

***trans*-2,3-Bis(2,4,5-trimethyl-3-thienyl)-but-2-enedinitrile**

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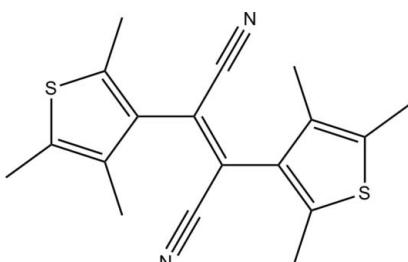
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Key indicators: single-crystal X-ray study; $T = 273\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$; R factor = 0.058; wR factor = 0.175; data-to-parameter ratio = 18.5.

In title compound, $\text{C}_{18}\text{H}_{18}\text{N}_2\text{S}_2$, the dihedral angle between two thiophene rings is $61.83(8)^\circ$.

Related literature

For related structures, see: Munakata *et al.* (1996); Han *et al.* (2006).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{18}\text{N}_2\text{S}_2$

$M_r = 326.46$

Triclinic, $P\bar{1}$
 $a = 8.8368(10)\text{ \AA}$
 $b = 9.1785(10)\text{ \AA}$
 $c = 11.4160(12)\text{ \AA}$
 $\alpha = 85.271(2)^\circ$
 $\beta = 71.058(2)^\circ$
 $\gamma = 77.171(2)^\circ$

$V = 853.88(16)\text{ \AA}^3$
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.31\text{ mm}^{-1}$
 $T = 273\text{ K}$
 $0.40 \times 0.32 \times 0.28\text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.886$, $T_{\max} = 0.918$

5025 measured reflections
3686 independent reflections
2264 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.175$
 $S = 1.06$
3686 reflections

199 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.28\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.23\text{ e \AA}^{-3}$

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: HG2788).

References

- Bruker (1998). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (1999). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Han, J., Nabei, A., Suenaga, Y., Maekawa, M., Isihara, H., Kuroda-Sowa, T. & Munakata, M. (2006). *Polyhedron*, **25**, 2483–2490.
- Munakata, M., Wu, L. P., Kuroda-Sowa, T., Maekawa, M., Suenaga, Y. & Furuchi, K. (1996). *J. Am. Chem. Soc.* **118**, 3305–3306.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.

supplementary materials

Acta Cryst. (2011). E67, o399 [doi:10.1107/S1600536811001176]

***trans*-2,3-Bis(2,4,5-trimethyl-3-thienyl)but-2-enedinitrile**

J. Bian, Y. Zhang and X. Yan

Comment

In the crystal structure of the title compound, two substituted thiophene rings are *trans* positioned with respect to the dicyano group. The ring skeleton of the molecule is not planar. This diarylethene with thiophene rings is prepared in an attempt to construct thermally irreversible photochromic systems. The dicyano group was selected to shift the absorption maxima of the dihydro-type isomers to longer wavelengths.

All bond lengths and angles in title compound are normal and good agreement with those previously reported. (Munakata, *et al.*, 1996; Han *et al.*, 2006). The dihedral angles between the two thiophene (S1/C12—C15 and S2/C1—C4) rings is 61.83°. No classical hydrogen bonds were found, the crystal structure was mainly stabilized by Van der Waals forces.

Experimental

To 20 ml of 50% NaOH aqueous solution containing triethylbenzylammonium chloride (0.21 g, 0.0010 mol) was added a mixture of 2,3,5-trimethyl-4-(cyanomethyl)thiophene (16 g, 0.10 mol) and CCl₄ (15 g, 0.10 mol) at 40 °C. The solution was stirred for 1.5 h at 45 °C. The reaction mixture was poured into water and the product was extracted with ether and chloroform. After the solvent was removed, the mixture of *trans* and *cis* forms was separated by column chromatography on silica gel with light petroleum-CHCl₃ (1: 1), collected the first yellow band, and then purified by recrystallization from a hexane-ether mixture. Single crystals suitable for X-ray measurements were obtained by recrystallization from methanol at room temperature for one week.

Refinement

H atoms bonded to C atoms were treated as riding atoms, with C—H distances of 0.96 Å and $U_{\text{iso}}(\text{H})$ values of 1.5 $U_{\text{eq}}(\text{C})$.

Figures

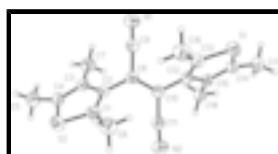


Fig. 1. View of the title compound (I), with displacement ellipsoids drawn at the 40% probability level.

***trans*-2,3-Bis(2,4,5-trimethyl-3-thienyl)but-2-enedinitrile**

Crystal data

| | |
|---------------------------------------------------------------|----------------|
| C ₁₈ H ₁₈ N ₂ S ₂ | Z = 2 |
| $M_r = 326.46$ | $F(000) = 344$ |

supplementary materials

| | |
|---------------------------------|---------------------------------------------------------|
| Triclinic, $P\bar{1}$ | $D_x = 1.270 \text{ Mg m}^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $a = 8.8368 (10) \text{ \AA}$ | Cell parameters from 2501 reflections |
| $b = 9.1785 (10) \text{ \AA}$ | $\theta = 2.3\text{--}25.1^\circ$ |
| $c = 11.4160 (12) \text{ \AA}$ | $\mu = 0.31 \text{ mm}^{-1}$ |
| $\alpha = 85.271 (2)^\circ$ | $T = 273 \text{ K}$ |
| $\beta = 71.058 (2)^\circ$ | Block, yellow |
| $\gamma = 77.171 (2)^\circ$ | $0.40 \times 0.32 \times 0.28 \text{ mm}$ |
| $V = 853.88 (16) \text{ \AA}^3$ | |

Data collection

| | |
|----------------------------------------------------------------------|---------------------------------------------------------------------|
| Bruker SMART CCD area-detector diffractometer | 3686 independent reflections |
| Radiation source: fine-focus sealed tube graphite | 2264 reflections with $I > 2\sigma(I)$ |
| φ and ω scans | $R_{\text{int}} = 0.020$ |
| Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996) | $\theta_{\text{max}} = 27.5^\circ, \theta_{\text{min}} = 1.9^\circ$ |
| $T_{\text{min}} = 0.886, T_{\text{max}} = 0.918$ | $h = -11 \rightarrow 9$ |
| 5025 measured reflections | $k = -11 \rightarrow 11$ |
| | $l = -13 \rightarrow 14$ |

Refinement

| | |
|---------------------------------|-------------------------------------------------------------------------------------|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.058$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.175$ | H-atom parameters constrained |
| $S = 1.06$ | $w = 1/[\sigma^2(F_o^2) + (0.0826P)^2 + 0.1249P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3686 reflections | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 199 parameters | $\Delta\rho_{\text{max}} = 0.28 \text{ e \AA}^{-3}$ |
| 0 restraints | $\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$ |

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|---------------|-------------|----------------------------------|
| S1 | 0.36871 (11) | 0.71963 (9) | 0.60411 (8) | 0.0553 (3) |
| S2 | 0.40282 (12) | -0.15478 (10) | 0.92480 (9) | 0.0616 (3) |
| C12 | 0.2777 (4) | 0.4790 (3) | 0.6886 (3) | 0.0409 (7) |
| C2 | 0.2998 (4) | 0.1229 (3) | 0.8994 (3) | 0.0428 (7) |
| C10 | 0.2760 (4) | 0.3248 (3) | 0.7386 (3) | 0.0420 (7) |
| C15 | 0.1480 (4) | 0.5656 (3) | 0.6474 (2) | 0.0410 (7) |
| C13 | 0.4056 (4) | 0.5472 (4) | 0.6719 (3) | 0.0474 (8) |
| C8 | 0.2843 (4) | 0.2788 (3) | 0.8535 (3) | 0.0438 (7) |
| C11 | 0.2615 (4) | 0.2192 (4) | 0.6591 (3) | 0.0481 (8) |
| C14 | 0.1819 (4) | 0.6995 (3) | 0.5987 (3) | 0.0459 (7) |
| C3 | 0.1900 (4) | 0.0800 (3) | 1.0143 (3) | 0.0457 (7) |
| C1 | 0.4219 (4) | 0.0072 (3) | 0.8411 (3) | 0.0481 (8) |
| C4 | 0.2314 (4) | -0.0692 (4) | 1.0389 (3) | 0.0527 (8) |
| C18 | -0.0090 (4) | 0.5183 (4) | 0.6644 (3) | 0.0556 (9) |
| H18A | -0.0777 | 0.5931 | 0.6298 | 0.083* |
| H18B | -0.0636 | 0.5061 | 0.7512 | 0.083* |
| H18C | 0.0133 | 0.4252 | 0.6232 | 0.083* |
| N2 | 0.2477 (4) | 0.1424 (3) | 0.5914 (3) | 0.0682 (9) |
| C9 | 0.2797 (5) | 0.3908 (4) | 0.9369 (3) | 0.0543 (8) |
| C7 | 0.0454 (5) | 0.1843 (4) | 1.0961 (3) | 0.0654 (10) |
| H7A | -0.0088 | 0.1304 | 1.1673 | 0.098* |
| H7B | -0.0292 | 0.2258 | 1.0509 | 0.098* |
| H7C | 0.0816 | 0.2635 | 1.1223 | 0.098* |
| N1 | 0.2708 (5) | 0.4759 (4) | 1.0067 (3) | 0.0814 (11) |
| C6 | 0.5626 (4) | 0.0063 (4) | 0.7253 (3) | 0.0651 (10) |
| H6A | 0.5563 | 0.1048 | 0.6892 | 0.098* |
| H6B | 0.5588 | -0.0623 | 0.6677 | 0.098* |
| H6C | 0.6632 | -0.0242 | 0.7444 | 0.098* |
| C17 | 0.0801 (5) | 0.8252 (4) | 0.5472 (3) | 0.0655 (10) |
| H17A | -0.0200 | 0.7979 | 0.5506 | 0.098* |
| H17B | 0.1395 | 0.8446 | 0.4628 | 0.098* |
| H17C | 0.0558 | 0.9133 | 0.5953 | 0.098* |
| C16 | 0.5635 (4) | 0.4920 (4) | 0.6983 (4) | 0.0648 (10) |
| H16A | 0.5649 | 0.3945 | 0.7361 | 0.097* |
| H16B | 0.5745 | 0.5595 | 0.7536 | 0.097* |
| H16C | 0.6526 | 0.4866 | 0.6223 | 0.097* |
| C5 | 0.1468 (6) | -0.1591 (4) | 1.1464 (3) | 0.0789 (12) |
| H5A | 0.0541 | -0.0947 | 1.2009 | 0.118* |
| H5B | 0.2214 | -0.2043 | 1.1906 | 0.118* |
| H5C | 0.1108 | -0.2356 | 1.1164 | 0.118* |

Atomic displacement parameters (\AA^2)

| | | | | | |
|----------|----------|----------|----------|----------|----------|
| U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----------|----------|----------|----------|----------|----------|

supplementary materials

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|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| S1 | 0.0595 (6) | 0.0513 (5) | 0.0576 (5) | -0.0242 (4) | -0.0145 (4) | 0.0040 (4) |
| S2 | 0.0718 (6) | 0.0429 (5) | 0.0699 (6) | -0.0036 (4) | -0.0276 (5) | -0.0013 (4) |
| C12 | 0.0455 (17) | 0.0419 (17) | 0.0338 (15) | -0.0106 (14) | -0.0097 (13) | -0.0001 (12) |
| C2 | 0.0490 (18) | 0.0417 (17) | 0.0398 (16) | -0.0079 (14) | -0.0178 (14) | -0.0006 (13) |
| C10 | 0.0425 (17) | 0.0417 (16) | 0.0412 (16) | -0.0105 (13) | -0.0110 (13) | -0.0025 (13) |
| C15 | 0.0431 (17) | 0.0462 (17) | 0.0327 (15) | -0.0112 (14) | -0.0094 (13) | -0.0006 (13) |
| C13 | 0.0443 (18) | 0.0493 (19) | 0.0475 (17) | -0.0128 (15) | -0.0104 (14) | -0.0026 (14) |
| C8 | 0.0510 (18) | 0.0394 (16) | 0.0399 (16) | -0.0092 (14) | -0.0126 (14) | -0.0028 (13) |
| C11 | 0.055 (2) | 0.0485 (19) | 0.0433 (17) | -0.0162 (15) | -0.0156 (15) | 0.0022 (15) |
| C14 | 0.0520 (19) | 0.0447 (18) | 0.0411 (16) | -0.0101 (15) | -0.0151 (14) | 0.0010 (14) |
| C3 | 0.0533 (19) | 0.0490 (18) | 0.0367 (16) | -0.0127 (15) | -0.0153 (14) | -0.0003 (13) |
| C1 | 0.0486 (19) | 0.0449 (18) | 0.0508 (18) | -0.0058 (15) | -0.0169 (15) | -0.0058 (15) |
| C4 | 0.069 (2) | 0.0485 (19) | 0.0479 (18) | -0.0186 (17) | -0.0261 (16) | 0.0059 (15) |
| C18 | 0.051 (2) | 0.063 (2) | 0.058 (2) | -0.0173 (17) | -0.0203 (16) | 0.0035 (17) |
| N2 | 0.084 (2) | 0.066 (2) | 0.0641 (19) | -0.0231 (17) | -0.0289 (17) | -0.0100 (17) |
| C9 | 0.073 (2) | 0.0437 (18) | 0.0458 (18) | -0.0077 (17) | -0.0213 (17) | -0.0013 (15) |
| C7 | 0.072 (2) | 0.065 (2) | 0.051 (2) | -0.0134 (19) | -0.0064 (18) | -0.0075 (17) |
| N1 | 0.130 (3) | 0.057 (2) | 0.060 (2) | -0.019 (2) | -0.032 (2) | -0.0110 (17) |
| C6 | 0.050 (2) | 0.064 (2) | 0.070 (2) | -0.0069 (18) | -0.0050 (18) | -0.0098 (19) |
| C17 | 0.084 (3) | 0.051 (2) | 0.063 (2) | -0.0120 (19) | -0.029 (2) | 0.0108 (17) |
| C16 | 0.050 (2) | 0.069 (2) | 0.081 (3) | -0.0162 (18) | -0.0243 (19) | -0.006 (2) |
| C5 | 0.117 (4) | 0.067 (3) | 0.060 (2) | -0.038 (2) | -0.031 (2) | 0.017 (2) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|-------------|------------|---------------|-----------|
| S1—C13 | 1.716 (3) | C4—C5 | 1.503 (5) |
| S1—C14 | 1.723 (3) | C18—H18A | 0.9600 |
| S2—C1 | 1.711 (3) | C18—H18B | 0.9600 |
| S2—C4 | 1.723 (4) | C18—H18C | 0.9600 |
| C12—C13 | 1.364 (4) | C9—N1 | 1.133 (4) |
| C12—C15 | 1.432 (4) | C7—H7A | 0.9600 |
| C12—C10 | 1.483 (4) | C7—H7B | 0.9600 |
| C2—C1 | 1.370 (4) | C7—H7C | 0.9600 |
| C2—C3 | 1.441 (4) | C6—H6A | 0.9600 |
| C2—C8 | 1.476 (4) | C6—H6B | 0.9600 |
| C10—C8 | 1.364 (4) | C6—H6C | 0.9600 |
| C10—C11 | 1.433 (4) | C17—H17A | 0.9600 |
| C15—C14 | 1.361 (4) | C17—H17B | 0.9600 |
| C15—C18 | 1.493 (4) | C17—H17C | 0.9600 |
| C13—C16 | 1.492 (5) | C16—H16A | 0.9600 |
| C8—C9 | 1.443 (4) | C16—H16B | 0.9600 |
| C11—N2 | 1.140 (4) | C16—H16C | 0.9600 |
| C14—C17 | 1.502 (4) | C5—H5A | 0.9600 |
| C3—C4 | 1.367 (4) | C5—H5B | 0.9600 |
| C3—C7 | 1.500 (5) | C5—H5C | 0.9600 |
| C1—C6 | 1.491 (5) | | |
| C13—S1—C14 | 92.95 (15) | H18A—C18—H18B | 109.5 |
| C1—S2—C4 | 93.19 (15) | C15—C18—H18C | 109.5 |
| C13—C12—C15 | 114.4 (3) | H18A—C18—H18C | 109.5 |

| | | | |
|-----------------|------------|-----------------|------------|
| C13—C12—C10 | 123.2 (3) | H18B—C18—H18C | 109.5 |
| C15—C12—C10 | 122.3 (3) | N1—C9—C8 | 176.8 (4) |
| C1—C2—C3 | 113.7 (3) | C3—C7—H7A | 109.5 |
| C1—C2—C8 | 124.0 (3) | C3—C7—H7B | 109.5 |
| C3—C2—C8 | 122.3 (3) | H7A—C7—H7B | 109.5 |
| C8—C10—C11 | 118.9 (3) | C3—C7—H7C | 109.5 |
| C8—C10—C12 | 124.9 (3) | H7A—C7—H7C | 109.5 |
| C11—C10—C12 | 116.2 (2) | H7B—C7—H7C | 109.5 |
| C14—C15—C12 | 111.4 (3) | C1—C6—H6A | 109.5 |
| C14—C15—C18 | 124.7 (3) | C1—C6—H6B | 109.5 |
| C12—C15—C18 | 123.8 (3) | H6A—C6—H6B | 109.5 |
| C12—C13—C16 | 130.3 (3) | C1—C6—H6C | 109.5 |
| C12—C13—S1 | 109.8 (2) | H6A—C6—H6C | 109.5 |
| C16—C13—S1 | 119.8 (2) | H6B—C6—H6C | 109.5 |
| C10—C8—C9 | 117.8 (3) | C14—C17—H17A | 109.5 |
| C10—C8—C2 | 125.3 (3) | C14—C17—H17B | 109.5 |
| C9—C8—C2 | 116.9 (3) | H17A—C17—H17B | 109.5 |
| N2—C11—C10 | 175.8 (3) | C14—C17—H17C | 109.5 |
| C15—C14—C17 | 129.5 (3) | H17A—C17—H17C | 109.5 |
| C15—C14—S1 | 111.4 (2) | H17B—C17—H17C | 109.5 |
| C17—C14—S1 | 119.1 (3) | C13—C16—H16A | 109.5 |
| C4—C3—C2 | 111.6 (3) | C13—C16—H16B | 109.5 |
| C4—C3—C7 | 123.7 (3) | H16A—C16—H16B | 109.5 |
| C2—C3—C7 | 124.6 (3) | C13—C16—H16C | 109.5 |
| C2—C1—C6 | 130.3 (3) | H16A—C16—H16C | 109.5 |
| C2—C1—S2 | 110.3 (2) | H16B—C16—H16C | 109.5 |
| C6—C1—S2 | 119.4 (2) | C4—C5—H5A | 109.5 |
| C3—C4—C5 | 128.6 (3) | C4—C5—H5B | 109.5 |
| C3—C4—S2 | 111.2 (2) | H5A—C5—H5B | 109.5 |
| C5—C4—S2 | 120.2 (3) | C4—C5—H5C | 109.5 |
| C15—C18—H18A | 109.5 | H5A—C5—H5C | 109.5 |
| C15—C18—H18B | 109.5 | H5B—C5—H5C | 109.5 |
| C13—C12—C10—C8 | 61.6 (4) | C12—C15—C14—C17 | -178.7 (3) |
| C15—C12—C10—C8 | -121.9 (3) | C18—C15—C14—C17 | -2.8 (5) |
| C13—C12—C10—C11 | -119.5 (3) | C12—C15—C14—S1 | -0.3 (3) |
| C15—C12—C10—C11 | 57.0 (4) | C18—C15—C14—S1 | 175.6 (2) |
| C13—C12—C15—C14 | 0.4 (4) | C13—S1—C14—C15 | 0.1 (2) |
| C10—C12—C15—C14 | -176.3 (3) | C13—S1—C14—C17 | 178.7 (3) |
| C13—C12—C15—C18 | -175.5 (3) | C1—C2—C3—C4 | -0.9 (4) |
| C10—C12—C15—C18 | 7.7 (4) | C8—C2—C3—C4 | -178.3 (3) |
| C15—C12—C13—C16 | -177.6 (3) | C1—C2—C3—C7 | -179.5 (3) |
| C10—C12—C13—C16 | -0.9 (5) | C8—C2—C3—C7 | 3.1 (5) |
| C15—C12—C13—S1 | -0.3 (3) | C3—C2—C1—C6 | -176.8 (3) |
| C10—C12—C13—S1 | 176.4 (2) | C8—C2—C1—C6 | 0.6 (5) |
| C14—S1—C13—C12 | 0.1 (2) | C3—C2—C1—S2 | 0.6 (3) |
| C14—S1—C13—C16 | 177.7 (3) | C8—C2—C1—S2 | 177.9 (2) |
| C11—C10—C8—C9 | -173.0 (3) | C4—S2—C1—C2 | -0.1 (3) |
| C12—C10—C8—C9 | 5.9 (5) | C4—S2—C1—C6 | 177.6 (3) |
| C11—C10—C8—C2 | 7.8 (5) | C2—C3—C4—C5 | -178.2 (3) |

supplementary materials

| | | | |
|----------------|------------|--------------|-----------|
| C12—C10—C8—C2 | -173.3 (3) | C7—C3—C4—C5 | 0.4 (5) |
| C1—C2—C8—C10 | 55.5 (5) | C2—C3—C4—S2 | 0.8 (3) |
| C3—C2—C8—C10 | -127.3 (3) | C7—C3—C4—S2 | 179.4 (3) |
| C1—C2—C8—C9 | -123.7 (3) | C1—S2—C4—C3 | -0.4 (3) |
| C3—C2—C8—C9 | 53.5 (4) | C1—S2—C4—C5 | 178.7 (3) |
| C8—C10—C11—N2 | 167 (5) | C10—C8—C9—N1 | 133 (7) |
| C12—C10—C11—N2 | -12 (5) | C2—C8—C9—N1 | -48 (7) |

Fig. 1

