

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

O-Propyl N-phenylthiocarbamate

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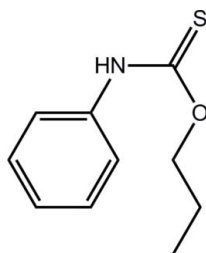
Received 11 May 2012; accepted 11 May 2012

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
R factor = 0.030; wR factor = 0.081; data-to-parameter ratio = 17.5.

Two independent molecules comprise the asymmetric unit in the title thiocarbamide derivative, $\text{C}_{10}\text{H}_{13}\text{NOS}$. These differ in the relative orientations of terminal ethyl groups [C—C—C—O torsion angles = -66.95 (13) and 55.92 (13)°, respectively]. The phenyl ring is twisted out of the plane of the central residue [C_q—N—C_{ph}—C_{ph} = -146.20 (12) and -144.15 (12)°, respectively; q = quaternary and ph = phenyl]. The independent molecules are linked into a dimeric aggregate by N—H···S hydrogen bonds and an eight-membered thioamide {···H—N—C=S}₂ synthon.

Related literature

For related thiocarbamaide structures, see: Ho *et al.* (2005); Kuan *et al.* (2007).



Experimental

Crystal data

$\text{C}_{10}\text{H}_{13}\text{NOS}$
 $M_r = 195.27$
Triclinic, $P\bar{1}$
 $a = 8.9230$ (4) Å

$b = 9.8752$ (4) Å
 $c = 12.9613$ (5) Å
 $\alpha = 98.037$ (3)°
 $\beta = 105.866$ (4)°

$\gamma = 104.533$ (4)°
 $V = 1036.46$ (7) Å³
 $Z = 4$
Cu $K\alpha$ radiation

$\mu = 2.45$ mm⁻¹
 $T = 100$ K
 $0.35 \times 0.30 \times 0.25$ mm

Data collection

Agilent SuperNova Dual
diffractometer with an Atlas
detector
Absorption correction: multi-scan
(*CrysAlis PRO*; Agilent, 2011)
 $T_{\min} = 0.772$, $T_{\max} = 1.000$

7531 measured reflections
4249 independent reflections
4049 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.014$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.081$
 $S = 1.04$
4249 reflections
243 parameters
2 restraints

H atoms treated by a mixture of
independent and constrained
refinement
 $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 _n ···S2	0.88 (1)	2.51 (1)	3.3667 (10)	164 (2)
N2—H2 _n ···S1	0.88 (1)	2.52 (1)	3.3765 (10)	167 (2)

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997), *DIAMOND* (Brandenburg, 2006) and *QMoI* (Gans & Shalloway, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

PS thanks the Development and Promotion of Science and Technology Talents Project (DPST), Thailand, for support to enable study at the University of Malaya. We also thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research scheme (UM.C/HIR/MOHE/SC/12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5228).

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supporting information

Acta Cryst. (2012). E68, o1774 [doi:10.1107/S160053681202140X]

O-Propyl N-phenylthiocarbamate

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S1. Comment

The title thiocarbamate, (I), was investigated as a continuation of systematic evaluation of the structural features of this class of compound (Ho *et al.*, 2005; Kuan *et al.*, 2007). In (I), Fig. 1, two independent molecules comprise the asymmetric unit, and these have very similar molecular conformations as seen in the overlay diagram, Fig. 2. The difference arises in the pseudo mirror relationship in the terminal ethyl group as seen in the C1—C2—C3—O1 and C11—C12—C13—O2 torsion angles of $-66.95(13)$ and $55.92(13)^\circ$, respectively. A further twist is evident in the molecule as seen in the value of the C4—N1—C5—C6 torsion angle of $-146.20(12)^\circ$; the equivalent torsion angle for the second independent molecule [C14—N2—C15—C16] is $-144.15(12)^\circ$. The geometric parameters match literature precedents (Ho *et al.*, 2005; Kuan *et al.*, 2007)

The independent molecules are linked into a dimeric aggregate by N—H \cdots S hydrogen bonds and an eight-membered thioamide $\{\cdots\text{H—N—C=S}\}_2$ synthon, Table 1, as found in most thiocarbamate structures (Kuan *et al.*, 2007). Molecules assemble into a three-dimensional architecture with no specific interactions between them.

S2. Experimental

Phenyl isothiocyanate (2 ml) was added drop-wise to a stirred solution of NaOH (1 mol equiv.) in *n*-propanol (20 ml) and stirred for 3 h. Excess HCl (5M) was then added and the solution was stirred for a further 1 h. The product was then extracted with CHCl₃ and left for evaporation at room temperature, yielding colourless crystals after 2 weeks. IR (KBr, cm⁻¹): $\nu(\text{N—H})$ 3211 (br); $\nu(\text{C—N})$ 1410 (s); $\nu(\text{C=S})$ 1221 (s); $\nu(\text{C—O})$ 1060 (s). ¹H NMR (CDCl₃, p.p.m.): δ 1.00 (t, J = 7.44 Hz, 3H, CH₃), 1.80 (sextet, J = 7.06 Hz, 2H, CH₂), 4.54 (br, 2H, CH₂O), 7.16 – 7.35 (br, m, 5H aryl-H), 8.85 (br, 1H NH). *M.pt.*: 311–312 K.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 0.99 Å, $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$] and were included in the refinement in the riding model approximation. The amino-H atoms were refined with the distance restraint N—H = 0.88±0.01 Å.

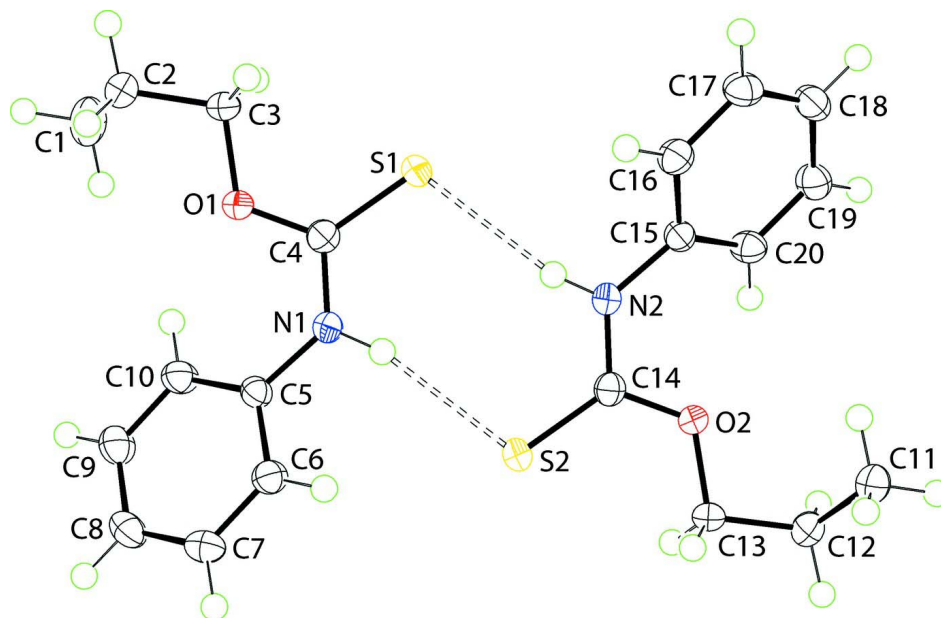


Figure 1

The molecular structures of the two independent molecules comprising (I) showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level. The dashed lines represent N—H hydrogen bonds.

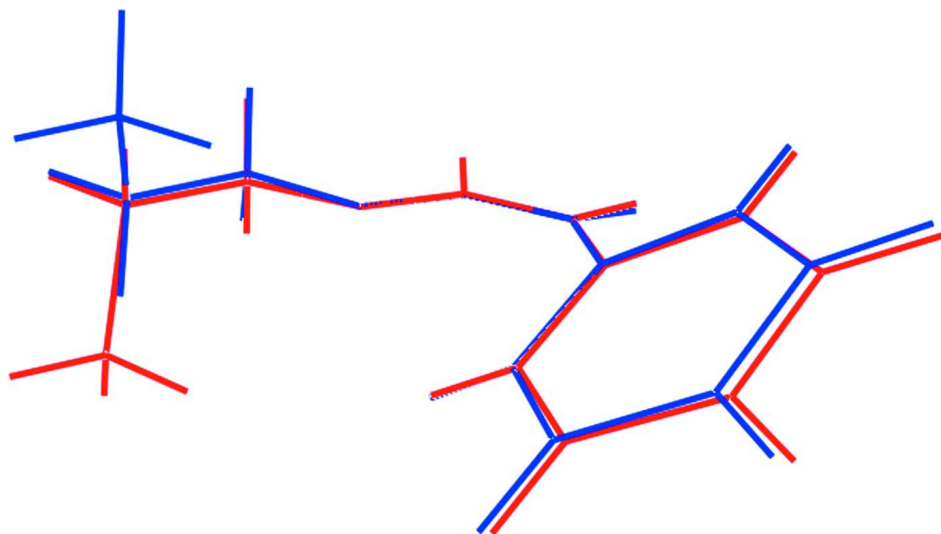


Figure 2

Overlay diagram of the two independent molecules comprising the asymmetric unit of (I). The first independent molecule (with the S1 atom) is shown in red and the second (S2) in blue. The S, O and N atoms in each molecule have been overlapped.

O-Propyl N-phenylthiocarbamate

Crystal data

$C_{10}H_{13}NOS$

$M_r = 195.27$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.9230(4)\ \text{\AA}$

$b = 9.8752(4)\ \text{\AA}$

$c = 12.9613 (5) \text{ \AA}$
 $\alpha = 98.037 (3)^\circ$
 $\beta = 105.866 (4)^\circ$
 $\gamma = 104.533 (4)^\circ$
 $V = 1036.46 (7) \text{ \AA}^3$
 $Z = 4$
 $F(000) = 416$
 $D_x = 1.251 \text{ Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$
 Cell parameters from 5287 reflections
 $\theta = 4.7\text{--}76.4^\circ$
 $\mu = 2.45 \text{ mm}^{-1}$
 $T = 100 \text{ K}$
 Prism, colourless
 $0.35 \times 0.30 \times 0.25 \text{ mm}$

Data collection

Agilent SuperNova Dual
 diffractometer with an Atlas detector
 Radiation source: SuperNova (Cu) X-ray
 Source
 Mirror monochromator
 Detector resolution: $10.4041 \text{ pixels mm}^{-1}$
 ω scan
 Absorption correction: multi-scan
 (*CrysAlis PRO*; Agilent, 2011)

$T_{\min} = 0.772, T_{\max} = 1.000$
 7531 measured reflections
 4249 independent reflections
 4049 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.014$
 $\theta_{\max} = 76.6^\circ, \theta_{\min} = 4.8^\circ$
 $h = -7 \rightarrow 11$
 $k = -11 \rightarrow 12$
 $l = -15 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.081$
 $S = 1.04$
 4249 reflections
 243 parameters
 2 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.325P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.22 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.26 \text{ e \AA}^{-3}$

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.71820 (3)	0.96137 (3)	0.53434 (2)	0.01838 (9)
S2	0.28880 (3)	0.57145 (3)	0.43767 (2)	0.01822 (9)
O1	0.69183 (10)	1.01848 (8)	0.33618 (6)	0.01621 (17)
O2	0.32823 (10)	0.50276 (9)	0.63279 (7)	0.01760 (18)
N1	0.50067 (12)	0.82607 (11)	0.33959 (8)	0.0170 (2)
N2	0.51265 (12)	0.70040 (10)	0.63170 (8)	0.0163 (2)
C1	0.92887 (18)	1.12337 (16)	0.22198 (11)	0.0293 (3)
H1A	0.9495	1.1744	0.1652	0.044*

H1B	0.8424	1.0319	0.1872	0.044*
H1C	1.0292	1.1051	0.2626	0.044*
C2	0.87524 (15)	1.21464 (13)	0.30110 (10)	0.0208 (2)
H2A	0.9631	1.3068	0.3359	0.025*
H2B	0.7769	1.2364	0.2590	0.025*
C3	0.83708 (14)	1.14212 (12)	0.38999 (10)	0.0178 (2)
H3A	0.9302	1.1107	0.4283	0.021*
H3B	0.8161	1.2092	0.4447	0.021*
C4	0.63469 (13)	0.93553 (12)	0.39794 (9)	0.0152 (2)
C5	0.41567 (14)	0.78782 (12)	0.22442 (9)	0.0152 (2)
C6	0.24671 (14)	0.72731 (12)	0.19297 (10)	0.0176 (2)
H6	0.1942	0.7184	0.2474	0.021*
C7	0.15509 (14)	0.68008 (13)	0.08232 (10)	0.0199 (2)
H7	0.0400	0.6378	0.0612	0.024*
C8	0.23078 (15)	0.69437 (13)	0.00225 (10)	0.0203 (2)
H8	0.1678	0.6631	-0.0735	0.024*
C9	0.39904 (15)	0.75463 (14)	0.03377 (10)	0.0219 (2)
H9	0.4511	0.7642	-0.0209	0.026*
C10	0.49257 (14)	0.80118 (13)	0.14456 (10)	0.0197 (2)
H10	0.6079	0.8417	0.1655	0.024*
C11	0.15346 (15)	0.40071 (14)	0.77344 (10)	0.0239 (3)
H11A	0.1401	0.3434	0.8281	0.036*
H11B	0.0630	0.4418	0.7546	0.036*
H11C	0.2573	0.4782	0.8040	0.036*
C12	0.15342 (15)	0.30544 (13)	0.67048 (10)	0.0197 (2)
H12A	0.2421	0.2610	0.6908	0.024*
H12B	0.0484	0.2272	0.6404	0.024*
C13	0.17672 (14)	0.38556 (12)	0.58226 (9)	0.0184 (2)
H13A	0.1841	0.3213	0.5192	0.022*
H13B	0.0838	0.4233	0.5555	0.022*
C14	0.38000 (14)	0.59088 (12)	0.57262 (9)	0.0152 (2)
C15	0.60105 (13)	0.72986 (12)	0.74636 (9)	0.0151 (2)
C16	0.66568 (14)	0.87358 (12)	0.80113 (10)	0.0183 (2)
H16	0.6453	0.9459	0.7630	0.022*
C17	0.76006 (15)	0.91136 (13)	0.91153 (10)	0.0203 (2)
H17	0.8049	1.0096	0.9487	0.024*
C18	0.78895 (14)	0.80571 (13)	0.96760 (10)	0.0204 (2)
H18	0.8531	0.8313	1.0432	0.025*
C19	0.72344 (14)	0.66214 (13)	0.91244 (10)	0.0201 (2)
H19	0.7424	0.5898	0.9509	0.024*
C20	0.63053 (14)	0.62339 (12)	0.80164 (10)	0.0180 (2)
H20	0.5877	0.5253	0.7641	0.022*
H1n	0.452 (2)	0.7739 (17)	0.3777 (13)	0.033 (4)*
H2n	0.5510 (19)	0.7633 (15)	0.5966 (12)	0.029 (4)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01728 (14)	0.02170 (15)	0.01217 (14)	0.00052 (11)	0.00352 (11)	0.00349 (11)
S2	0.01900 (15)	0.02037 (15)	0.01232 (14)	0.00178 (11)	0.00402 (11)	0.00404 (11)
O1	0.0153 (4)	0.0165 (4)	0.0133 (4)	0.0003 (3)	0.0035 (3)	0.0025 (3)
O2	0.0161 (4)	0.0186 (4)	0.0134 (4)	-0.0014 (3)	0.0034 (3)	0.0037 (3)
N1	0.0150 (4)	0.0206 (5)	0.0132 (5)	0.0010 (4)	0.0050 (4)	0.0042 (4)
N2	0.0173 (5)	0.0166 (5)	0.0138 (5)	0.0023 (4)	0.0046 (4)	0.0051 (4)
C1	0.0328 (7)	0.0362 (7)	0.0263 (7)	0.0113 (6)	0.0175 (6)	0.0128 (6)
C2	0.0217 (6)	0.0192 (5)	0.0188 (6)	0.0016 (4)	0.0056 (5)	0.0065 (5)
C3	0.0173 (5)	0.0159 (5)	0.0151 (5)	-0.0012 (4)	0.0037 (4)	0.0012 (4)
C4	0.0134 (5)	0.0178 (5)	0.0157 (5)	0.0056 (4)	0.0060 (4)	0.0034 (4)
C5	0.0167 (5)	0.0143 (5)	0.0133 (5)	0.0044 (4)	0.0037 (4)	0.0023 (4)
C6	0.0165 (5)	0.0176 (5)	0.0178 (6)	0.0040 (4)	0.0056 (4)	0.0032 (4)
C7	0.0152 (5)	0.0198 (6)	0.0206 (6)	0.0041 (4)	0.0019 (4)	0.0019 (4)
C8	0.0237 (6)	0.0195 (5)	0.0143 (5)	0.0072 (5)	0.0015 (4)	0.0010 (4)
C9	0.0242 (6)	0.0256 (6)	0.0158 (6)	0.0067 (5)	0.0082 (5)	0.0026 (5)
C10	0.0161 (5)	0.0236 (6)	0.0168 (6)	0.0028 (4)	0.0055 (4)	0.0015 (4)
C11	0.0232 (6)	0.0278 (6)	0.0193 (6)	0.0025 (5)	0.0103 (5)	0.0042 (5)
C12	0.0211 (6)	0.0178 (5)	0.0186 (6)	0.0021 (4)	0.0068 (5)	0.0051 (4)
C13	0.0169 (5)	0.0177 (5)	0.0146 (5)	-0.0017 (4)	0.0028 (4)	0.0017 (4)
C14	0.0155 (5)	0.0164 (5)	0.0154 (5)	0.0059 (4)	0.0068 (4)	0.0037 (4)
C15	0.0128 (5)	0.0183 (5)	0.0138 (5)	0.0039 (4)	0.0046 (4)	0.0032 (4)
C16	0.0195 (5)	0.0163 (5)	0.0194 (6)	0.0054 (4)	0.0061 (5)	0.0046 (4)
C17	0.0219 (6)	0.0162 (5)	0.0197 (6)	0.0040 (4)	0.0054 (5)	-0.0003 (4)
C18	0.0193 (6)	0.0243 (6)	0.0152 (5)	0.0057 (5)	0.0035 (4)	0.0024 (5)
C19	0.0201 (5)	0.0207 (6)	0.0188 (6)	0.0071 (4)	0.0036 (5)	0.0063 (5)
C20	0.0179 (5)	0.0152 (5)	0.0188 (6)	0.0046 (4)	0.0037 (4)	0.0025 (4)

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

S1—C4	1.6745 (12)	C7—H7	0.9500
S2—C14	1.6758 (12)	C8—C9	1.3869 (17)
O1—C4	1.3298 (14)	C8—H8	0.9500
O1—C3	1.4596 (13)	C9—C10	1.3920 (16)
O2—C14	1.3280 (14)	C9—H9	0.9500
O2—C13	1.4543 (13)	C10—H10	0.9500
N1—C4	1.3412 (15)	C11—C12	1.5213 (17)
N1—C5	1.4233 (14)	C11—H11A	0.9800
N1—H1n	0.881 (9)	C11—H11B	0.9800
N2—C14	1.3370 (15)	C11—H11C	0.9800
N2—C15	1.4277 (15)	C12—C13	1.5090 (16)
N2—H2n	0.876 (9)	C12—H12A	0.9900
C1—C2	1.5230 (18)	C12—H12B	0.9900
C1—H1A	0.9800	C13—H13A	0.9900
C1—H1B	0.9800	C13—H13B	0.9900
C1—H1C	0.9800	C15—C20	1.3908 (16)

C2—C3	1.5096 (16)	C15—C16	1.3909 (16)
C2—H2A	0.9900	C16—C17	1.3893 (17)
C2—H2B	0.9900	C16—H16	0.9500
C3—H3A	0.9900	C17—C18	1.3884 (17)
C3—H3B	0.9900	C17—H17	0.9500
C5—C10	1.3931 (16)	C18—C19	1.3910 (17)
C5—C6	1.3928 (16)	C18—H18	0.9500
C6—C7	1.3868 (16)	C19—C20	1.3901 (16)
C6—H6	0.9500	C19—H19	0.9500
C7—C8	1.3891 (18)	C20—H20	0.9500
C4—O1—C3	118.40 (9)	C10—C9—H9	119.6
C14—O2—C13	119.24 (9)	C9—C10—C5	119.44 (11)
C4—N1—C5	129.52 (10)	C9—C10—H10	120.3
C4—N1—H1n	116.3 (11)	C5—C10—H10	120.3
C5—N1—H1n	113.9 (12)	C12—C11—H11A	109.5
C14—N2—C15	128.33 (10)	C12—C11—H11B	109.5
C14—N2—H2n	116.9 (11)	H11A—C11—H11B	109.5
C15—N2—H2n	114.8 (11)	C12—C11—H11C	109.5
C2—C1—H1A	109.5	H11A—C11—H11C	109.5
C2—C1—H1B	109.5	H11B—C11—H11C	109.5
H1A—C1—H1B	109.5	C13—C12—C11	113.18 (10)
C2—C1—H1C	109.5	C13—C12—H12A	108.9
H1A—C1—H1C	109.5	C11—C12—H12A	108.9
H1B—C1—H1C	109.5	C13—C12—H12B	108.9
C3—C2—C1	112.87 (11)	C11—C12—H12B	108.9
C3—C2—H2A	109.0	H12A—C12—H12B	107.8
C1—C2—H2A	109.0	O2—C13—C12	106.33 (9)
C3—C2—H2B	109.0	O2—C13—H13A	110.5
C1—C2—H2B	109.0	C12—C13—H13A	110.5
H2A—C2—H2B	107.8	O2—C13—H13B	110.5
O1—C3—C2	107.03 (9)	C12—C13—H13B	110.5
O1—C3—H3A	110.3	H13A—C13—H13B	108.7
C2—C3—H3A	110.3	O2—C14—N2	112.77 (10)
O1—C3—H3B	110.3	O2—C14—S2	124.50 (9)
C2—C3—H3B	110.3	N2—C14—S2	122.71 (9)
H3A—C3—H3B	108.6	C20—C15—C16	120.28 (11)
O1—C4—N1	112.98 (10)	C20—C15—N2	123.06 (10)
O1—C4—S1	124.75 (8)	C16—C15—N2	116.58 (10)
N1—C4—S1	122.27 (9)	C17—C16—C15	120.03 (11)
C10—C5—C6	119.92 (11)	C17—C16—H16	120.0
C10—C5—N1	123.81 (10)	C15—C16—H16	120.0
C6—C5—N1	116.20 (10)	C16—C17—C18	120.08 (11)
C7—C6—C5	120.09 (11)	C16—C17—H17	120.0
C7—C6—H6	120.0	C18—C17—H17	120.0
C5—C6—H6	120.0	C17—C18—C19	119.60 (11)
C6—C7—C8	120.30 (11)	C17—C18—H18	120.2
C6—C7—H7	119.9	C19—C18—H18	120.2

C8—C7—H7	119.9	C20—C19—C18	120.74 (11)
C9—C8—C7	119.50 (11)	C20—C19—H19	119.6
C9—C8—H8	120.2	C18—C19—H19	119.6
C7—C8—H8	120.2	C19—C20—C15	119.27 (11)
C8—C9—C10	120.75 (11)	C19—C20—H20	120.4
C8—C9—H9	119.6	C15—C20—H20	120.4
C4—O1—C3—C2	179.25 (10)	C14—O2—C13—C12	179.29 (10)
C1—C2—C3—O1	-66.95 (13)	C11—C12—C13—O2	55.92 (13)
C3—O1—C4—N1	179.65 (9)	C13—O2—C14—N2	174.58 (9)
C3—O1—C4—S1	-0.49 (14)	C13—O2—C14—S2	-4.13 (15)
C5—N1—C4—O1	0.59 (17)	C15—N2—C14—O2	0.88 (17)
C5—N1—C4—S1	-179.27 (9)	C15—N2—C14—S2	179.63 (9)
C4—N1—C5—C10	37.09 (18)	C14—N2—C15—C20	39.15 (18)
C4—N1—C5—C6	-146.20 (12)	C14—N2—C15—C16	-144.15 (12)
C10—C5—C6—C7	0.15 (17)	C20—C15—C16—C17	-0.04 (17)
N1—C5—C6—C7	-176.70 (10)	N2—C15—C16—C17	-176.84 (10)
C5—C6—C7—C8	-0.78 (18)	C15—C16—C17—C18	-0.51 (18)
C6—C7—C8—C9	0.79 (18)	C16—C17—C18—C19	0.26 (18)
C7—C8—C9—C10	-0.17 (19)	C17—C18—C19—C20	0.53 (18)
C8—C9—C10—C5	-0.46 (19)	C18—C19—C20—C15	-1.07 (18)
C6—C5—C10—C9	0.47 (18)	C16—C15—C20—C19	0.82 (17)
N1—C5—C10—C9	177.06 (11)	N2—C15—C20—C19	177.41 (10)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1 <i>n</i> ...S2	0.88 (1)	2.51 (1)	3.3667 (10)	164 (2)
N2—H2 <i>n</i> ...S1	0.88 (1)	2.52 (1)	3.3765 (10)	167 (2)