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1,1,2-Trichloro-4,4-bis(4-methylphenylsulfanyl)-3-nitrobuta-1,3-diene

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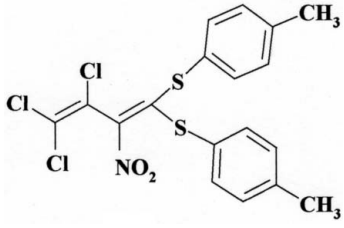
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.036; wR factor = 0.049; data-to-parameter ratio = 12.1.

The title compound, $C_{18}H_{14}Cl_3NO_2S_2$, was synthesized by the reaction of 1,1,2,4-tetrachloro-4-(4-methylphenylsulfanyl)-3-nitrobuta-1,3-diene with ethanedithiol. The butadiene unit is not completely planar as would be expected if the two double bonds were fully conjugated The torsion angle of the butadiene unit is −82.2 (5)°.

Related literature

For related literature, see: Ibis (1996); Ibis & Deniz (2006, 2007*a*,*b*); Carruthers & Watkin (1979).



Experimental

Crystal data

$C_{18}H_{14}Cl_3NO_2S_2$
M_r = 446.79
Monoclinic, $P2_1/n$
a = 13.885 (1) Å
b = 6.8246 (6) Å
c = 21.313 (2) Å
β = 98.630 (5)°
V = 1996.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 293.5 K
0.40 × 0.20 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID S diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.849, T_{max} = 0.935
69322 measured reflections
3653 independent reflections
3254 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.086

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.049
S = 1.12
3254 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2003); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2039).

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Carruthers, J. R. & Watkin, D. J. (1979). *Acta Cryst.* A**35**, 698–699.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Ibis, C. (1996). *Bull. Soc. Chim. Belg.* **105**, 317–320.
Ibis, C. & Deniz, N. G. (2006). *Acta Cryst.* E**62**, o5373–o5374.
Ibis, C. & Deniz, N. G. (2007*a*). *Indian J. Chem.* **46**, 674–680.
Ibis, C. & Deniz, N. G. (2007*b*). *Acta Cryst.* E**63**, o3058.
Rigaku/MSC (2003). *CrystalStructure* Version 3.5.1. Rigaku/MSC, The Woodlands, Texas, USA.
Rigaku/MSC (2005). *CrystalClear* Version 1.3.6. Rigaku/MSC Inc., The Woodlands, Texas, USA.

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supplementary materials

Acta Cryst. (2007). E**63**, o4394 [**doi:10.1107/S1600536807050957**]

1,1,2-Trichloro-4,4-bis(4-methylphenylsulfanyl)-3-nitrobuta-1,3-diene

C. Ibis and N. G. Deniz

Comment

The chemistry of compounds exhibiting nitro and additional halogen substituents, has been intensively studied in recent decades. These highly reactive substances have been used to develop preparative methods for the synthesis of complex polyfunctional derivatives of different classes. The synthesis of unsaturated thio-substituted halogenated organic compounds from the reaction of various halogenated alkenes and dienes with a number of thiols were published (Ibis & Deniz, 2007*a*). The aim in this study was to determine the conformation of 1,1,2-trichloro-4,4-bis(4'-methylphenylsulfanyl)-3-nitro-buta-1,3-diene (Ibis, 1996). The butadiene unit is not completely planar as it would be expected if the two double bonds were fully conjugated. The torsional angle of the butadiene unit (C1—C2—C3—C4) is −82.2 (5)°. The C—C bond lengths of the butadiene chain agree well with corresponding distances in a similar compound. (Ibis & Deniz, 2006, 2007*b*). Both phenyl rings are planar with maximum deviations of 0.0087 (1) Å and 0.0101 (1) Å and are inclined at an angle of 15.1 (1)°.

Experimental

A mixture of 1,1,2,4-tetrachloro-4-(4-methylphenylsulfanyl)-3-nitro- buta-1,3-diene (1.98 g, 5.52 mmol) and ethanedithiol (0.52 g, 5.52 mmol) was stirred in ethanol (35 ml) and 2 g sodium hydroxide in 10 ml water was added at room temperature. The mixture was stirred for another 2 h. Chloroform (50 ml) was added to the reaction mixture. The organic layer was separated and washed with water (4x30 ml), and dried with $MgSO_4$. The solvent was evaporated and the residue was purified by column chromatography on silica gel (0.063–0.20 mm; E. Merck). The title compound was obtained as a side product next to the main product 2-(4-methylphenylsulfanyl)-3-nitro-4,5-dichloro-1,6-dithia-octane-2,4-diene during this reaction sequence (Ibis *et al.*, 1996). Yellow crystals of (I) suitable for X-ray diffraction analysis were obtained by slow evaporation of an ethanolic solution at room temperature (yield: 0.19 g, 8%; m.p. 392–393 K).

Refinement

The non-hydrogen atoms were refined anisotropically. H atoms were located in geometrically idealized positions C—H = 0.95 (6) Å and treated as riding and U_{iso}(H) = 1.2U_{eq}(C).

Figures

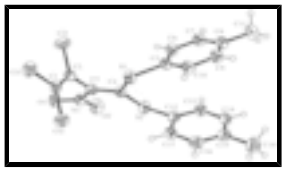


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

1,1,2-Trichloro-4,4-bis(4-methylphenylsulfanyl)-3-nitrobuta-1,3-diene

Crystal data

$C_{18}H_{14}Cl_3NO_2S_2$	F_{000} = 912.00
M_r = 446.79	D_x = 1.486 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 392-393 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.7107 Å
a = 13.885 (1) Å	Cell parameters from 5659 reflections
b = 6.8246 (6) Å	θ = 2.9–25.3º
c = 21.313 (2) Å	μ = 0.68 mm^{-1}
β = 98.630 (5)º	T = 293.5 K
V = 1996.7 (3) Å^3	Needle, yellow
Z = 4	0.40 × 0.20 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID S diffractometer	3254 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 10.00 pixels mm^{-1}	R_{int} = 0.086
ω scans	θ_{max} = 25.3º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	h = −16→16
T_{min} = 0.849, T_{max} = 0.935	k = −8→7
69322 measured reflections	l = −25→25
3653 independent reflections	

Refinement

Refinement on F	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.036	Chebychev polynomial *w*ith 3 parameters (Carruthers & Watkin, 1979) 14.9656 -4.4915 13.6461
$wR(F^2)$ = 0.049	$(\Delta/\sigma)_{max}$ = 0.026
S = 1.12	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
3254 reflections	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
235 parameters	Extinction correction: none

Special details

Geometry. Least Squares Planes

———— Plane number 1 ————

Atoms Defining Plane Distance e.s.d. C1 [1;0;0;0] −0.1397 0.0013 C2 [1;0;0;0] 0.3219 0.0029 C3 [1;0;0;0] −0.2390 0.0022 C4 [1;0;0;0] 0.0847 0.0008

Additional Atoms Distance e.s.d.

Mean deviation from plane is 0.1963 angstrom Chi-squared: 12552.825

————— Plane number 2 —————

Atoms Defining Plane Distance e.s.d. C5 [1;0;0;0] 0.0121 0.0028 C6 [1;0;0;0] −0.0118 0.0029 C7 [1;0;0;0] −0.0009 0.0031 C8 [1;0;0;0] 0.0136 0.0030 C9 [1;0;0;0] −0.0135 0.0031 C10 [1;0;0;0] −0.0004 0.0027

Additional Atoms Distance e.s.d.

Mean deviation from plane is 0.0087 angstrom Chi-squared: 37.790

————— Plane number 3 —————

Atoms Defining Plane Distance e.s.d. C12 [1;0;0;0] −0.0141 0.0030 C13 [1;0;0;0] 0.0049 0.0031 C14 [1;0;0;0] 0.0115 0.0037 C15 [1;0;0;0] −0.0165 0.0038 C16 [1;0;0;0] 0.0021 0.0034 C17 [1;0;0;0] 0.0116 0.0031

Additional Atoms Distance e.s.d.

Mean deviation from plane is 0.0101 angstrom Chi-squared: 33.959

Dihedral angles between least-squares planes ————————————————

plane plane angle e.s.d. 1 2 142.942 0.132 1 3 152.025 0.166 2 3 15.008 0.151

Refinement. Refinement using reflections with $F^2 > 3.0$ sigma(F^2). The weighted *R*-factor(*wR*), goodness of fit (S) and *R*-factor (gt) are based on F, with F set to zero for negative F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating *R*-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S(1)	0.56841 (7)	0.0359 (2)	0.88785 (4)	0.0565 (3)
Cl(1)	0.34904 (7)	−0.2935 (2)	0.74876 (5)	0.0720 (3)
Cl(2)	0.55665 (8)	−0.3657 (2)	0.76900 (5)	0.0700 (3)
S(2)	0.74902 (7)	0.2064 (2)	0.83810 (4)	0.0595 (3)
Cl(3)	0.38832 (8)	0.1596 (2)	0.74025 (7)	0.0830 (4)
O(1)	0.5776 (2)	0.0536 (5)	0.65928 (12)	0.0732 (9)
O(2)	0.6947 (2)	0.2191 (5)	0.71320 (13)	0.0775 (10)
N(1)	0.6211 (2)	0.1190 (5)	0.7097 (1)	0.0564 (10)
C(10)	0.6222 (3)	0.1431 (6)	1.0105 (2)	0.0556 (11)
C(5)	0.6007 (3)	0.2113 (6)	0.9486 (2)	0.0502 (10)
C(3)	0.5809 (3)	0.0756 (5)	0.7665 (2)	0.0487 (10)
C(2)	0.4828 (2)	−0.0080 (6)	0.7558 (2)	0.0508 (10)
C(7)	0.6249 (3)	0.5388 (6)	0.9868 (2)	0.0621 (12)
C(4)	0.6323 (2)	0.1088 (5)	0.8259 (2)	0.0473 (10)
C(6)	0.6005 (3)	0.4103 (6)	0.9371 (2)	0.0590 (11)
C(12)	0.7987 (3)	0.1309 (6)	0.9161 (2)	0.0539 (11)
C(13)	0.8408 (3)	0.2735 (7)	0.9576 (2)	0.0615 (12)
C(14)	0.8875 (3)	0.2180 (8)	1.0170 (2)	0.0682 (13)

C(8)	0.6484 (3)	0.4734 (6)	1.0485 (2)	0.0594 (12)
C(1)	0.4645 (3)	−0.1987 (6)	0.7574 (2)	0.0526 (11)
C(15)	0.8917 (3)	0.0225 (8)	1.0359 (2)	0.0663 (13)
C(16)	0.8512 (3)	−0.1173 (7)	0.9926 (2)	0.0677 (13)
C(9)	0.6447 (3)	0.2746 (6)	1.0595 (2)	0.0604 (12)
C(17)	0.8053 (3)	−0.0643 (7)	0.9327 (2)	0.0602 (12)
C(11)	0.6771 (4)	0.6177 (8)	1.1021 (2)	0.082
C(18)	0.9416 (4)	−0.0351 (9)	1.1015 (2)	0.091
H(1)	0.5825 (3)	0.4578 (6)	0.8951 (2)	0.071*
H(2)	0.6258 (3)	0.6758 (6)	0.9791 (2)	0.075*
H(3)	0.6583 (3)	0.2279 (6)	1.1018 (2)	0.073*
H(4)	0.6200 (3)	0.0062 (6)	1.0182 (2)	0.068*
H(5)	0.6919 (4)	0.5500 (8)	1.1413 (2)	0.099*
H(6)	0.7323 (4)	0.6911 (8)	1.0944 (2)	0.099*
H(7)	0.6239 (4)	0.7038 (8)	1.1038 (2)	0.099*
H(8)	0.8383 (3)	0.4066 (7)	0.9444 (2)	0.074*
H(9)	0.9154 (3)	0.3151 (8)	1.0461 (2)	0.082*
H(10)	0.8549 (3)	−0.2514 (7)	1.0047 (2)	0.082*
H(11)	0.7786 (3)	−0.1610 (7)	0.9030 (2)	0.072*
H(12)	0.9391 (4)	−0.1731 (9)	1.1068 (2)	0.109*
H(13)	1.0077 (4)	0.0061 (9)	1.1063 (2)	0.109*
H(14)	0.9099 (4)	0.0275 (9)	1.1326 (2)	0.109*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S(1)	0.0593 (5)	0.0684 (7)	0.0447 (5)	−0.0163 (5)	0.0170 (4)	−0.0056 (4)
Cl(1)	0.0565 (6)	0.0882 (8)	0.0716 (6)	−0.0201 (5)	0.0110 (5)	−0.0034 (6)
Cl(2)	0.0672 (6)	0.0618 (7)	0.0794 (7)	0.0068 (5)	0.0056 (5)	0.0047 (5)
S(2)	0.0539 (5)	0.0762 (7)	0.0493 (5)	−0.0174 (5)	0.0112 (4)	0.0020 (5)
Cl(3)	0.0571 (6)	0.0748 (8)	0.1148 (9)	0.0163 (5)	0.0057 (6)	−0.0009 (6)
O(1)	0.075 (2)	0.100 (2)	0.045 (1)	−0.002 (2)	0.0105 (12)	−0.007 (2)
O(2)	0.079 (2)	0.100 (2)	0.057 (2)	−0.026 (2)	0.021 (1)	0.011 (2)
N(1)	0.056 (2)	0.073 (2)	0.042 (2)	0.002 (2)	0.011 (1)	0.005 (1)
C(10)	0.071 (2)	0.053 (2)	0.046 (2)	−0.001 (2)	0.015 (2)	0.003 (2)
C(5)	0.053 (2)	0.059 (2)	0.040 (2)	0.000 (2)	0.013 (1)	−0.001 (2)
C(3)	0.051 (2)	0.052 (2)	0.045 (2)	0.000 (2)	0.014 (2)	−0.001 (2)
C(2)	0.047 (2)	0.063 (3)	0.043 (2)	0.002 (2)	0.010 (1)	−0.005 (2)
C(7)	0.072 (2)	0.056 (2)	0.059 (2)	0.004 (2)	0.011 (2)	−0.001 (2)
C(4)	0.048 (2)	0.052 (2)	0.044 (2)	−0.003 (2)	0.013 (1)	0.000 (2)
C(6)	0.070 (2)	0.066 (3)	0.040 (2)	0.005 (2)	0.006 (2)	0.006 (2)
C(12)	0.046 (2)	0.070 (3)	0.048 (2)	−0.004 (2)	0.012 (2)	−0.001 (2)
C(13)	0.052 (2)	0.072 (3)	0.059 (2)	−0.008 (2)	0.007 (2)	−0.008 (2)
C(14)	0.058 (2)	0.091 (4)	0.055 (2)	−0.005 (2)	0.007 (2)	−0.022 (2)
C(8)	0.065 (2)	0.070 (3)	0.045 (2)	0.002 (2)	0.010 (2)	−0.005 (2)
C(1)	0.050 (2)	0.065 (3)	0.042 (2)	−0.008 (2)	0.007 (1)	−0.003 (2)
C(15)	0.050 (2)	0.095 (4)	0.055 (2)	0.008 (2)	0.013 (2)	−0.004 (2)
C(16)	0.070 (3)	0.074 (3)	0.062 (2)	0.011 (2)	0.018 (2)	0.005 (2)

C(9)	0.073 (3)	0.065 (3)	0.043 (2)	0.003 (2)	0.010 (2)	0.004 (2)
C(17)	0.060 (2)	0.070 (3)	0.051 (2)	0.000 (2)	0.010 (2)	−0.012 (2)
C(11)	0.102 (4)	0.077 (3)	0.066 (3)	−0.007 (3)	0.015 (2)	−0.013 (2)
C(18)	0.079 (3)	0.131 (5)	0.062 (3)	0.008 (3)	0.004 (2)	0.003 (3)

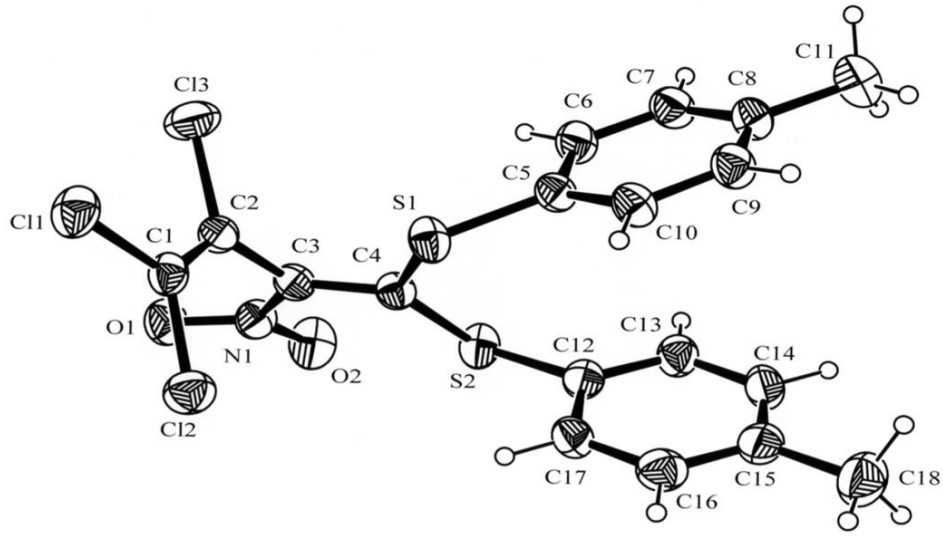
Geometric parameters (Å, °)

S(1)—C(5)	1.771 (4)	C(12)—C(13)	1.384 (6)
S(1)—C(4)	1.768 (4)	C(12)—C(17)	1.377 (6)
Cl(1)—C(1)	1.713 (4)	C(13)—C(14)	1.386 (5)
Cl(2)—C(1)	1.703 (4)	C(13)—H(8)	0.950 (6)
S(2)—C(4)	1.736 (3)	C(14)—C(15)	1.392 (7)
S(2)—C(12)	1.779 (4)	C(14)—H(9)	0.950 (6)
Cl(3)—C(2)	1.734 (4)	C(8)—C(9)	1.379 (6)
O(1)—N(1)	1.235 (4)	C(8)—C(11)	1.516 (6)
O(2)—N(1)	1.221 (5)	C(15)—C(16)	1.387 (6)
N(1)—C(3)	1.437 (5)	C(15)—C(18)	1.517 (6)
C(10)—C(5)	1.387 (5)	C(16)—C(17)	1.387 (5)
C(10)—C(9)	1.377 (5)	C(16)—H(10)	0.950 (7)
C(10)—H(4)	0.950 (6)	C(9)—H(3)	0.950 (5)
C(5)—C(6)	1.380 (6)	C(17)—H(11)	0.950 (6)
C(3)—C(2)	1.462 (5)	C(11)—H(5)	0.950 (7)
C(3)—C(4)	1.377 (5)	C(11)—H(6)	0.950 (8)
C(2)—C(1)	1.328 (6)	C(11)—H(7)	0.950 (8)
C(7)—C(6)	1.379 (5)	C(18)—H(12)	0.950 (9)
C(7)—C(8)	1.379 (5)	C(18)—H(13)	0.950 (7)
C(7)—H(2)	0.950 (6)	C(18)—H(14)	0.950 (7)
C(6)—H(1)	0.950 (5)		
C(5)—S(1)—C(4)	104.8 (2)	C(15)—C(14)—C(13)	121.3 (4)
C(4)—S(2)—C(12)	104.6 (2)	H(9)—C(14)—C(13)	119.7 (6)
C(3)—N(1)—O(1)	117.2 (3)	C(9)—C(8)—C(11)	121.6 (3)
C(3)—N(1)—O(2)	119.4 (3)	C(9)—C(8)—C(7)	118.1 (3)
O(1)—N(1)—O(2)	123.4 (3)	C(11)—C(8)—C(7)	120.4 (4)
C(5)—C(10)—C(9)	119.6 (4)	Cl(1)—C(1)—Cl(2)	115.7 (2)
C(5)—C(10)—H(4)	119.2 (4)	Cl(1)—C(1)—C(2)	123.2 (3)
C(9)—C(10)—H(4)	121.2 (4)	Cl(2)—C(1)—C(2)	121.1 (3)
C(6)—C(5)—S(1)	122.7 (3)	C(16)—C(15)—C(18)	121.3 (5)
C(6)—C(5)—C(10)	119.6 (3)	C(16)—C(15)—C(14)	118.2 (4)
S(1)—C(5)—C(10)	117.6 (3)	C(18)—C(15)—C(14)	120.6 (4)
C(2)—C(3)—C(4)	123.3 (3)	C(17)—C(16)—H(10)	119.9 (5)
C(2)—C(3)—N(1)	114.8 (3)	C(17)—C(16)—C(15)	121.2 (4)
C(4)—C(3)—N(1)	121.8 (3)	H(10)—C(16)—C(15)	118.9 (5)
C(1)—C(2)—Cl(3)	120.6 (3)	H(3)—C(9)—C(10)	119.5 (5)
C(1)—C(2)—C(3)	123.8 (3)	H(3)—C(9)—C(8)	119.0 (5)
Cl(3)—C(2)—C(3)	115.6 (3)	C(10)—C(9)—C(8)	121.5 (3)
C(6)—C(7)—C(8)	121.5 (4)	H(11)—C(17)—C(12)	119.8 (4)
C(6)—C(7)—H(2)	120.1 (4)	H(11)—C(17)—C(16)	120.8 (5)
C(8)—C(7)—H(2)	118.4 (4)	C(12)—C(17)—C(16)	119.5 (4)
S(1)—C(4)—S(2)	123.9 (2)	H(5)—C(11)—H(6)	109.5 (6)

S(1)—C(4)—C(3)	113.1 (3)	H(5)—C(11)—H(7)	109.5 (7)
S(2)—C(4)—C(3)	123.0 (3)	H(5)—C(11)—C(8)	110.2 (5)
H(1)—C(6)—C(5)	119.8 (4)	H(6)—C(11)—H(7)	109.5 (7)
H(1)—C(6)—C(7)	120.5 (5)	H(6)—C(11)—C(8)	109.9 (5)
C(5)—C(6)—C(7)	119.7 (3)	H(7)—C(11)—C(8)	108.3 (5)
C(13)—C(12)—C(17)	120.7 (3)	H(12)—C(18)—H(13)	109.5 (7)
C(13)—C(12)—S(2)	117.5 (3)	H(12)—C(18)—H(14)	109.5 (7)
C(17)—C(12)—S(2)	121.4 (3)	H(12)—C(18)—C(15)	110.3 (5)
C(14)—C(13)—H(8)	121.5 (5)	H(13)—C(18)—H(14)	109.5 (7)
C(14)—C(13)—C(12)	119.1 (4)	H(13)—C(18)—C(15)	108.8 (5)
H(8)—C(13)—C(12)	119.4 (4)	H(14)—C(18)—C(15)	109.3 (5)
C(15)—C(14)—H(9)	119.0 (5)		
C(4)—S(1)—C(5)—C(10)	−136.8 (3)	H(2)—C(7)—C(8)—C(9)	178.5 (5)
C(4)—S(1)—C(5)—C(6)	46.5 (3)	H(2)—C(7)—C(8)—C(11)	−1.4 (7)
C(5)—S(1)—C(4)—S(2)	37.1 (3)	S(2)—C(12)—C(13)—C(14)	−174.7 (3)
C(5)—S(1)—C(4)—C(3)	−144.4 (3)	S(2)—C(12)—C(13)—H(8)	4.0 (6)
C(12)—S(2)—C(4)—S(1)	20.6 (3)	C(17)—C(12)—C(13)—C(14)	−1.8 (6)
C(12)—S(2)—C(4)—C(3)	−157.7 (3)	C(17)—C(12)—C(13)—H(8)	176.8 (5)
C(4)—S(2)—C(12)—C(13)	−129.4 (3)	S(2)—C(12)—C(17)—C(16)	175.2 (3)
C(4)—S(2)—C(12)—C(17)	57.9 (3)	S(2)—C(12)—C(17)—H(11)	−4.6 (6)
O(1)—N(1)—C(3)—C(2)	−11.5 (5)	C(13)—C(12)—C(17)—C(16)	2.6 (6)
O(1)—N(1)—C(3)—C(4)	167.6 (4)	C(13)—C(12)—C(17)—H(11)	−177.2 (5)
O(2)—N(1)—C(3)—C(2)	167.5 (3)	C(12)—C(13)—C(14)—C(15)	−0.8 (6)
O(2)—N(1)—C(3)—C(4)	−13.4 (6)	C(12)—C(13)—C(14)—H(9)	−178.8 (5)
C(9)—C(10)—C(5)—S(1)	−178.0 (3)	H(8)—C(13)—C(14)—C(15)	−179.4 (5)
C(9)—C(10)—C(5)—C(6)	−1.1 (6)	H(8)—C(13)—C(14)—H(9)	2.6 (8)
H(4)—C(10)—C(5)—S(1)	0.9 (6)	C(13)—C(14)—C(15)—C(16)	2.5 (6)
H(4)—C(10)—C(5)—C(6)	177.8 (5)	C(13)—C(14)—C(15)—C(18)	−179.0 (4)
C(5)—C(10)—C(9)—C(8)	−1.4 (6)	H(9)—C(14)—C(15)—C(16)	−179.5 (5)
C(5)—C(10)—C(9)—H(3)	178.8 (5)	H(9)—C(14)—C(15)—C(18)	−1.0 (7)
H(4)—C(10)—C(9)—C(8)	179.7 (5)	C(7)—C(8)—C(9)—C(10)	2.6 (6)
H(4)—C(10)—C(9)—H(3)	−0.0 (8)	C(7)—C(8)—C(9)—H(3)	−177.6 (5)
S(1)—C(5)—C(6)—C(7)	178.9 (3)	C(11)—C(8)—C(9)—C(10)	−177.5 (4)
S(1)—C(5)—C(6)—H(1)	−0.1 (7)	C(11)—C(8)—C(9)—H(3)	2.3 (7)
C(10)—C(5)—C(6)—C(7)	2.2 (6)	C(7)—C(8)—C(11)—H(5)	−179.2 (6)
C(10)—C(5)—C(6)—H(1)	−176.8 (5)	C(7)—C(8)—C(11)—H(6)	−58.4 (7)
N(1)—C(3)—C(2)—Cl(3)	−83.0 (4)	C(7)—C(8)—C(11)—H(7)	61.1 (7)
N(1)—C(3)—C(2)—C(1)	96.9 (4)	C(9)—C(8)—C(11)—H(5)	1.0 (8)
C(4)—C(3)—C(2)—Cl(3)	97.8 (4)	C(9)—C(8)—C(11)—H(6)	121.7 (6)
C(4)—C(3)—C(2)—C(1)	−82.2 (5)	C(9)—C(8)—C(11)—H(7)	−118.8 (6)
N(1)—C(3)—C(4)—S(1)	−178.0 (3)	C(14)—C(15)—C(16)—C(17)	−1.7 (6)
N(1)—C(3)—C(4)—S(2)	0.4 (5)	C(14)—C(15)—C(16)—H(10)	178.7 (5)
C(2)—C(3)—C(4)—S(1)	1.1 (5)	C(18)—C(15)—C(16)—C(17)	179.8 (4)
C(2)—C(3)—C(4)—S(2)	179.5 (3)	C(18)—C(15)—C(16)—H(10)	0.2 (7)
Cl(3)—C(2)—C(1)—Cl(1)	−3.4 (4)	C(14)—C(15)—C(18)—H(12)	−179.2 (5)
Cl(3)—C(2)—C(1)—Cl(2)	177.0 (2)	C(14)—C(15)—C(18)—H(13)	−59.1 (7)
C(3)—C(2)—C(1)—Cl(1)	176.6 (3)	C(14)—C(15)—C(18)—H(14)	60.4 (7)
C(3)—C(2)—C(1)—Cl(2)	−3.0 (5)	C(16)—C(15)—C(18)—H(12)	−0.8 (7)
C(8)—C(7)—C(6)—C(5)	−1.0 (6)	C(16)—C(15)—C(18)—H(13)	119.4 (7)

C(8)—C(7)—C(6)—H(1)	178.0 (5)	C(16)—C(15)—C(18)—H(14)	−121.2 (6)
H(2)—C(7)—C(6)—C(5)	179.1 (5)	C(15)—C(16)—C(17)—C(12)	−0.8 (6)
H(2)—C(7)—C(6)—H(1)	−1.9 (8)	C(15)—C(16)—C(17)—H(11)	179.0 (5)
C(6)—C(7)—C(8)—C(9)	−1.4 (6)	H(10)—C(16)—C(17)—C(12)	178.8 (5)
C(6)—C(7)—C(8)—C(11)	178.7 (4)	H(10)—C(16)—C(17)—H(11)	−1.5 (8)

Fig. 1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C18