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4-(2-Cyanoethylsulfanyl)-5′-(pyridin-4-yl)tetrathiafulvalene

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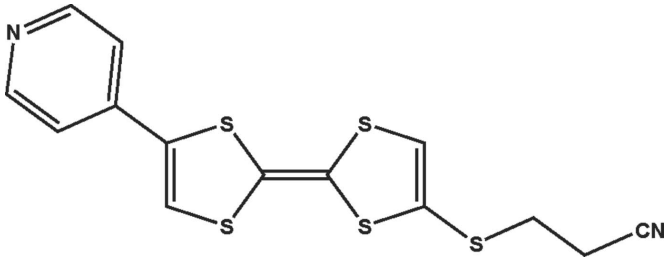
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.006 Å; R factor = 0.061; wR factor = 0.126; data-to-parameter ratio = 15.0.

In the title compound, $C_{14}H_{10}N_2S_5$ [systematic name; 3-({2-[4-(pyridin-4-yl)-2*H*-1,3-dithiol-2-ylidene]-2*H*-1,3-dithiol-4-yl}sulfanyl)propanenitrile], all of the non-H atoms except for the cyanoethylsulfanyl group, are approximately coplanar [maxium deviation = 0.090 (3) Å]. The two five-membered 1,3-dithiole rings are twisted by 2.6 (2)°. Weak intermolecular S···S interactions occur [3.586 (4) and 3.530 (4) Å].

Related literature

For background to the chemistry of prridine-based tetrathiafulvalenes, see: Fabre (2004); Zhu *et al.* (2007). For the preparation of the title compound, see: Jia *et al.* (2001); Zhu *et al.* (2010). For related structures, see: Han *et al.* (2007); Zhao *et al.* (2008).



Experimental

Crystal data

$C_{14}H_{10}N_2S_5$
M_r = 366.54
Monoclinic, $P2_1/c$
a = 14.6231 (18) Å
b = 10.7197 (12) Å
c = 9.9211 (12) Å
β = 94.775 (4)°
V = 1549.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.74 mm^{-1}
T = 223 K
0.50 × 0.20 × 0.20 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
T_{min} = 0.613, T_{max} = 0.856
7658 measured reflections
2869 independent reflections
2268 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.126
S = 1.11
2869 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5167).

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supporting information

Acta Cryst. (2011). E**67**, o1467 [doi:10.1107/S1600536811018800]

4-(2-Cyanoethylsulfanyl)-5′-(pyridin-4-yl)tetrathiafulvalene

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S1. Comment

Tetrathiafulvalene (TTF) and its derivatives are strong electron donors (D). Many electron acceptors (A) have been connected to TTF to afford electron D—A system to build molecular level devices, such as molecular rectifiers and molecular switches. In order to obtain materials in molecular electronics, currently, our research is focus on the synthesis and crystal structures of TTF derivatives. In the title compound, the substituent group of the TTF core are located in opposite direction, resulting in chair-like molecular comformations. All bonds lengths and bond angles are found to within the range for neutral TTF (Han *et al.* 2007). In addition, the pyridyl group and tetrathiafulvalene motif are coplanar, the non-H atoms of the two group lie on a plan [maxium deviation is 0.0908 (33)?Å] (Fig.1). Inter-molecular interaction involving S(2)···S(1) 3.586 (4) Å and S(2)···S(3) 3.530 (4) Å are present consolidating the crystal packing. (Fig.2).

S2. Experimental

The title compound was prepared according to the literature (Jia *et al.*,2001) (Zhu *et al.*,2007). Red crystals were obtained from slow evaporation of a dichloromethane solution at room temperature.

S3. Refinement

H atoms were positioned geometrically [C–H = 0.93–0.98 Å] and refined using a riding model, with U_{iso}(H) = 1.2Ueq(C).

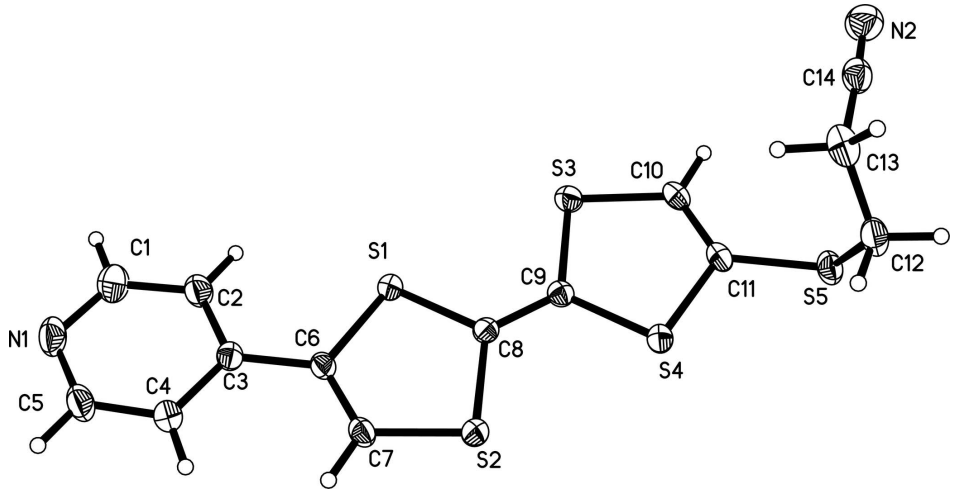

Figure 1

The molecular structure of the title compound.Displacement ellipsoids are drawn at the 30% probability level.

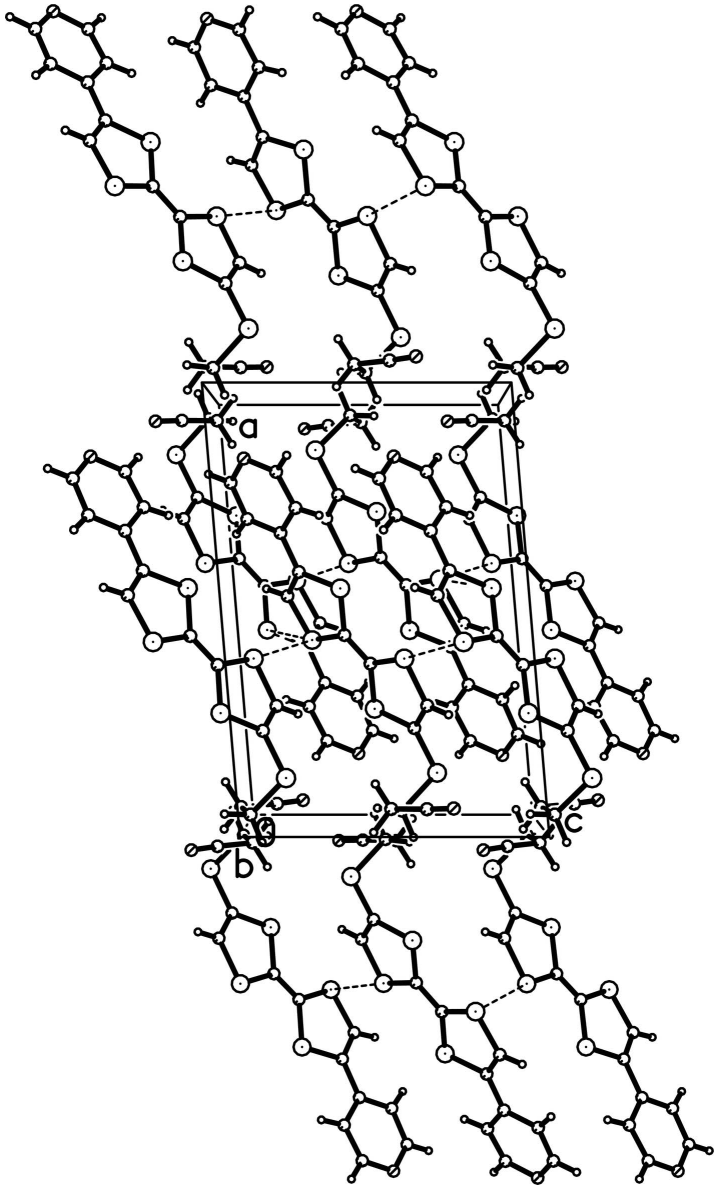

Figure 2

The crystal packing diagram view along the crystallographic *b*-axis.

3-({2-[4-(pyridin-4-yl)-2*H*-1,3-dithiol-2-ylidene]-2*H*-1,3-dithiol- 4-yl}sulfanyl)propanenitrile

Crystal data

$C_{14}H_{10}N_2S_5$
M_r = 366.54
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 14.6231 (18) Å
b = 10.7197 (12) Å
c = 9.9211 (12) Å
β = 94.775 (4)°
V = 1549.8 (3) Å^3
Z = 4
$F(000)$ = 752
D_x = 1.571 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 5787 reflections
θ = 3.1–27.5°
μ = 0.74 mm^{-1}
T = 223 K
Block, red
0.50 × 0.20 × 0.20 mm

Data collection

Rigaku Saturn diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 14.63 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (REQAB; Jacobson, 1998)
T_{min} = 0.613, T_{max} = 0.856
7658 measured reflections
2869 independent reflections
2268 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.5°, θ_{min} = 3.1°
h = −17→16
k = −12→12
l = −12→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.126
S = 1.11
2869 reflections
191 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
$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 1.3388P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 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.

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.45140 (7)	0.17432 (9)	0.11234 (11)	0.0324 (3)
S2	0.57042 (7)	−0.02950 (10)	0.22543 (11)	0.0362 (3)
S3	0.61033 (7)	0.25532 (10)	−0.08148 (12)	0.0377 (3)
S4	0.72869 (7)	0.05022 (10)	0.03146 (11)	0.0361 (3)
S5	0.87437 (8)	0.10167 (11)	−0.16139 (12)	0.0438 (3)
N1	0.1558 (3)	0.1902 (4)	0.3981 (5)	0.0555 (11)
N2	0.9396 (3)	0.4512 (4)	−0.1998 (5)	0.0619 (12)
C1	0.1881 (3)	0.2455 (5)	0.2923 (6)	0.0601 (14)
H1	0.1532	0.3107	0.2508	0.072*
C2	0.2690 (3)	0.2145 (4)	0.2386 (5)	0.0459 (12)
H2	0.2865	0.2562	0.1615	0.055*
C3	0.3240 (3)	0.1224 (4)	0.2984 (4)	0.0323 (9)
C4	0.2907 (3)	0.0618 (4)	0.4090 (5)	0.0451 (12)
H4	0.3242	−0.0035	0.4528	0.054*
C5	0.2082 (3)	0.0989 (5)	0.4532 (5)	0.0529 (14)
H5	0.1873	0.0568	0.5278	0.063*

C6	0.4131 (3)	0.0883 (4)	0.2484 (4)	0.0321 (9)
C7	0.4680 (3)	−0.0036 (4)	0.2963 (4)	0.0345 (10)
H7	0.4512	−0.0538	0.3680	0.041*
C8	0.5581 (2)	0.0973 (3)	0.1123 (4)	0.0284 (9)
C9	0.6232 (3)	0.1293 (4)	0.0326 (4)	0.0298 (9)
C10	0.7170 (3)	0.2350 (4)	−0.1449 (4)	0.0348 (10)
H10	0.7363	0.2886	−0.2120	0.042*
C11	0.7705 (3)	0.1427 (4)	−0.0967 (4)	0.0350 (10)
C12	0.9586 (3)	0.1601 (5)	−0.0324 (5)	0.0484 (12)
H12A	0.9549	0.1103	0.0498	0.058*
H12B	1.0199	0.1478	−0.0632	0.058*
C13	0.9480 (3)	0.2965 (5)	0.0034 (5)	0.0511 (13)
H13A	0.8915	0.3064	0.0491	0.061*
H13B	0.9995	0.3207	0.0676	0.061*
C14	0.9445 (3)	0.3823 (5)	−0.1136 (5)	0.0458 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0303 (5)	0.0311 (5)	0.0363 (6)	0.0025 (4)	0.0064 (4)	0.0022 (4)
S2	0.0359 (6)	0.0343 (6)	0.0396 (7)	0.0060 (5)	0.0090 (5)	0.0060 (5)
S3	0.0350 (6)	0.0345 (6)	0.0439 (7)	0.0004 (5)	0.0048 (5)	0.0076 (5)
S4	0.0306 (5)	0.0372 (6)	0.0413 (7)	0.0026 (5)	0.0079 (5)	0.0050 (5)
S5	0.0359 (6)	0.0507 (7)	0.0469 (8)	−0.0030 (5)	0.0165 (5)	−0.0037 (6)
N1	0.036 (2)	0.063 (3)	0.070 (3)	−0.005 (2)	0.020 (2)	−0.014 (2)
N2	0.069 (3)	0.056 (3)	0.062 (3)	0.004 (2)	0.014 (2)	0.003 (2)
C1	0.036 (3)	0.066 (3)	0.080 (4)	0.007 (2)	0.011 (3)	0.004 (3)
C2	0.037 (2)	0.051 (3)	0.051 (3)	0.003 (2)	0.010 (2)	0.010 (2)
C3	0.027 (2)	0.032 (2)	0.037 (3)	−0.0060 (17)	0.0039 (18)	−0.0083 (18)
C4	0.044 (3)	0.042 (3)	0.051 (3)	0.000 (2)	0.017 (2)	0.002 (2)
C5	0.047 (3)	0.056 (3)	0.060 (3)	−0.013 (3)	0.025 (3)	−0.007 (3)
C6	0.031 (2)	0.030 (2)	0.036 (2)	−0.0051 (18)	0.0087 (18)	−0.0032 (18)
C7	0.037 (2)	0.038 (2)	0.030 (2)	−0.0037 (19)	0.0103 (18)	0.0014 (19)
C8	0.0252 (19)	0.027 (2)	0.033 (2)	−0.0019 (16)	−0.0001 (17)	−0.0029 (17)
C9	0.030 (2)	0.030 (2)	0.030 (2)	−0.0032 (17)	0.0018 (17)	−0.0028 (17)
C10	0.036 (2)	0.039 (2)	0.030 (2)	−0.0086 (19)	0.0072 (19)	0.0033 (19)
C11	0.031 (2)	0.039 (2)	0.036 (3)	−0.0080 (19)	0.0085 (19)	0.000 (2)
C12	0.031 (2)	0.063 (3)	0.052 (3)	0.000 (2)	0.009 (2)	0.007 (3)
C13	0.041 (3)	0.069 (3)	0.043 (3)	−0.010 (2)	0.007 (2)	−0.007 (3)
C14	0.039 (3)	0.050 (3)	0.049 (3)	−0.003 (2)	0.010 (2)	−0.013 (3)

Geometric parameters (Å, º)

S1—C6	1.764 (4)	C3—C4	1.398 (6)
S1—C8	1.765 (4)	C3—C6	1.478 (5)
S2—C7	1.729 (4)	C4—C5	1.376 (6)
S2—C8	1.762 (4)	C4—H4	0.9400
S3—C10	1.744 (4)	C5—H5	0.9400

S3—C9	1.762 (4)	C6—C7	1.333 (6)
S4—C9	1.761 (4)	C7—H7	0.9400
S4—C11	1.761 (4)	C8—C9	1.333 (5)
S5—C11	1.753 (4)	C10—C11	1.326 (6)
S5—C12	1.812 (5)	C10—H10	0.9400
N1—C1	1.327 (7)	C12—C13	1.515 (6)
N1—C5	1.331 (7)	C12—H12A	0.9800
N2—C14	1.128 (6)	C12—H12B	0.9800
C1—C2	1.377 (6)	C13—C14	1.479 (7)
C1—H1	0.9400	C13—H13A	0.9800
C2—C3	1.377 (6)	C13—H13B	0.9800
C2—H2	0.9400		

C6—S1—C8	95.29 (18)	S2—C7—H7	120.3
C7—S2—C8	95.10 (19)	C9—C8—S2	122.4 (3)
C10—S3—C9	94.88 (19)	C9—C8—S1	123.7 (3)
C9—S4—C11	95.20 (19)	S2—C8—S1	113.8 (2)
C11—S5—C12	102.3 (2)	C8—C9—S4	123.3 (3)
C1—N1—C5	115.0 (4)	C8—C9—S3	122.3 (3)
N1—C1—C2	124.8 (5)	S4—C9—S3	114.3 (2)
N1—C1—H1	117.6	C11—C10—S3	118.8 (3)
C2—C1—H1	117.6	C11—C10—H10	120.6
C3—C2—C1	119.8 (4)	S3—C10—H10	120.6
C3—C2—H2	120.1	C10—C11—S5	123.9 (3)
C1—C2—H2	120.1	C10—C11—S4	116.8 (3)
C2—C3—C4	116.2 (4)	S5—C11—S4	119.1 (2)
C2—C3—C6	122.2 (4)	C13—C12—S5	115.0 (3)
C4—C3—C6	121.6 (4)	C13—C12—H12A	108.5
C5—C4—C3	119.2 (4)	S5—C12—H12A	108.5
C5—C4—H4	120.4	C13—C12—H12B	108.5
C3—C4—H4	120.4	S5—C12—H12B	108.5
N1—C5—C4	124.9 (5)	H12A—C12—H12B	107.5
N1—C5—H5	117.6	C14—C13—C12	114.5 (4)
C4—C5—H5	117.6	C14—C13—H13A	108.6
C7—C6—C3	125.8 (4)	C12—C13—H13A	108.6
C7—C6—S1	116.0 (3)	C14—C13—H13B	108.6
C3—C6—S1	118.2 (3)	C12—C13—H13B	108.6
C6—C7—S2	119.3 (3)	H13A—C13—H13B	107.6
C6—C7—H7	120.3	N2—C14—C13	177.0 (5)

C5—N1—C1—C2	0.3 (8)	C6—S1—C8—S2	6.1 (2)
N1—C1—C2—C3	−2.1 (8)	S2—C8—C9—S4	−0.5 (5)
C1—C2—C3—C4	2.7 (7)	S1—C8—C9—S4	−178.9 (2)
C1—C2—C3—C6	−177.7 (4)	S2—C8—C9—S3	179.4 (2)
C2—C3—C4—C5	−1.7 (6)	S1—C8—C9—S3	1.0 (5)
C6—C3—C4—C5	178.7 (4)	C11—S4—C9—C8	178.6 (4)
C1—N1—C5—C4	0.7 (8)	C11—S4—C9—S3	−1.4 (3)
C3—C4—C5—N1	0.0 (8)	C10—S3—C9—C8	−179.1 (4)

C2—C3—C6—C7	−176.5 (4)	C10—S3—C9—S4	0.8 (3)
C4—C3—C6—C7	3.1 (7)	C9—S3—C10—C11	0.3 (4)
C2—C3—C6—S1	2.9 (6)	S3—C10—C11—S5	173.8 (2)
C4—C3—C6—S1	−177.5 (3)	S3—C10—C11—S4	−1.4 (5)
C8—S1—C6—C7	−4.2 (4)	C12—S5—C11—C10	106.0 (4)
C8—S1—C6—C3	176.3 (3)	C12—S5—C11—S4	−79.0 (3)
C3—C6—C7—S2	−179.7 (3)	C9—S4—C11—C10	1.6 (4)
S1—C6—C7—S2	0.9 (5)	C9—S4—C11—S5	−173.7 (3)
C8—S2—C7—C6	3.0 (4)	C11—S5—C12—C13	−53.5 (4)
C7—S2—C8—C9	175.7 (4)	S5—C12—C13—C14	−53.5 (5)
C7—S2—C8—S1	−5.7 (3)	C12—C13—C14—N2	152 (11)
C6—S1—C8—C9	−175.4 (4)		