



Crystal structure of 4-methyl-*N*-{(*E*)-methyl[(3*aR*,8*aS*)-2-oxo-3,3*a*,8,8*a*-tetrahydro-2*H*-indeno[1,2-*d*][1,3]oxazol-3-yl]- λ^4 -sulfanylidene}benzenesulfonamide

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The formulation that the title compound, C₁₈H₁₈N₂O₄S₂, adopts is a zwitterionic core with the charge separated to the sulfilimine S and N atoms and is supported by the two different S–N bond distances about the sulfinimine N atom [1.594 (2) and 1.631 (2) Å, respectively] that are typical for such bonds. The notably unusual bond is S–N(oxazolidinone) [1.692 (2) Å] that is longer than a typical S–N bond [1.603 (18) Å, *Mogul* analysis; Macrae *et al.* (2008). *J. Appl. Cryst.* **41**, 466–470]. The bond-angle sum about sulfilimine sulfur (308.35°) reflects the trigonal–pyramidal geometry of this atom. Two of the angles are less than 100°. Despite the pyramidalization of this sulfur, there are no significant intermolecular interactions, beyond usual van der Waals contacts, in the crystal packing.

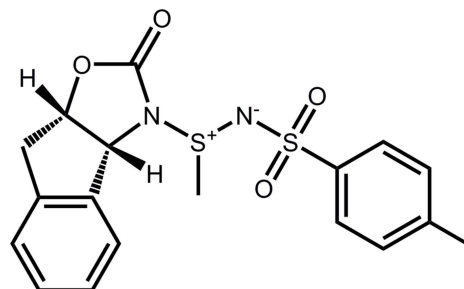
Keywords: oxazolidinone; vinyl sulfonamide; crystal structure.

CCDC reference: 1444186

1. Related literature

Oxazolidinone sulfilimines are synthesized as precursors of vinyl sulfilimines which are used in the γ -lactamization reaction to generate chiral pyrrolidinones with medicinal chemistry interest. For the synthesis, see: Celentano & Colonna (1998); Silveira & Marino (2013). For sulfonyl oxazolidinone structures, see: Barbey *et al.* (2012); Berredjem *et al.* (2010); Bonnaud *et al.* (1987); Dewynter *et al.* (1997). For related vinyl sulfonamide chemistry, see: Silveira *et al.* (2013). For related

oxazolidinone sulfinime structures, see: Silveira *et al.* (2012, 2014). For the Hooft parameter, see: Hooft *et al.* (2008).



2. Experimental

2.1. Crystal data

C ₁₈ H ₁₈ N ₂ O ₄ S ₂	$V = 1700.30 (5) \text{ \AA}^3$
$M_r = 390.46$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Cu $K\alpha$ radiation
$a = 6.8841 (1) \text{ \AA}$	$\mu = 3.09 \text{ mm}^{-1}$
$b = 12.2326 (2) \text{ \AA}$	$T = 100 \text{ K}$
$c = 20.1911 (4) \text{ \AA}$	$0.42 \times 0.40 \times 0.34 \text{ mm}$

2.2. Data collection

Bruker SMART APEX CCD diffractometer	11963 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)	3004 independent reflections
$T_{\min} = 0.701$, $T_{\max} = 0.929$	2984 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.032$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$	$\Delta\rho_{\min} = -0.36 \text{ e \AA}^{-3}$
$wR(F^2) = 0.070$	Absolute structure: Flack x
$S = 1.11$	determined using 1183 quotients
3004 reflections	$[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons
237 parameters	<i>et al.</i> , 2013)
H-atom parameters constrained	Absolute structure parameter:
$\Delta\rho_{\max} = 0.29 \text{ e \AA}^{-3}$	0.052 (4)

Table 1
Selected geometric parameters (Å, °).

S1–N2	1.594 (2)	S2–O3	1.451 (2)
S1–N1	1.692 (2)	S2–N2	1.631 (2)
S1–C11	1.782 (3)	S2–C12	1.768 (2)
S2–O4	1.4430 (19)		
N2–S1–N1	110.58 (11)	O3–S2–N2	112.27 (11)
N2–S1–C11	99.43 (12)	O4–S2–C12	107.93 (11)
N1–S1–C11	98.34 (11)	O3–S2–C12	108.03 (12)
O4–S2–O3	117.24 (12)	N2–S2–C12	103.67 (12)
O4–S2–N2	106.79 (12)		

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2* and *SAINT* (Bruker, 2007); data reduction: *SAINT* and *XPREF* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *XCIF* (Sheldrick, 2008) and *pubCIF* (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: NK2234).

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supporting information

Acta Cryst. (2015). E71, o1097–o1098 [https://doi.org/10.1107/S2056989015024779]

Crystal structure of 4-methyl-*N*-{(*E*)-methyl[(3*aR*,8*aS*)-2-oxo-3,3*a*,8,8*a*-tetrahydro-2*H*-indeno[1,2-*d*][1,3]oxazol-3-yl]- λ^4 -sulfanylidene}benzenesulfonamide

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S1. Commentary

Oxazolidinone sulfilimines are synthesized as precursors of vinyl sulfilimines which are used in the γ -lactamization reaction (Silveira & Marino, 2013) to generate chiral pyrrolidinones with medicinal chemistry interest. This compound represents one of only five other oxazolidinone compounds that incorporate an N—S—N backbone (Barbey *et al.*, 2012; Berredjem *et al.*, 2010; Bonnaud *et al.*, 1987; Dewynter *et al.*, 1997). It is the only reported structure that does not have a sulfonyl bridging the oxazolidinone ring to the second nitrogen atom. Related sulfur-containing oxazolidinones have been reported previously by us (Silveira *et al.*, 2012; 2014). We have also reported a related sulfur-containing indole as a precursor of physostigmine alkaloid. (Silveira *et al.*, 2013).

S2. Synthesis and crystallization

Following literature preparative methods (Celentano *et al.*, 1998; Silveira & Marino, 2013): chloramine-T (951 mg, 4.18 mmol) and hexadecyltributylphosphonium bromide (100 mg, 0.20 mmol) were added to a solution of oxazolidinone sulfide (840 mg, 3.80 mmol) in toluene (25 mL) at 295 K. After overnight stirring, ethyl acetate (25 mL) was added and the mixture washed (2 x 30 mL water; 1 x 30 mL brine), dried over anhydrous sodium sulfate, filtered, and the mixture of solvents rota-evaporated at reduced pressure. To the resulting dry, crude product, silica gel (6 g) and methylene chloride (5 mL) were added and this slurry was rota-evaporated to yield the crude product on silica. This mixture was separated and purified through flash chromatography with elution (70% ethyl acetate / 30% hexanes). After slow evaporation of the ethyl acetate / hexanes elutant, the more polar sulfilimine was obtained as white crystals (688 mg). Two sulfilimine diastereoisomers were obtained in a ratio of 2.5:1 (total of 65% yield).

S3. Refinement details

The structure was modeled routinely with all non-hydrogen atoms included with an anisotropic model. Hydrogen atoms were included in calculated positions riding on the atom to which they are bonded (C—H = 0.99 Å for methyl, 0.95 Å for methyne and aromatic. $U_{\text{iso}}(\text{H})$ was set = $1.5U_{\text{eq}}(\text{C})$ for methyl and $1.2U_{\text{eq}}(\text{C})$ for all others.

The absolute configuration from synthesis was confirmed by comparison of intensities of Friedel pairs of reflections yielding a Flack x parameter = 0.052 (4) (Parsons *et al.*, 2013) and a Hooft γ parameter = 0.050 (6) (Hooft *et al.*, 2008).

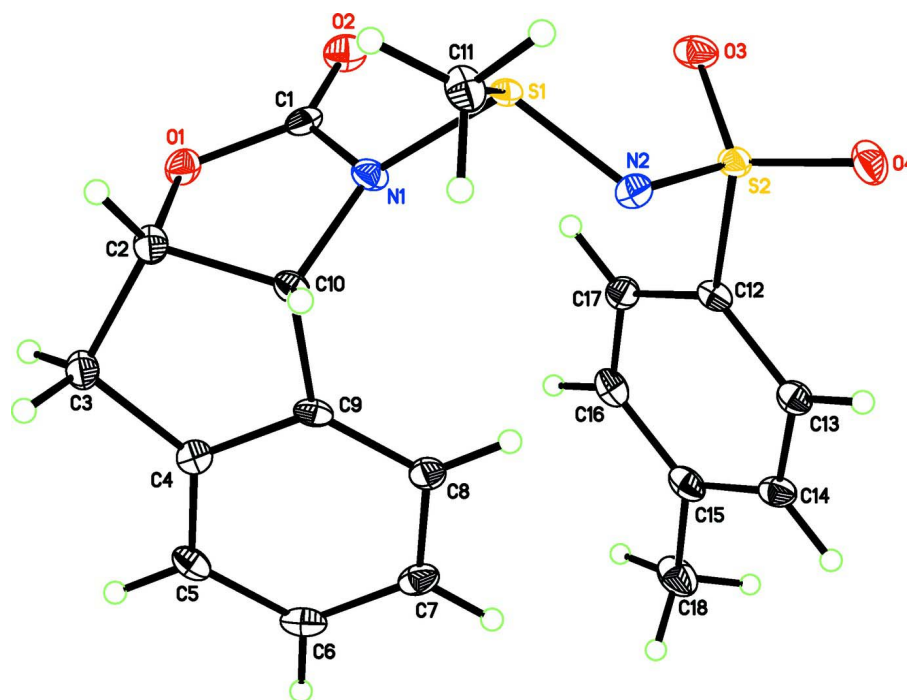


Figure 1

Labeling diagram of the title compound. Atomic displacement ellipsoids depicted at the 50% probability level. Hydrogen atoms depicted as spheres of an arbitrary radius.

4-Methyl-N-((E)-methyl[(3aR,8aS)-2-oxo-3,3a,8,8a-tetrahydro-2H-indeno[1,2-d][1,3]oxazol-3-yl)]-λ⁴-sulfanylidene)benzenesulfonamide

Crystal data

C₁₈H₁₈N₂O₄S₂

M_r = 390.46

Orthorhombic, *P*2₁2₁2₁

a = 6.8841 (1) Å

b = 12.2326 (2) Å

c = 20.1911 (4) Å

V = 1700.30 (5) Å³

Z = 4

F(000) = 816

D_x = 1.525 Mg m⁻³

Cu *K*α radiation, λ = 1.54178 Å

Cell parameters from 9988 reflections

θ = 4.2–69.2°

μ = 3.09 mm⁻¹

T = 100 K

Parallelepiped, clear colorless

0.42 × 0.40 × 0.34 mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube,
Siemens KFFCU2K-90

Graphite monochromator

Detector resolution: 8.33 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Krause *et al.*, 2015)

*T*_{min} = 0.701, *T*_{max} = 0.929

11963 measured reflections

3004 independent reflections

2984 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.032

θ_{max} = 69.5°, θ_{min} = 4.2°

h = -8→8

k = -14→14

l = -24→22

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.028$ $wR(F^2) = 0.070$ $S = 1.11$

3004 reflections

237 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.5066P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.36 \text{ e } \text{\AA}^{-3}$ Absolute structure: Flack x determined using
1183 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons *et al.*, 2013)

Absolute structure parameter: 0.052 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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	0.45871 (9)	0.55630 (5)	0.77781 (3)	0.00978 (15)
S2	0.67201 (9)	0.69687 (5)	0.85264 (3)	0.01185 (16)
O1	0.3825 (3)	0.25928 (14)	0.82183 (9)	0.0148 (4)
O2	0.6694 (3)	0.34297 (15)	0.80444 (9)	0.0176 (4)
O3	0.8276 (3)	0.63677 (15)	0.82056 (9)	0.0175 (4)
O4	0.6751 (3)	0.81443 (15)	0.84687 (9)	0.0185 (4)
N1	0.3831 (3)	0.44084 (18)	0.81606 (11)	0.0127 (5)
N2	0.4579 (3)	0.65675 (17)	0.82812 (11)	0.0132 (5)
C1	0.4975 (4)	0.3476 (2)	0.81239 (12)	0.0129 (5)
C2	0.1767 (4)	0.2920 (2)	0.82310 (13)	0.0136 (5)
H2	0.1106	0.2809	0.7795	0.016*
C3	0.0725 (4)	0.2347 (2)	0.87983 (13)	0.0148 (6)
H3A	-0.0688	0.2299	0.8713	0.018*
H3B	0.1246	0.1601	0.8867	0.018*
C4	0.1142 (4)	0.3068 (2)	0.93859 (13)	0.0124 (5)
C5	0.0916 (4)	0.2842 (2)	1.00541 (13)	0.0140 (6)
H5	0.0423	0.2157	1.0198	0.017*
C6	0.1431 (4)	0.3648 (2)	1.05088 (13)	0.0161 (6)
H6	0.1258	0.3512	1.0968	0.019*
C7	0.2188 (4)	0.4644 (2)	1.03076 (14)	0.0157 (6)
H7	0.2569	0.5170	1.0628	0.019*
C8	0.2393 (4)	0.4875 (2)	0.96324 (14)	0.0141 (5)
H8	0.2899	0.5558	0.9488	0.017*
C9	0.1843 (4)	0.4088 (2)	0.91814 (13)	0.0117 (5)
C10	0.1900 (4)	0.41298 (19)	0.84277 (13)	0.0116 (5)
H10	0.0833	0.4584	0.8234	0.014*
C11	0.2421 (4)	0.5860 (2)	0.73290 (13)	0.0149 (6)

H11A	0.1358	0.5997	0.7641	0.022*
H11B	0.2089	0.5237	0.7046	0.022*
H11C	0.2627	0.6510	0.7054	0.022*
C12	0.6749 (4)	0.6636 (2)	0.93784 (12)	0.0112 (5)
C13	0.6177 (4)	0.7407 (2)	0.98430 (13)	0.0136 (5)
H13	0.5750	0.8110	0.9706	0.016*
C14	0.6237 (4)	0.7138 (2)	1.05134 (13)	0.0153 (6)
H14	0.5858	0.7664	1.0834	0.018*
C15	0.6846 (4)	0.6107 (2)	1.07178 (13)	0.0157 (5)
C16	0.7366 (4)	0.5341 (2)	1.02403 (14)	0.0152 (6)
H16	0.7745	0.4628	1.0376	0.018*
C17	0.7344 (4)	0.5596 (2)	0.95710 (14)	0.0147 (5)
H17	0.7727	0.5071	0.9250	0.018*
C18	0.6940 (5)	0.5854 (2)	1.14496 (14)	0.0231 (6)
H18A	0.7504	0.5126	1.1514	0.035*
H18B	0.5628	0.5871	1.1637	0.035*
H18C	0.7752	0.6400	1.1672	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0116 (3)	0.0111 (3)	0.0066 (3)	-0.0007 (2)	0.0007 (2)	0.0007 (2)
S2	0.0124 (3)	0.0139 (3)	0.0093 (3)	-0.0022 (2)	0.0002 (2)	-0.0003 (2)
O1	0.0189 (10)	0.0105 (8)	0.0151 (9)	0.0019 (7)	0.0014 (7)	-0.0003 (7)
O2	0.0161 (9)	0.0186 (9)	0.0179 (9)	0.0046 (8)	0.0011 (8)	0.0004 (8)
O3	0.0116 (9)	0.0269 (10)	0.0140 (9)	-0.0032 (8)	0.0015 (8)	-0.0017 (8)
O4	0.0251 (10)	0.0161 (9)	0.0143 (9)	-0.0067 (8)	-0.0028 (8)	0.0036 (7)
N1	0.0141 (11)	0.0108 (10)	0.0133 (10)	0.0016 (9)	0.0039 (9)	0.0032 (9)
N2	0.0135 (11)	0.0141 (10)	0.0118 (10)	0.0004 (9)	0.0001 (9)	-0.0013 (9)
C1	0.0170 (14)	0.0137 (12)	0.0080 (12)	0.0023 (10)	0.0010 (10)	-0.0015 (10)
C2	0.0157 (13)	0.0129 (12)	0.0121 (12)	-0.0016 (11)	-0.0025 (11)	0.0014 (10)
C3	0.0173 (14)	0.0137 (12)	0.0134 (13)	-0.0036 (10)	-0.0014 (11)	0.0008 (11)
C4	0.0116 (11)	0.0133 (12)	0.0121 (12)	0.0020 (10)	-0.0014 (10)	0.0006 (11)
C5	0.0109 (12)	0.0164 (13)	0.0149 (13)	0.0002 (10)	0.0010 (10)	0.0059 (10)
C6	0.0122 (13)	0.0256 (14)	0.0106 (12)	0.0041 (11)	0.0015 (10)	0.0017 (11)
C7	0.0107 (13)	0.0218 (13)	0.0145 (13)	0.0024 (10)	-0.0001 (10)	-0.0054 (11)
C8	0.0114 (12)	0.0135 (12)	0.0174 (13)	0.0023 (10)	0.0033 (10)	-0.0010 (11)
C9	0.0090 (11)	0.0148 (12)	0.0111 (12)	0.0030 (10)	0.0025 (11)	0.0023 (10)
C10	0.0112 (12)	0.0120 (12)	0.0117 (12)	0.0003 (9)	0.0010 (11)	0.0030 (9)
C11	0.0168 (13)	0.0158 (12)	0.0122 (13)	-0.0026 (10)	-0.0057 (10)	0.0050 (10)
C12	0.0087 (11)	0.0168 (12)	0.0080 (11)	-0.0023 (10)	-0.0023 (10)	0.0024 (9)
C13	0.0106 (12)	0.0158 (12)	0.0142 (13)	-0.0013 (10)	-0.0004 (10)	0.0011 (11)
C14	0.0116 (12)	0.0215 (13)	0.0127 (12)	-0.0028 (10)	0.0013 (10)	-0.0013 (10)
C15	0.0111 (12)	0.0223 (13)	0.0136 (13)	-0.0054 (11)	-0.0024 (11)	0.0031 (11)
C16	0.0107 (12)	0.0156 (12)	0.0192 (13)	-0.0008 (10)	-0.0024 (10)	0.0050 (11)
C17	0.0103 (12)	0.0158 (12)	0.0180 (13)	-0.0003 (10)	0.0015 (10)	-0.0028 (11)
C18	0.0263 (16)	0.0287 (15)	0.0144 (13)	-0.0091 (12)	-0.0016 (13)	0.0049 (11)

Geometric parameters (Å, °)

S1—N2	1.594 (2)	C7—C8	1.399 (4)
S1—N1	1.692 (2)	C7—H7	0.9500
S1—C11	1.782 (3)	C8—C9	1.378 (4)
S2—O4	1.4430 (19)	C8—H8	0.9500
S2—O3	1.451 (2)	C9—C10	1.523 (3)
S2—N2	1.631 (2)	C10—H10	1.0000
S2—C12	1.768 (2)	C11—H11A	0.9800
O1—C1	1.353 (3)	C11—H11B	0.9800
O1—C2	1.472 (3)	C11—H11C	0.9800
O2—C1	1.195 (3)	C12—C13	1.387 (4)
N1—C1	1.388 (3)	C12—C17	1.392 (4)
N1—C10	1.475 (3)	C13—C14	1.394 (4)
C2—C3	1.522 (4)	C13—H13	0.9500
C2—C10	1.535 (3)	C14—C15	1.391 (4)
C2—H2	1.0000	C14—H14	0.9500
C3—C4	1.506 (4)	C15—C16	1.392 (4)
C3—H3A	0.9900	C15—C18	1.511 (4)
C3—H3B	0.9900	C16—C17	1.387 (4)
C4—C5	1.386 (4)	C16—H16	0.9500
C4—C9	1.400 (4)	C17—H17	0.9500
C5—C6	1.393 (4)	C18—H18A	0.9800
C5—H5	0.9500	C18—H18B	0.9800
C6—C7	1.386 (4)	C18—H18C	0.9800
C6—H6	0.9500		
N2—S1—N1	110.58 (11)	C9—C8—H8	120.8
N2—S1—C11	99.43 (12)	C7—C8—H8	120.8
N1—S1—C11	98.34 (11)	C8—C9—C4	121.5 (2)
O4—S2—O3	117.24 (12)	C8—C9—C10	129.0 (2)
O4—S2—N2	106.79 (12)	C4—C9—C10	109.5 (2)
O3—S2—N2	112.27 (11)	N1—C10—C9	113.4 (2)
O4—S2—C12	107.93 (11)	N1—C10—C2	100.5 (2)
O3—S2—C12	108.03 (12)	C9—C10—C2	103.0 (2)
N2—S2—C12	103.67 (12)	N1—C10—H10	113.0
C1—O1—C2	110.39 (19)	C9—C10—H10	113.0
C1—N1—C10	110.0 (2)	C2—C10—H10	113.0
C1—N1—S1	119.14 (18)	S1—C11—H11A	109.5
C10—N1—S1	129.59 (17)	S1—C11—H11B	109.5
S1—N2—S2	114.97 (13)	H11A—C11—H11B	109.5
O2—C1—O1	124.1 (2)	S1—C11—H11C	109.5
O2—C1—N1	127.5 (2)	H11A—C11—H11C	109.5
O1—C1—N1	108.5 (2)	H11B—C11—H11C	109.5
O1—C2—C3	110.0 (2)	C13—C12—C17	121.0 (2)
O1—C2—C10	102.1 (2)	C13—C12—S2	119.9 (2)
C3—C2—C10	106.1 (2)	C17—C12—S2	119.0 (2)
O1—C2—H2	112.7	C12—C13—C14	119.2 (2)

C3—C2—H2	112.7	C12—C13—H13	120.4
C10—C2—H2	112.7	C14—C13—H13	120.4
C4—C3—C2	103.5 (2)	C15—C14—C13	120.7 (3)
C4—C3—H3A	111.1	C15—C14—H14	119.6
C2—C3—H3A	111.1	C13—C14—H14	119.6
C4—C3—H3B	111.1	C14—C15—C16	118.9 (2)
C2—C3—H3B	111.1	C14—C15—C18	119.3 (3)
H3A—C3—H3B	109.0	C16—C15—C18	121.9 (3)
C5—C4—C9	120.2 (2)	C17—C16—C15	121.3 (2)
C5—C4—C3	128.9 (2)	C17—C16—H16	119.3
C9—C4—C3	110.8 (2)	C15—C16—H16	119.3
C4—C5—C6	118.1 (2)	C16—C17—C12	118.8 (2)
C4—C5—H5	120.9	C16—C17—H17	120.6
C6—C5—H5	120.9	C12—C17—H17	120.6
C7—C6—C5	121.6 (2)	C15—C18—H18A	109.5
C7—C6—H6	119.2	C15—C18—H18B	109.5
C5—C6—H6	119.2	H18A—C18—H18B	109.5
C6—C7—C8	120.1 (3)	C15—C18—H18C	109.5
C6—C7—H7	120.0	H18A—C18—H18C	109.5
C8—C7—H7	120.0	H18B—C18—H18C	109.5
C9—C8—C7	118.3 (2)		
