Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*S*)-*O*-[4-(2,2,4-Trimethylchroman-4-yl)-phenyl] *N*,*N*-dimethylthiocarbamate

Tia Jacobs* and Martin W. Bredenkamp

Department of Chemistry, University of Stellenbosch, Private Bag X1, Matieland, South Africa
Correspondence e-mail: tj@sun.ac.za

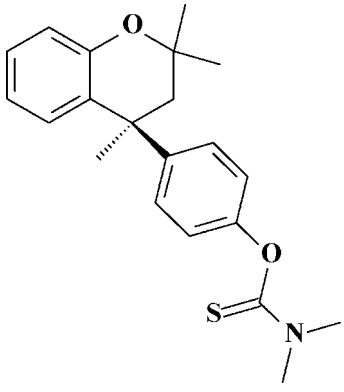
Received 30 July 2007; accepted 23 October 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.109; data-to-parameter ratio = 15.7.

Crystallization of the (*S*)-enantiomer of the title compound, $C_{21}H_{26}NO_2S$, from methanol gave an unsolvated crystal structure in which one-dimensional strands of molecules are formed through a series of C—H···O and C—H···S hydrogen bonds, and C—H···π interactions.

Related literature

For related literature, see: Esterhuysen *et al.* (2005); Flippen *et al.* (1970); Hardy *et al.* (1979); Jacobs *et al.* (2006); Lloyd & Bredenkamp (2005); Lloyd, Alen, Bredenkamp *et al.* (2006); Lloyd, Alen, Jacobs *et al.* (2006); Lloyd *et al.* (2005); de Vries *et al.* (2005); Brienne & Jacques (1975).



Experimental

Crystal data

$C_{21}H_{25}NO_2S$
M_r = 355.48
Monoclinic, $P2_1$
a = 6.5858 (5) Å
b = 7.1397 (5) Å
c = 19.996 (1) Å
β = 94.780 (1)°
V = 936.95 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 100 (2) K
0.21 × 0.18 × 0.15 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: none
5663 measured reflections
3574 independent reflections
3479 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.109
S = 1.04
3574 reflections
228 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), 1404 Friedel pairs
Flack parameter: 0.01 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1^{i}	0.95	2.55	3.414 (2)	151
C20—H20B···S^{ii}	0.98	2.73	3.671 (2)	160

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z$; (ii) $x, y+1, z$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001; Atwood & Barbour, 2003); software used to prepare material for publication: *X-SEED*.

The authors thank the National Research Foundation of South Africa for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2021).

References

Atwood, J. L. & Barbour, L. J. (2003). *Cryst. Growth Des.* **3**, 3–8.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Brienne, M. J. & Jacques, J. (1975). *Tetrahedron Lett.*, pp. 2349–2352.
Bruker (2002). *SMART*. Version 5.628. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT*. Version 6.45. Bruker AXS Inc., Madison, Wisconsin, USA.
Esterhuysen, C., Bredenkamp, M. W. & Lloyd, G. O. (2005). *Acta Cryst.* C**61**, o32–o34.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Flippen, J. L., Karle, J. & Karle, I. L. (1970). *J. Am. Chem. Soc.* **92**, 3749–3755.
Hardy, A. D. U., McKendrick, J. J., MacNicol, D. D. & Wilson, D. R. (1979). *J. Chem. Soc. Perkin Trans. 2*, pp. 729–734.
Jacobs, T., Lloyd, G. O. & Bredenkamp, M. W. (2006). *Acta Cryst.* E**62**, o4400–o4402.
Lloyd, G. O., Alen, J., Bredenkamp, M. W., de Vries, E. J. C., Esterhuysen, C. & Barbour, L. J. (2006). *Angew. Chem. Int. Ed.* **45**, 5354–5358.
Lloyd, G. O., Alen, J., Jacobs, T., Bredenkamp, M. W. & de Vries, E. J. C. (2006). *Acta Cryst.* E**62**, o691–o693.
Lloyd, G. O. & Bredenkamp, M. W. (2005). *Acta Cryst.* E**61**, o1512–o1514.
Lloyd, G. O., Bredenkamp, M. W. & Barbour, L. J. (2005). *Chem. Commun.* pp. 4053–4055.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Vries, E. J. C. de, Bredenkamp, M. W., Jacobs, T. & Lloyd, G. O. (2005). *Acta Cryst.* E**61**, o2871–o2872.

  doi:10.1107/S160053680705249X

supplementary materials

Acta Cryst. (2007). E**63**, o4444 [**doi:10.1107/S160053680705249X**]

(*S*)-*O*-[4-(2,2,4-Trimethylchroman-4-yl)phenyl] *N*,*N*-dimethylthiocarbamate

T. Jacobs and M. W. Bredenkamp

Comment

In an ongoing investigation of Dianin's compound (4-*p*-hydroxyphenyl-2,2,4-trimethylchroman) (Flippen *et al.*, 1970) and the inclusion chemistry of its derivatives, we synthesized the title compound (Fig. 1, I) (Esterhuysen *et al.*, 2005; Lloyd *et al.*,2005; Lloyd & Bredenkamp, 2005; Lloyd *et al.*, 2006; Jacobs *et al.*, 2006).

The title compound was synthesized as a chirally pure intermediate from (*S*)-4-(4-Hydroxyphenyl)-2,2,4-trimethylchroman in the preparation of the resolved thiol derivative of Dianin's compound. Here we report the structure of the resolved dimethylthiocarbamate derivative, which is very different from the corresponding racemic structure (de Vries *et al.*, 2005). The molecules form bilayer-type sheets in the [100] plane (Fig 2). The molecule packing is stabilized by C—H···O and C—H···S hydrogen bonds, and intermolecular C—H···π interactions (Table 1, *Cg* is the centroid of the C10—C15 benzene ring), with the dimethylthiocarbamate moieties associating and the chroman moieties pointing towards each other.

Experimental

(*S*)-4-*p*-hydroxyphenyl-2,2,4-trimethylchroman was chirally resolved according to the literature method (Brienne & Jacques, 1975) from a racemic mixture of the compound. This chirally pure species was then converted into the title compound according to the literature method (Hardy *et al.*, 1979). Single crystals suitable for X-ray analysis were obtained by slow evaporation from a methanol solution.

Refinement

All the H atoms were included in the riding-model approximation, with C—H = 0.95–0.98, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C) (C20 and C21).

Figures

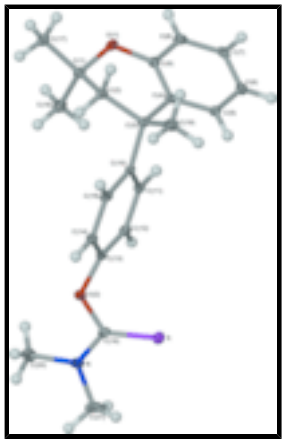


Fig. 1. The molecular structure of (I), showing atom labels and 50% probability displacement ellipsoids for non-H atoms.

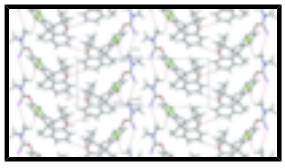


Fig. 2. The bilayer-type packing of compound I, intermolecular interactions are shown as red dashed lines. *Cg* denotes the ring centroid. [Symmetry codes: (i) 1 − *x*, *y* − 1/2, −*z*; (ii) *x*, 1 + *y*, *z*; (iii) *x*, *y* − 1, *z*; (iv) 1 − *x*, *y* + 1/2, −*z*.]

(*S*)-*O*-[4-(2,2,4-Trimethylchroman-4-yl)phenyl] *N*,*N*-dimethylthiocarbamate

Crystal data

$C_{21}H_{25}NO_2S$	F_{000} = 380
M_r = 355.48	D_x = 1.260 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 1032 reflections
a = 6.5858 (5) Å	θ = 2.3–19.3º
b = 7.1397 (5) Å	μ = 0.19 mm^{-1}
c = 19.996 (1) Å	*T* = 100 (2) K
β = 94.780 (1)º	Blocks, colourless
V = 936.95 (11) Å^3	0.21 × 0.18 × 0.15 mm
Z = 2	

Data collection

Bruker APEX CCD area-detector diffractometer	3574 independent reflections
Radiation source: fine-focus sealed tube	3479 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.0º
T = 100(2) K	θ_{min} = 1.0º
ω scans	*h* = −6→8
Absorption correction: none	*k* = −8→9
5663 measured reflections	*l* = −25→23

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0762P)^2 + 0.15P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.109$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.46$ e Å^{-3}
3574 reflections	$\Delta\rho_{min} = -0.26$ e Å^{-3}
228 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1358 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.01 (7)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2$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}
S	0.28200 (7)	0.52502 (8)	0.44057 (2)	0.02235 (14)
O1	0.8148 (2)	0.1302 (2)	0.07012 (7)	0.0197 (3)
O2	0.5200 (2)	0.7164 (2)	0.36253 (7)	0.0236 (3)
N	0.3274 (3)	0.8928 (3)	0.42094 (9)	0.0228 (4)
C1	0.9298 (3)	0.2663 (3)	0.11193 (9)	0.0179 (4)
C2	0.9973 (3)	0.1746 (3)	0.17922 (9)	0.0162 (4)
H2A	1.0753	0.2678	0.2076	0.019*
H2B	1.0911	0.0702	0.1710	0.019*
C3	0.8242 (3)	0.0978 (3)	0.21874 (9)	0.0148 (4)
C4	0.6675 (3)	0.0035 (3)	0.16921 (9)	0.0151 (4)
C5	0.5173 (3)	−0.1144 (3)	0.19136 (9)	0.0170 (4)
H5	0.5098	−0.1308	0.2382	0.020*
C6	0.3786 (3)	−0.2084 (3)	0.14704 (10)	0.0198 (4)
H6	0.2777	−0.2870	0.1636	0.024*
C7	0.3887 (3)	−0.1864 (3)	0.07831 (10)	0.0189 (4)
H7	0.2949	−0.2500	0.0476	0.023*

C8	0.5361 (3)	−0.0713 (3)	0.05506 (9)	0.0186 (4)
H8	0.5438	−0.0568	0.0081	0.022*
C9	0.6736 (3)	0.0237 (3)	0.09965 (9)	0.0159 (3)
C10	0.7311 (3)	0.2545 (3)	0.25958 (9)	0.0147 (4)
C11	0.5289 (3)	0.3112 (3)	0.24875 (9)	0.0165 (4)
H11	0.4411	0.2478	0.2161	0.020*
C12	0.4517 (3)	0.4591 (3)	0.28479 (10)	0.0179 (4)
H12	0.3137	0.4972	0.2765	0.021*
C13	0.5801 (3)	0.5485 (3)	0.33256 (9)	0.0181 (4)
C14	0.7813 (3)	0.4949 (3)	0.34578 (9)	0.0187 (4)
H14	0.8673	0.5576	0.3791	0.022*
C15	0.8553 (3)	0.3475 (3)	0.30932 (9)	0.0177 (4)
H15	0.9929	0.3090	0.3183	0.021*
C16	0.3755 (3)	0.7167 (3)	0.40763 (9)	0.0167 (4)
C17	1.1158 (3)	0.3091 (3)	0.07366 (10)	0.0224 (4)
H17A	1.0710	0.3600	0.0294	0.027*
H17B	1.1933	0.1937	0.0683	0.027*
H17C	1.2023	0.4010	0.0988	0.027*
C18	0.8008 (3)	0.4421 (3)	0.11708 (11)	0.0227 (4)
H18A	0.6748	0.4104	0.1374	0.027*
H18B	0.7672	0.4940	0.0721	0.027*
H18C	0.8773	0.5351	0.1450	0.027*
C19	0.9192 (3)	−0.0513 (3)	0.26836 (10)	0.0205 (4)
H19A	1.0249	0.0072	0.2989	0.025*
H19B	0.9799	−0.1517	0.2432	0.025*
H19C	0.8130	−0.1037	0.2944	0.025*
C20	0.4249 (4)	1.0515 (3)	0.39042 (11)	0.0298 (5)
H20A	0.5669	1.0611	0.4091	0.045*
H20B	0.3522	1.1670	0.3999	0.045*
H20C	0.4210	1.0328	0.3418	0.045*
C21	0.1799 (4)	0.9357 (4)	0.46943 (12)	0.0313 (5)
H21A	0.0415	0.9238	0.4477	0.047*
H21B	0.2015	1.0640	0.4859	0.047*
H21C	0.1978	0.8480	0.5072	0.047*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0260 (2)	0.0186 (2)	0.0239 (2)	−0.0034 (2)	0.01069 (18)	−0.0010 (2)
O1	0.0236 (7)	0.0221 (7)	0.0143 (6)	−0.0046 (6)	0.0065 (5)	−0.0005 (6)
O2	0.0322 (8)	0.0145 (7)	0.0267 (7)	−0.0010 (7)	0.0171 (6)	−0.0043 (6)
N	0.0322 (10)	0.0172 (9)	0.0205 (8)	0.0033 (8)	0.0119 (7)	−0.0025 (7)
C1	0.0183 (9)	0.0181 (10)	0.0178 (9)	−0.0012 (8)	0.0045 (7)	−0.0020 (8)
C2	0.0151 (8)	0.0158 (10)	0.0184 (9)	0.0018 (7)	0.0051 (6)	−0.0007 (7)
C3	0.0157 (9)	0.0152 (9)	0.0138 (8)	0.0002 (8)	0.0030 (7)	−0.0017 (7)
C4	0.0174 (8)	0.0121 (9)	0.0161 (8)	0.0022 (8)	0.0033 (6)	−0.0029 (8)
C5	0.0210 (9)	0.0158 (9)	0.0149 (8)	−0.0003 (8)	0.0058 (7)	−0.0008 (7)
C6	0.0212 (9)	0.0140 (9)	0.0252 (10)	−0.0009 (8)	0.0070 (8)	−0.0022 (8)

C7	0.0201 (9)	0.0137 (9)	0.0228 (9)	0.0007 (8)	0.0010 (7)	−0.0046 (8)
C8	0.0224 (9)	0.0188 (10)	0.0151 (8)	0.0038 (8)	0.0040 (7)	−0.0017 (8)
C9	0.0166 (8)	0.0142 (8)	0.0175 (8)	0.0024 (9)	0.0052 (6)	−0.0003 (8)
C10	0.0191 (9)	0.0126 (9)	0.0132 (8)	−0.0001 (8)	0.0068 (7)	0.0004 (7)
C11	0.0191 (9)	0.0157 (10)	0.0152 (8)	−0.0008 (8)	0.0043 (7)	−0.0013 (7)
C12	0.0176 (9)	0.0170 (10)	0.0201 (9)	0.0037 (8)	0.0078 (7)	0.0022 (7)
C13	0.0263 (9)	0.0119 (10)	0.0175 (8)	−0.0009 (8)	0.0106 (7)	−0.0017 (7)
C14	0.0235 (9)	0.0175 (10)	0.0157 (8)	−0.0043 (8)	0.0049 (7)	−0.0020 (7)
C15	0.0186 (9)	0.0203 (10)	0.0146 (8)	0.0009 (8)	0.0044 (7)	0.0012 (7)
C16	0.0183 (9)	0.0187 (10)	0.0137 (8)	0.0007 (8)	0.0043 (7)	−0.0008 (7)
C17	0.0235 (10)	0.0217 (11)	0.0234 (10)	−0.0022 (9)	0.0108 (8)	−0.0001 (8)
C18	0.0248 (10)	0.0198 (10)	0.0245 (10)	0.0045 (9)	0.0077 (8)	0.0050 (8)
C19	0.0232 (9)	0.0192 (10)	0.0193 (9)	0.0045 (9)	0.0017 (7)	0.0002 (8)
C20	0.0473 (13)	0.0154 (11)	0.0285 (11)	0.0012 (10)	0.0128 (9)	0.0003 (8)
C21	0.0375 (12)	0.0286 (12)	0.0305 (11)	0.0058 (11)	0.0188 (10)	−0.0068 (10)

Geometric parameters (Å, °)

S—C16	1.659 (2)	C8—H8	0.9500
O1—C9	1.372 (2)	C10—C11	1.391 (3)
O1—C1	1.452 (2)	C10—C15	1.401 (3)
O2—C16	1.365 (2)	C11—C12	1.398 (3)
O2—C13	1.411 (2)	C11—H11	0.9500
N—C16	1.329 (3)	C12—C13	1.379 (3)
N—C20	1.461 (3)	C12—H12	0.9500
N—C21	1.461 (3)	C13—C14	1.383 (3)
C1—C18	1.525 (3)	C14—C15	1.392 (3)
C1—C17	1.529 (3)	C14—H14	0.9500
C1—C2	1.529 (3)	C15—H15	0.9500
C2—C3	1.541 (2)	C17—H17A	0.9800
C2—H2A	0.9900	C17—H17B	0.9800
C2—H2B	0.9900	C17—H17C	0.9800
C3—C4	1.526 (2)	C18—H18A	0.9800
C3—C10	1.542 (3)	C18—H18B	0.9800
C3—C19	1.551 (3)	C18—H18C	0.9800
C4—C5	1.399 (3)	C19—H19A	0.9800
C4—C9	1.402 (2)	C19—H19B	0.9800
C5—C6	1.391 (3)	C19—H19C	0.9800
C5—H5	0.9500	C20—H20A	0.9800
C6—C7	1.390 (3)	C20—H20B	0.9800
C6—H6	0.9500	C20—H20C	0.9800
C7—C8	1.382 (3)	C21—H21A	0.9800
C7—H7	0.9500	C21—H21B	0.9800
C8—C9	1.393 (3)	C21—H21C	0.9800
C9—O1—C1	117.53 (14)	C12—C11—H11	119.2
C16—O2—C13	121.16 (15)	C13—C12—C11	118.60 (18)
C16—N—C20	121.99 (17)	C13—C12—H12	120.7
C16—N—C21	120.92 (19)	C11—C12—H12	120.7
C20—N—C21	117.04 (18)	C12—C13—C14	121.78 (18)

O1—C1—C18	108.83 (17)	C12—C13—O2	120.66 (18)
O1—C1—C17	104.27 (15)	C14—C13—O2	116.86 (18)
C18—C1—C17	110.09 (17)	C13—C14—C15	118.75 (18)
O1—C1—C2	108.65 (16)	C13—C14—H14	120.6
C18—C1—C2	114.59 (16)	C15—C14—H14	120.6
C17—C1—C2	109.87 (16)	C14—C15—C10	121.39 (19)
C1—C2—C3	115.50 (16)	C14—C15—H15	119.3
C1—C2—H2A	108.4	C10—C15—H15	119.3
C3—C2—H2A	108.4	N—C16—O2	108.95 (17)
C1—C2—H2B	108.4	N—C16—S	126.74 (15)
C3—C2—H2B	108.4	O2—C16—S	124.30 (15)
H2A—C2—H2B	107.5	C1—C17—H17A	109.5
C4—C3—C2	108.26 (14)	C1—C17—H17B	109.5
C4—C3—C10	112.73 (15)	H17A—C17—H17B	109.5
C2—C3—C10	110.92 (16)	C1—C17—H17C	109.5
C4—C3—C19	109.12 (16)	H17A—C17—H17C	109.5
C2—C3—C19	107.21 (15)	H17B—C17—H17C	109.5
C10—C3—C19	108.45 (15)	C1—C18—H18A	109.5
C5—C4—C9	117.09 (17)	C1—C18—H18B	109.5
C5—C4—C3	121.19 (16)	H18A—C18—H18B	109.5
C9—C4—C3	121.65 (17)	C1—C18—H18C	109.5
C6—C5—C4	122.19 (17)	H18A—C18—H18C	109.5
C6—C5—H5	118.9	H18B—C18—H18C	109.5
C4—C5—H5	118.9	C3—C19—H19A	109.5
C7—C6—C5	119.49 (19)	C3—C19—H19B	109.5
C7—C6—H6	120.3	H19A—C19—H19B	109.5
C5—C6—H6	120.3	C3—C19—H19C	109.5
C8—C7—C6	119.52 (18)	H19A—C19—H19C	109.5
C8—C7—H7	120.2	H19B—C19—H19C	109.5
C6—C7—H7	120.2	N—C20—H20A	109.5
C7—C8—C9	120.77 (17)	N—C20—H20B	109.5
C7—C8—H8	119.6	H20A—C20—H20B	109.5
C9—C8—H8	119.6	N—C20—H20C	109.5
O1—C9—C8	114.96 (15)	H20A—C20—H20C	109.5
O1—C9—C4	124.07 (17)	H20B—C20—H20C	109.5
C8—C9—C4	120.93 (18)	N—C21—H21A	109.5
C11—C10—C15	117.86 (17)	N—C21—H21B	109.5
C11—C10—C3	123.12 (17)	H21A—C21—H21B	109.5
C15—C10—C3	119.02 (17)	N—C21—H21C	109.5
C10—C11—C12	121.60 (18)	H21A—C21—H21C	109.5
C10—C11—H11	119.2	H21B—C21—H21C	109.5
C9—O1—C1—C18	−81.6 (2)	C5—C4—C9—C8	−0.5 (3)
C9—O1—C1—C17	160.98 (17)	C3—C4—C9—C8	176.53 (18)
C9—O1—C1—C2	43.8 (2)	C4—C3—C10—C11	−4.1 (3)
O1—C1—C2—C3	−58.0 (2)	C2—C3—C10—C11	117.48 (19)
C18—C1—C2—C3	63.9 (2)	C19—C3—C10—C11	−125.04 (19)
C17—C1—C2—C3	−171.53 (17)	C4—C3—C10—C15	177.00 (16)
C1—C2—C3—C4	40.8 (2)	C2—C3—C10—C15	−61.4 (2)
C1—C2—C3—C10	−83.3 (2)	C19—C3—C10—C15	56.1 (2)

C1—C2—C3—C19	158.42 (16)	C15—C10—C11—C12	1.6 (3)
C2—C3—C4—C5	165.70 (17)	C3—C10—C11—C12	−177.26 (17)
C10—C3—C4—C5	−71.2 (2)	C10—C11—C12—C13	−0.7 (3)
C19—C3—C4—C5	49.3 (2)	C11—C12—C13—C14	−0.4 (3)
C2—C3—C4—C9	−11.2 (3)	C11—C12—C13—O2	169.79 (16)
C10—C3—C4—C9	111.9 (2)	C16—O2—C13—C12	72.1 (2)
C19—C3—C4—C9	−127.53 (19)	C16—O2—C13—C14	−117.3 (2)
C9—C4—C5—C6	−0.1 (3)	C12—C13—C14—C15	0.5 (3)
C3—C4—C5—C6	−177.08 (19)	O2—C13—C14—C15	−170.06 (17)
C4—C5—C6—C7	0.4 (3)	C13—C14—C15—C10	0.5 (3)
C5—C6—C7—C8	−0.1 (3)	C11—C10—C15—C14	−1.6 (3)
C6—C7—C8—C9	−0.4 (3)	C3—C10—C15—C14	177.39 (17)
C1—O1—C9—C8	165.62 (18)	C20—N—C16—O2	−0.9 (3)
C1—O1—C9—C4	−16.5 (3)	C21—N—C16—O2	−178.18 (19)
C7—C8—C9—O1	178.71 (18)	C20—N—C16—S	177.94 (17)
C7—C8—C9—C4	0.7 (3)	C21—N—C16—S	0.7 (3)
C5—C4—C9—O1	−178.26 (18)	C13—O2—C16—N	−171.51 (18)
C3—C4—C9—O1	−1.3 (3)	C13—O2—C16—S	9.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{i}	0.95	2.55	3.414 (2)	151
C20—H20B···S^{ii}	0.98	2.73	3.671 (2)	160
C20—H20C···Cg^{ii}	0.98	3.22	3.543 (3)	101

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*; (ii) *x*, *y*+1, *z*.

Fig. 1

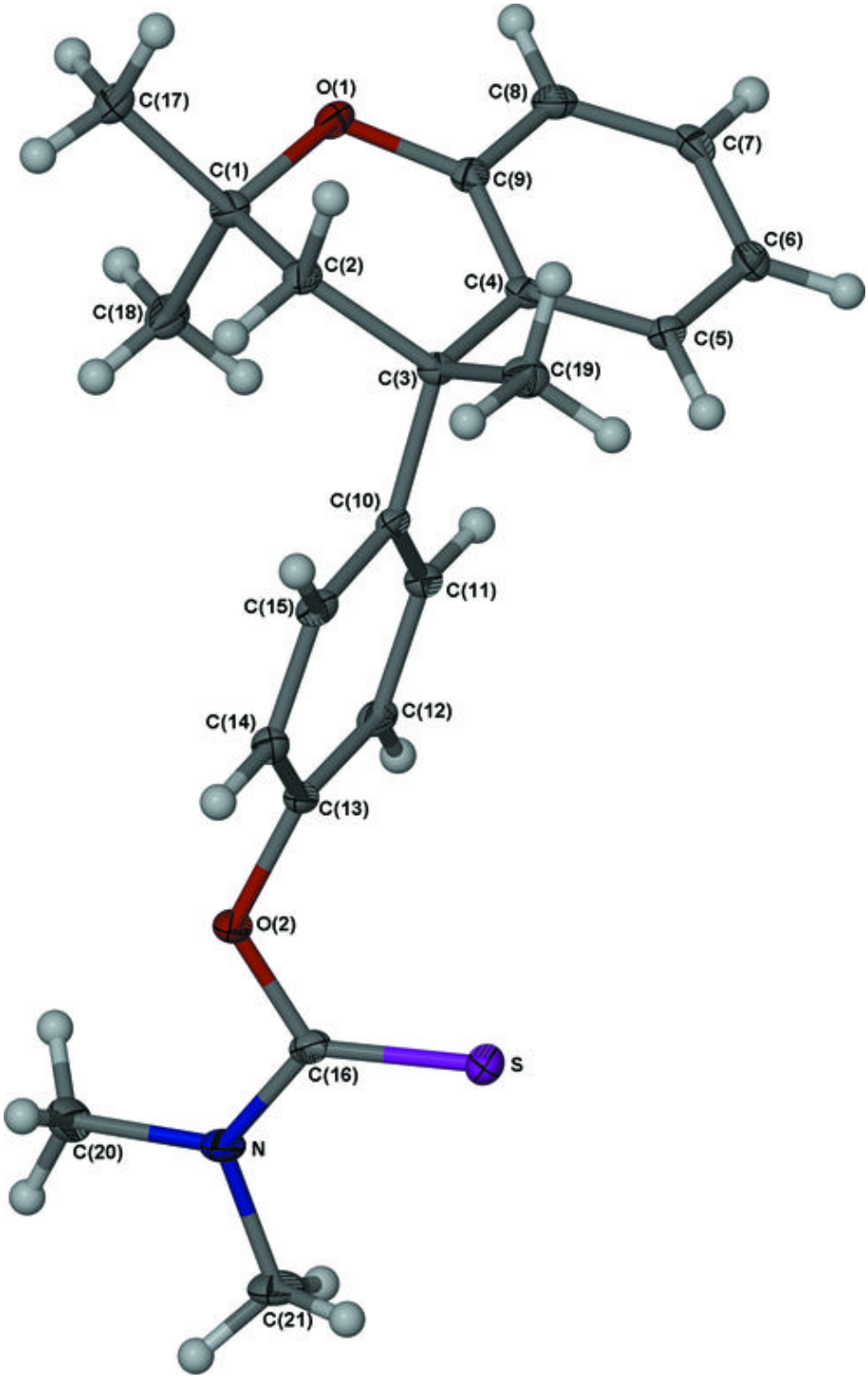

C(17)
O(1)
C(8)
C(7)
C(1)
C(9)
C(6)
C(2)
C(4)
C(18)
C(5)
C(3)
C(19)
C(10)
C(11)
C(15)
C(12)
C(14)
C(13)
O(2)
S
C(16)
C(20)
N
C(21)

Fig. 2