08 (14)
C2—S2—C5	95.87 (6)	C14—C15—H15	120.0
C2—C1—S1	118.33 (10)	C16—C15—H15	120.0

C2—C1—S3	125.24 (10)	C15—C16—C11	120.10 (14)
S1—C1—S3	116.43 (8)	C15—C16—H16	120.0
C1—C2—S2	116.56 (10)	C11—C16—H16	120.0
C1—C2—S4	118.41 (10)	O4—C4—C21	123.74 (12)
S2—C2—S4	125.03 (8)	O4—C4—S4	122.32 (11)
C1—S3—C3	98.68 (6)	C21—C4—S4	113.90 (9)
C2—S4—C4	104.47 (6)	C26—C21—C22	119.54 (12)
O1—C5—S1	124.37 (11)	C26—C21—C4	122.96 (12)
O1—C5—S2	122.25 (11)	C22—C21—C4	117.49 (12)
S1—C5—S2	113.37 (7)	C23—C22—C21	120.26 (13)
O3—C3—C11	124.83 (13)	C23—C22—H22	119.9
O3—C3—S3	120.76 (11)	C21—C22—H22	119.9
C11—C3—S3	114.40 (10)	C22—C23—C24	119.96 (13)
C16—C11—C12	119.66 (13)	C22—C23—H23	120.0
C16—C11—C3	122.80 (13)	C24—C23—H23	120.0
C12—C11—C3	117.54 (13)	C25—C24—C23	119.99 (13)
C13—C12—C11	119.97 (14)	C25—C24—H24	120.0
C13—C12—H12	120.0	C23—C24—H24	120.0
C11—C12—H12	120.0	C24—C25—C26	120.41 (13)
C14—C13—C12	120.19 (14)	C24—C25—H25	119.8
C14—C13—H13	119.9	C26—C25—H25	119.8
C12—C13—H13	119.9	C25—C26—C21	119.81 (13)
C15—C14—C13	119.99 (13)	C25—C26—H26	120.1
C15—C14—H14	120.0	C21—C26—H26	120.1
C13—C14—H14	120.0		

C5—S1—C1—C2	1.96 (12)	C16—C11—C12—C13	0.7 (2)
C5—S1—C1—S3	−177.98 (8)	C3—C11—C12—C13	−179.09 (14)
S1—C1—C2—S2	−1.50 (15)	C11—C12—C13—C14	−0.4 (2)
S3—C1—C2—S2	178.44 (8)	C12—C13—C14—C15	0.0 (2)
S1—C1—C2—S4	178.93 (7)	C13—C14—C15—C16	0.1 (2)
S3—C1—C2—S4	−1.13 (17)	C14—C15—C16—C11	0.3 (3)
C5—S2—C2—C1	0.19 (12)	C12—C11—C16—C15	−0.7 (2)
C5—S2—C2—S4	179.73 (9)	C3—C11—C16—C15	179.17 (15)
C2—C1—S3—C3	85.59 (13)	C2—S4—C4—O4	5.12 (14)
S1—C1—S3—C3	−94.47 (9)	C2—S4—C4—C21	−176.91 (10)
C1—C2—S4—C4	178.56 (11)	O4—C4—C21—C26	−176.12 (14)
S2—C2—S4—C4	−0.97 (10)	S4—C4—C21—C26	5.94 (17)
C1—S1—C5—O1	178.99 (13)	O4—C4—C21—C22	4.5 (2)
C1—S1—C5—S2	−1.71 (9)	S4—C4—C21—C22	−173.46 (10)
C2—S2—C5—O1	−179.58 (12)	C26—C21—C22—C23	−1.0 (2)
C2—S2—C5—S1	1.11 (9)	C4—C21—C22—C23	178.37 (12)
C1—S3—C3—O3	−10.74 (14)	C21—C22—C23—C24	−0.5 (2)
C1—S3—C3—C11	170.29 (10)	C22—C23—C24—C25	1.6 (2)
O3—C3—C11—C16	176.25 (15)	C23—C24—C25—C26	−1.2 (2)
S3—C3—C11—C16	−4.83 (19)	C24—C25—C26—C21	−0.4 (2)
O3—C3—C11—C12	−3.9 (2)	C22—C21—C26—C25	1.5 (2)
S3—C3—C11—C12	175.00 (11)	C4—C21—C26—C25	−177.93 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···S3	0.95	2.59	3.0392 (15)	109
C26—H26···S4	0.95	2.58	3.0146 (14)	108