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1,1-Dichloro-3-(6,1,3-oxadithiaoctocan-2-ylidene)-3-nitro-2-(4-methylphenylsulfanyl)propene

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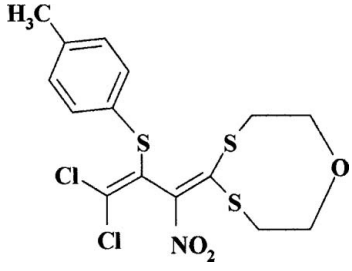
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.027; data-to-parameter ratio = 8.7.

The molecule of the title compound, $C_{15}H_{15}Cl_2NO_3S_3$, is not planar. The butadiene group and the 4-methylphenyl ring are inclined at an angle of 57.9 (1)°.

Related literature

For general background, see: Edema *et al.* (1993). The C—C bond lengths of the butadiene unit are similar to those in related compounds (Ibis & Deniz, 2006, 2007; Ibis *et al.*, 2006). For related literature, see: Ibis (1996).



Experimental

Crystal data

$C_{15}H_{15}Cl_2NO_3S_3$
M_r = 424.37
Orthorhombic, $P2_12_12$
a = 13.5112 (5) Å
b = 18.0213 (6) Å
c = 7.5559 (2) Å
V = 1839.78 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.71 mm^{-1}
T = 293.5 K
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID S diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.772, T_{max} = 0.869
69828 measured reflections
1897 independent reflections
1886 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.027
S = 1.13
1886 reflections
217 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 11 Friedel pairs
Flack parameter: 0.07 (5)

Table 1
Selected torsion angles (°).

C1—C2—C3—C4	−97.2 (3)	O3—C7—C8—S3	−59.0 (4)
O3—C6—C5—S2	−74.0 (4)		

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: XU2259).

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supplementary materials

Acta Cryst. (2007). E**63**, o3058 [**doi:10.1107/S1600536807025731**]

1,1-Dichloro-3-(6,1,3-oxadithiaoctocan-2-ylidene)-3-nitro-2-(4-methylphenylsulfanyl)propene

C. Ibis and N. G. Deniz

Comment

Compounds with conjugated double bonds are fairly reactive because of their strained structures, thus, effective synthesis of these compounds are still challenging in organic chemistry. Macrocyclic thio-crown ethers are particular interest, among other reasons, as potential heavy-metal receptors and could be useful for treatment of heavy-metal poisoning (Edema *et al.*, 1993). The aim of this study was to determine the conformation of the 4,4-dichloro-2-nitro-3-(4-methylphenylsulfanyl)-1,1-(*cyclo*-oxydiethanesulfanyl) -buta-1,3-diene (Ibis, 1996). The butadiene group and the 4-methylphenyl ring are inclined at an angle of 57.9 (1)°. The butadiene unit has assumed a configuration close to *cisoid*, but is not completely planar as would be if the two double bounds were fully conjugated. Torsion angle of C4—C3—C2—C1 is −97.2 (3)°.

Experimental

To a mixture of 2-nitro-1,3,4,4-tetrachloro-1-(4-methylphenylthio) −1,3-butadiene (2 g, 5.57 mmol) and 2,2'-oxydiethane-thiol, $HSCH_2CH_2OCH_2CH_2SH$, (0.77 g, 5.57 mmol) were stirred in ethanol (35 ml) and 2 g sodium hydroxide in 10 ml water was added at room temperature. The mixture was stirred for 2 h. Chloroform (50 ml) was added to the reaction mixture. The organic layer was separated and washed with water (4x30 ml), and dried $MgSO_4$. The solvent was evaporated and residue was purified by column chromatography on silica gel (0.063–0.20 mm). The yellow crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution at the room temperature; yield 0.60 g, 25%.

Refinement

H atoms were treated as riding, with C—H = 0.95 (6)Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

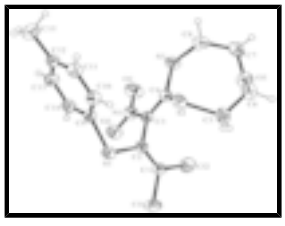


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

1,1-Dichloro-3-(6,1,3-oxadithiaoctocan-2-ylidene)-3-nitro- 2-(4-methylphenylsulfanyl)propene

Crystal data

$C_{15}H_{15}Cl_2NO_3S_3$	D_x = 1.532 Mg m^{-3}
M_r = 424.37	Melting point: 418-420 K

Orthorhombic, $P2_12_12$	Mo $K\alpha$ radiation $\lambda = 0.7107$ Å
Hall symbol: P 2 2ab	Cell parameters from 10401 reflections
$a = 13.5112$ (5) Å	$\theta = 2.7–25.0°$
$b = 18.0213$ (6) Å	$\mu = 0.71$ mm^{-1}
$c = 7.5559$ (2) Å	$T = 293.5$ K
$V = 1839.78$ (10) Å^3	Block, yellow
$Z = 4$	0.40 × 0.30 × 0.20 mm
$F_{000} = 872.00$	

Data collection

Rigaku R-AXIS RAPID S diffractometer	1886 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 10.00 pixels mm^{-1}	$R_{int} = 0.034$
ω scans	$\theta_{max} = 25.1°$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -16\rightarrow16$
$T_{min} = 0.772$, $T_{max} = 0.869$	$k = -21\rightarrow21$
69828 measured reflections	$l = -8\rightarrow8$
1897 independent reflections	

Refinement

Refinement on F	Chebychev polynomial *w*ith 3 parameters (Carruthers & Watkin (1979). Acta Cryst. A35, 698–699) 4.7778 -2.5240 3.7682
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} = 0.011$
$wR(F^2) = 0.027$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
$S = 1.13$	$\Delta\rho_{min} = -0.20$ e Å^{-3}
1886 reflections	Extinction correction: none
217 parameters	Absolute structure: Flack (1983), 11 Friedel pairs
H atoms treated by a mixture of independent and constrained refinement	Flack parameter: 0.07 (5)

Special details

Geometry. Least Squares Planes

———— Plane number 1 ————

Atoms Defining Plane Distance e.s.d. C1 [1;0;0;0] −0.1475 0.0008 C2 [1;0;0;0] 0.2949 0.0017 C3 [1;0;0;0] −0.3380 0.0019 C4 [1;0;0;0] 0.1243 0.0007

Additional Atoms Distance e.s.d.

Mean deviation from plane is 0.2262 angstrom Chi-squared: 30910.697

———— Plane number 2 ————

Atoms Defining Plane Distance e.s.d. C9 [1;0;0;0] 0.0065 0.0020 C10 [1;0;0;0] −0.0062 0.0022 C11 [1;0;0;0] −0.0039 0.0024 C12 [1;0;0;0] 0.0113 0.0021 C13 [1;0;0;0] −0.0110 0.0023 C14 [1;0;0;0] 0.0007 0.0021

Additional Atoms Distance e.s.d.

Mean deviation from plane is 0.0066 angstrom Chi-squared: 36.706

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

plane plane angle e.s.d. 1 2 57.939 0.179

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(2)	0.91725 (5)	0.26150 (4)	1.20586 (11)	0.0540 (2)
S(1)	0.84229 (6)	0.44795 (4)	1.09641 (10)	0.0555 (2)
S(3)	0.82153 (6)	0.16803 (4)	0.91382 (11)	0.0616 (2)
Cl(1)	0.67918 (7)	0.45722 (5)	1.38723 (12)	0.0775 (3)
Cl(2)	0.60463 (6)	0.31134 (5)	1.2969 (1)	0.0780 (3)
O(3)	0.8220 (2)	0.09720 (12)	1.2966 (3)	0.0685 (6)
O(2)	0.6445 (2)	0.36598 (12)	0.8510 (3)	0.0680 (7)
N(1)	0.6947 (2)	0.30988 (13)	0.8709 (3)	0.0550 (7)
C(12)	1.0330 (2)	0.3895 (1)	0.6181 (4)	0.0504 (8)
O(1)	0.6907 (2)	0.25714 (13)	0.7694 (3)	0.0866 (8)
C(2)	0.7595 (2)	0.37355 (13)	1.1325 (4)	0.0452 (7)
C(9)	0.9120 (2)	0.41788 (13)	0.9113 (4)	0.0468 (7)
C(11)	1.0693 (2)	0.3824 (2)	0.7885 (4)	0.0561 (8)
C(3)	0.7635 (2)	0.3066 (1)	1.0190 (4)	0.0446 (7)
C(4)	0.8237 (2)	0.24795 (13)	1.0448 (3)	0.0435 (7)
C(14)	0.8750 (2)	0.4239 (2)	0.7403 (4)	0.0538 (8)
C(13)	0.9349 (2)	0.4091 (2)	0.5970 (4)	0.0566 (8)
C(10)	1.0099 (2)	0.3963 (2)	0.9345 (4)	0.0530 (8)
C(1)	0.6910 (2)	0.3792 (2)	1.2578 (4)	0.0540 (8)
C(6)	0.8883 (3)	0.1338 (2)	1.4124 (5)	0.0684 (10)
C(5)	0.8718 (3)	0.2166 (2)	1.4040 (4)	0.0645 (9)
C(7)	0.8667 (3)	0.0581 (2)	1.1558 (5)	0.0684 (10)
C(8)	0.9115 (2)	0.1069 (2)	1.0145 (5)	0.0623 (9)
C(15)	1.0992 (3)	0.3795 (2)	0.4603 (4)	0.0729 (10)
H(1)	0.8085 (2)	0.4397 (2)	0.7242 (4)	0.0645*
H(2)	0.9074 (2)	0.4117 (2)	0.4815 (4)	0.0680*
H(3)	1.1367 (2)	0.3693 (2)	0.8068 (4)	0.0672*
H(4)	1.0358 (2)	0.3910 (2)	1.0507 (4)	0.0636*
H(5)	0.9025 (3)	0.2397 (2)	1.5029 (4)	0.077*
H(6)	0.8022 (3)	0.2238 (2)	1.4104 (4)	0.077*
H(7)	0.8786 (3)	0.1156 (2)	1.5291 (5)	0.082*

H(8)	0.9545 (3)	0.1244 (2)	1.3765 (5)	0.082*
H(9)	0.9401 (2)	0.0766 (2)	0.9254 (5)	0.075*
H(10)	0.9615 (2)	0.1364 (2)	1.0679 (5)	0.075*
H(11)	0.9164 (3)	0.0264 (2)	1.2026 (5)	0.082*
H(12)	0.8166 (3)	0.0290 (2)	1.1010 (5)	0.082*
H(13)	1.1272 (3)	0.3312 (2)	0.4628 (4)	0.088*
H(14)	1.0614 (3)	0.3854 (2)	0.3551 (4)	0.088*
H(15)	1.1506 (3)	0.4155 (2)	0.4628 (4)	0.088*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S(2)	0.0532 (4)	0.0441 (3)	0.0646 (4)	−0.0069 (3)	−0.0154 (4)	0.0018 (3)
S(1)	0.0689 (5)	0.0436 (3)	0.0540 (4)	−0.0054 (3)	0.0049 (4)	−0.0090 (3)
S(3)	0.0740 (5)	0.0499 (4)	0.0609 (5)	0.0050 (3)	−0.0072 (4)	−0.0153 (4)
Cl(1)	0.0919 (6)	0.0718 (5)	0.0687 (5)	0.0196 (5)	0.0132 (5)	−0.0181 (4)
Cl(2)	0.0658 (5)	0.0829 (5)	0.0854 (6)	−0.0053 (4)	0.0223 (5)	0.0040 (5)
O(3)	0.0600 (12)	0.0708 (12)	0.075 (1)	−0.0143 (11)	0.0024 (13)	−0.0024 (12)
O(2)	0.0595 (12)	0.0694 (12)	0.075 (2)	0.0109 (11)	−0.0168 (12)	0.0018 (11)
N(1)	0.056 (1)	0.0562 (13)	0.053 (1)	−0.0019 (11)	−0.0094 (12)	−0.0043 (12)
C(12)	0.052 (2)	0.045 (1)	0.054 (2)	−0.0051 (12)	0.002 (1)	−0.0044 (13)
O(1)	0.106 (2)	0.079 (2)	0.075 (2)	0.013 (1)	−0.040 (2)	−0.025 (1)
C(2)	0.048 (1)	0.0429 (13)	0.045 (2)	0.0031 (11)	−0.0034 (13)	0.0003 (12)
C(9)	0.054 (2)	0.0384 (11)	0.048 (2)	−0.0049 (12)	0.000 (1)	0.0008 (12)
C(11)	0.047 (2)	0.060 (2)	0.062 (2)	−0.0012 (13)	−0.006 (2)	0.001 (2)
C(3)	0.047 (1)	0.0446 (13)	0.042 (1)	−0.0022 (12)	−0.0028 (12)	−0.0025 (12)
C(4)	0.0447 (13)	0.0409 (12)	0.045 (2)	−0.0068 (11)	−0.0012 (12)	−0.0026 (11)
C(14)	0.050 (2)	0.054 (2)	0.057 (2)	0.0027 (13)	−0.004 (1)	0.001 (1)
C(13)	0.064 (2)	0.061 (2)	0.045 (2)	0.001 (1)	−0.006 (2)	−0.004 (1)
C(10)	0.057 (2)	0.052 (2)	0.050 (2)	−0.0083 (13)	−0.009 (1)	0.0006 (13)
C(1)	0.059 (2)	0.053 (1)	0.050 (2)	0.0072 (13)	0.007 (1)	−0.0019 (12)
C(6)	0.079 (2)	0.060 (2)	0.066 (2)	−0.007 (2)	−0.012 (2)	0.010 (2)
C(5)	0.079 (2)	0.059 (2)	0.055 (2)	−0.001 (2)	−0.015 (2)	0.003 (2)
C(7)	0.068 (2)	0.045 (2)	0.093 (3)	−0.003 (1)	−0.010 (2)	−0.005 (2)
C(8)	0.056 (2)	0.050 (2)	0.081 (2)	0.007 (1)	0.005 (2)	−0.016 (2)
C(15)	0.065 (2)	0.091 (2)	0.062 (2)	−0.007 (2)	0.008 (2)	−0.011 (2)

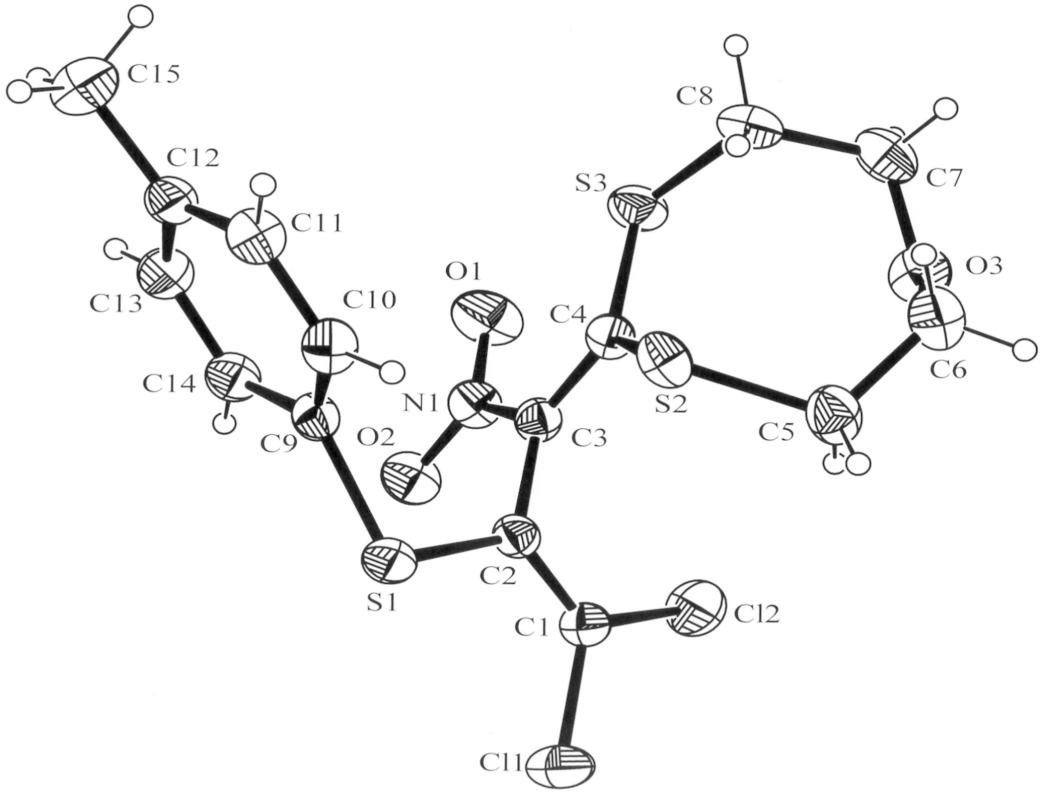
Geometric parameters (Å, °)

S(2)—C(4)	1.771 (3)	C(11)—C(10)	1.387 (4)
S(2)—C(5)	1.809 (3)	C(11)—H(3)	0.950 (4)
S(1)—C(2)	1.767 (3)	C(3)—C(4)	1.348 (4)
S(1)—C(9)	1.771 (3)	C(14)—C(13)	1.377 (4)
S(3)—C(4)	1.748 (2)	C(14)—H(1)	0.950 (4)
S(3)—C(8)	1.808 (3)	C(13)—H(2)	0.950 (4)
Cl(1)—C(1)	1.720 (3)	C(10)—H(4)	0.950 (4)
Cl(2)—C(1)	1.716 (3)	C(6)—C(5)	1.510 (4)
O(3)—C(6)	1.415 (4)	C(6)—H(7)	0.950 (5)
O(3)—C(7)	1.412 (4)	C(6)—H(8)	0.950 (5)

O(2)—N(1)	1.227 (3)	C(5)—H(5)	0.950 (5)
N(1)—O(1)	1.222 (3)	C(5)—H(6)	0.950 (5)
N(1)—C(3)	1.455 (4)	C(7)—C(8)	1.510 (5)
C(12)—C(11)	1.384 (4)	C(7)—H(11)	0.950 (5)
C(12)—C(13)	1.381 (4)	C(7)—H(12)	0.950 (5)
C(12)—C(15)	1.501 (5)	C(8)—H(9)	0.950 (5)
C(2)—C(3)	1.481 (4)	C(8)—H(10)	0.950 (4)
C(2)—C(1)	1.328 (4)	C(15)—H(13)	0.950 (5)
C(9)—C(14)	1.389 (4)	C(15)—H(14)	0.950 (5)
C(9)—C(10)	1.390 (4)	C(15)—H(15)	0.950 (5)
C(4)—S(2)—C(5)	105.4 (1)	Cl(1)—C(1)—Cl(2)	114.9 (2)
C(2)—S(1)—C(9)	103.1 (1)	Cl(1)—C(1)—C(2)	122.2 (2)
C(4)—S(3)—C(8)	104.6 (1)	Cl(2)—C(1)—C(2)	122.8 (2)
C(6)—O(3)—C(7)	115.4 (2)	C(5)—C(6)—H(7)	111.1 (4)
O(1)—N(1)—C(3)	118.6 (2)	C(5)—C(6)—H(8)	107.6 (4)
O(1)—N(1)—O(2)	122.6 (3)	C(5)—C(6)—O(3)	110.0 (3)
C(3)—N(1)—O(2)	118.8 (2)	H(7)—C(6)—H(8)	109.5 (5)
C(11)—C(12)—C(13)	118.1 (3)	H(7)—C(6)—O(3)	109.0 (4)
C(11)—C(12)—C(15)	121.1 (3)	H(8)—C(6)—O(3)	109.7 (4)
C(13)—C(12)—C(15)	120.7 (3)	H(5)—C(5)—H(6)	109.5 (4)
C(3)—C(2)—C(1)	120.1 (2)	H(5)—C(5)—S(2)	107.9 (3)
C(3)—C(2)—S(1)	120.4 (2)	H(5)—C(5)—C(6)	109.6 (3)
C(1)—C(2)—S(1)	119.5 (2)	H(6)—C(5)—S(2)	108.5 (3)
C(14)—C(9)—C(10)	118.8 (3)	H(6)—C(5)—C(6)	106.1 (3)
C(14)—C(9)—S(1)	121.3 (2)	S(2)—C(5)—C(6)	115.2 (2)
C(10)—C(9)—S(1)	119.5 (2)	C(8)—C(7)—H(11)	109.3 (4)
C(10)—C(11)—H(3)	118.9 (4)	C(8)—C(7)—H(12)	107.4 (4)
C(10)—C(11)—C(12)	121.1 (3)	C(8)—C(7)—O(3)	114.4 (2)
H(3)—C(11)—C(12)	119.9 (4)	H(11)—C(7)—H(12)	109.5 (4)
C(4)—C(3)—N(1)	121.9 (2)	H(11)—C(7)—O(3)	108.8 (4)
C(4)—C(3)—C(2)	125.2 (2)	H(12)—C(7)—O(3)	107.4 (4)
N(1)—C(3)—C(2)	112.9 (2)	H(9)—C(8)—H(10)	109.5 (4)
S(2)—C(4)—S(3)	121.0 (1)	H(9)—C(8)—S(3)	109.0 (3)
S(2)—C(4)—C(3)	115.0 (2)	H(9)—C(8)—C(7)	109.2 (3)
S(3)—C(4)—C(3)	123.6 (2)	H(10)—C(8)—S(3)	108.4 (3)
C(13)—C(14)—H(1)	120.8 (3)	H(10)—C(8)—C(7)	108.1 (4)
C(13)—C(14)—C(9)	120.3 (3)	S(3)—C(8)—C(7)	112.5 (2)
H(1)—C(14)—C(9)	118.8 (3)	H(13)—C(15)—H(14)	109.5 (5)
H(2)—C(13)—C(12)	119.6 (3)	H(13)—C(15)—H(15)	109.5 (5)
H(2)—C(13)—C(14)	118.9 (3)	H(13)—C(15)—C(12)	109.3 (4)
C(12)—C(13)—C(14)	121.5 (3)	H(14)—C(15)—H(15)	109.5 (5)
H(4)—C(10)—C(9)	119.7 (3)	H(14)—C(15)—C(12)	109.3 (4)
H(4)—C(10)—C(11)	120.2 (4)	H(15)—C(15)—C(12)	109.7 (4)
C(9)—C(10)—C(11)	120.1 (3)		
C(5)—S(2)—C(4)—S(3)	−87.1 (2)	S(1)—C(2)—C(1)—Cl(1)	0.3 (4)
C(5)—S(2)—C(4)—C(3)	100.1 (2)	S(1)—C(2)—C(1)—Cl(2)	177.5 (2)
C(4)—S(2)—C(5)—C(6)	82.4 (3)	C(3)—C(2)—C(1)—Cl(1)	−177.1 (2)
C(4)—S(2)—C(5)—H(5)	−154.9 (3)	C(3)—C(2)—C(1)—Cl(2)	0.1 (4)

C(4)—S(2)—C(5)—H(6)	−36.4 (3)	S(1)—C(9)—C(14)—C(13)	171.7 (2)
C(9)—S(1)—C(2)—C(3)	1.2 (2)	S(1)—C(9)—C(14)—H(1)	−6.6 (4)
C(9)—S(1)—C(2)—C(1)	−176.2 (2)	C(10)—C(9)—C(14)—C(13)	−0.3 (4)
C(2)—S(1)—C(9)—C(14)	80.2 (2)	C(10)—C(9)—C(14)—H(1)	−178.6 (3)
C(2)—S(1)—C(9)—C(10)	−107.8 (2)	S(1)—C(9)—C(10)—C(11)	−171.2 (2)
C(8)—S(3)—C(4)—S(2)	10.9 (2)	S(1)—C(9)—C(10)—H(4)	9.1 (4)
C(8)—S(3)—C(4)—C(3)	−176.9 (2)	C(14)—C(9)—C(10)—C(11)	1.0 (4)
C(4)—S(3)—C(8)—C(7)	89.4 (2)	C(14)—C(9)—C(10)—H(4)	−178.7 (3)
C(4)—S(3)—C(8)—H(9)	−149.3 (3)	C(12)—C(11)—C(10)—C(9)	0.0 (4)
C(4)—S(3)—C(8)—H(10)	−30.2 (4)	C(12)—C(11)—C(10)—H(4)	179.7 (3)
C(7)—O(3)—C(6)—C(5)	116.5 (3)	H(3)—C(11)—C(10)—C(9)	177.9 (3)
C(7)—O(3)—C(6)—H(7)	−121.5 (4)	H(3)—C(11)—C(10)—H(4)	−2.3 (5)
C(7)—O(3)—C(6)—H(8)	−1.7 (4)	N(1)—C(3)—C(4)—S(2)	168.8 (2)
C(6)—O(3)—C(7)—C(8)	−71.2 (3)	N(1)—C(3)—C(4)—S(3)	−3.8 (4)
C(6)—O(3)—C(7)—H(11)	51.4 (4)	C(2)—C(3)—C(4)—S(2)	−10.8 (4)
C(6)—O(3)—C(7)—H(12)	169.7 (3)	C(2)—C(3)—C(4)—S(3)	176.7 (2)
O(2)—N(1)—C(3)—C(2)	2.2 (4)	C(9)—C(14)—C(13)—C(12)	−1.4 (4)
O(2)—N(1)—C(3)—C(4)	−177.3 (3)	C(9)—C(14)—C(13)—H(2)	177.6 (3)
O(1)—N(1)—C(3)—C(2)	−179.1 (2)	H(1)—C(14)—C(13)—C(12)	176.9 (3)
O(1)—N(1)—C(3)—C(4)	1.3 (4)	H(1)—C(14)—C(13)—H(2)	−4.2 (5)
C(13)—C(12)—C(11)—C(10)	−1.7 (4)	O(3)—C(6)—C(5)—S(2)	−74.0 (4)
C(13)—C(12)—C(11)—H(3)	−179.6 (3)	O(3)—C(6)—C(5)—H(5)	164.1 (4)
C(15)—C(12)—C(11)—C(10)	175.8 (3)	O(3)—C(6)—C(5)—H(6)	46.1 (4)
C(15)—C(12)—C(11)—H(3)	−2.1 (5)	H(7)—C(6)—C(5)—S(2)	165.2 (4)
C(11)—C(12)—C(13)—C(14)	2.3 (4)	H(7)—C(6)—C(5)—H(5)	43.4 (6)
C(11)—C(12)—C(13)—H(2)	−176.6 (3)	H(7)—C(6)—C(5)—H(6)	−74.7 (5)
C(15)—C(12)—C(13)—C(14)	−175.1 (3)	H(8)—C(6)—C(5)—S(2)	45.4 (4)
C(15)—C(12)—C(13)—H(2)	6.0 (5)	H(8)—C(6)—C(5)—H(5)	−76.4 (5)
C(11)—C(12)—C(15)—H(13)	58.9 (5)	H(8)—C(6)—C(5)—H(6)	165.5 (4)
C(11)—C(12)—C(15)—H(14)	178.8 (4)	O(3)—C(7)—C(8)—S(3)	−59.0 (4)
C(11)—C(12)—C(15)—H(15)	−61.1 (5)	O(3)—C(7)—C(8)—H(9)	179.7 (4)
C(13)—C(12)—C(15)—H(13)	−123.7 (4)	O(3)—C(7)—C(8)—H(10)	60.7 (4)
C(13)—C(12)—C(15)—H(14)	−3.9 (5)	H(11)—C(7)—C(8)—S(3)	178.7 (3)
C(13)—C(12)—C(15)—H(15)	116.2 (4)	H(11)—C(7)—C(8)—H(9)	57.5 (5)
S(1)—C(2)—C(3)—N(1)	−94.2 (3)	H(11)—C(7)—C(8)—H(10)	−61.6 (5)
S(1)—C(2)—C(3)—C(4)	85.4 (3)	H(12)—C(7)—C(8)—S(3)	60.0 (4)
C(1)—C(2)—C(3)—N(1)	83.2 (3)	H(12)—C(7)—C(8)—H(9)	−61.2 (5)
C(1)—C(2)—C(3)—C(4)	−97.2 (3)	H(12)—C(7)—C(8)—H(10)	179.8 (4)

Fig. 1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S2
C5
C3
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Cl2
Cl1