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# 6-(Hex-5-enyloxy)naphthalene-2-carboxylic acid

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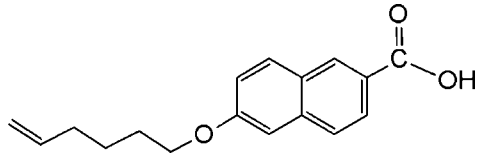
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.002 Å; disorder in main residue; $R$ factor = 0.045; $wR$ factor = 0.152; data-to-parameter ratio = 11.7.

The asymmetric unit of the title compound, $C_{17}H_{18}O_3$, comprises three independent molecules with similar geometries. In each molecule, the carbonyl group is twisted away from the napthalene ring system, making dihedral angles of 1.0 (2), 1.05 (19)° and 1.5 (2)°. The butene group in all three molecules are disordered over two sets of sites, with a refined occupancy ratio of 0.664 (6):0.336 (6). In the crystal, molecules are oriented with respect to their carbonyl groups, forming head-to-head dimers *via* O—H···O hydrogen bonds. Adjacent dimers are further interconnected by C—H···O hydrogen bonds into chains along the *a*-axis direction. The crystal structure is further stabilized by weak C—H···$\pi$ interactions.

## Related literature

For liquid crystal properties of carbonyl and naphthalene derivatives, see: Lee *et al.* (2001); Drzewinski (2013); Achalkumar *et al.* (2011). For naphthalene carboxylic acid derivatives, see: Rahman *et al.* (2013); Kozmik *et al.* (2005). For the synthesis of the title compound, see: Gopalakrishnan & Sadashiva (1998). For related structures, see: Fitzgerald & Gerkin (1993); Blackburn & Gerkin (1997); Lynch *et al.* (1998). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987).



## Experimental

### Crystal data

$C_{17}H_{18}O_3$
$M_r$ = 270.31
Triclinic, $P\overline{1}$
$a$ = 9.5018 (2) Å
$b$ = 14.8695 (2) Å
$c$ = 17.6757 (3) Å
$\alpha$ = 113.638 (1)°
$\beta$ = 102.188 (1)°
$\gamma$ = 93.127 (1)°
$V$ = 2209.06 (7) Å$^3$
$Z$ = 6
Cu $K\alpha$ radiation
$\mu$ = 0.67 mm$^{-1}$
$T$ = 298 K
0.53 × 0.21 × 0.18 mm

### Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.719, $T_{max}$ = 0.890
25536 measured reflections
6763 independent reflections
5768 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.152
$S$ = 1.06
6763 reflections
580 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2$A$—H1···O1$C^{i}$ | 0.97 | 1.65 | 2.6150 (16) | 174 |
| O2$B$—H2···O1$B^{ii}$ | 0.85 | 1.80 | 2.6342 (15) | 168 |
| O2$C$—H3···O1$A^{i}$ | 0.93 | 1.69 | 2.6133 (16) | 177 |
| C6$A$—H6$AA$···O1$A^{iii}$ | 0.93 | 2.50 | 3.3032 (19) | 144 |
| C6$B$—H6$BA$···O1$B^{iii}$ | 0.93 | 2.56 | 3.3666 (19) | 145 |
| C6$C$—H6$CA$···O1$C^{iii}$ | 0.93 | 2.56 | 3.3547 (18) | 144 |
| C5$A$—H5$AA$···O2$C^{iv}$ | 0.93 | 2.59 | 3.421 (2) | 149 |
| C5$B$—H5$BA$···O2$B^{v}$ | 0.93 | 2.65 | 3.520 (2) | 156 |
| C5$C$—H5$CA$···O2$A^{iv}$ | 0.93 | 2.61 | 3.472 (2) | 154 |
| C17$B$—H17$C$···$Cg1^{vi}$ | 0.93 | 2.93 | 3.736 (5) | 146 |

Symmetry codes: (i) $-x+2, -y+2, -z+1$; (ii) $-x+3, -y+2, -z$; (iii) $x-1, y, z$; (iv) $-x+1, -y+2, -z+1$; (v) $-x+2, -y+2, -z$; (vi) $-x+1, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: KP2470).

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# supporting information

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## 6-(Hex-5-enyloxy)naphthalene-2-carboxylic acid

**Md. Lutfor Rahman, H. T. Srinivasa, Mashitah Mohd. Yusoff, Huey Chong Kwong and Ching Kheng Quah**

### S1. Comment

The title compound is considered a potential candidate for material chemistry study comprising a polymerizable vinyl group at one end and a free carboxylic acid group at the other end of the molecule. In general, the free carboxylic acid group favours to form the hydrogen-bonded cyclic dimers in the liquid crystalline phases and most of the dimers exhibited enantiotropic liquid crystalline behavior (Lee *et al.* 2001). Considerable amount of work has been carried out in naphthalene derivatives to achieve application oriented SmC phase in low molar mass and polymeric liquid crystals with an azo/ester group (Drzewinski 2013; Achalkumar *et al.* 2011). These materials often studied in the view of their interesting optical properties, which enable applications such as optical switching, holography and optical storage devices (Rahman *et al.* 2013; Kozmik *et al.* 2005). This paper presents synthesis and crystal structure analysis of naphthalene based liquid crystalline precursor.

The asymmetry unit of the title compound (Fig. 1) comprises three crystallographically independent molecules (*A*, *B* and *C*) of similar geometries. The bonds lengths (Allen *et al.* 1987) and angles have normal values and comparable with the closely related structures (Fitzgerald & Gerkin 1993; Blackburn & Gerkin 1997; Lynch *et al.* 1998). In each molecule, the carbonyl group is almost coplanar with the attached naphthalene ring. The carbonyl group (O1—C1—O2) is slightly twisted away from the naphthalene ring system, with the dihedral angles of 1.00 (20)° in molecule *A*, 1.05 (19)° in molecule *B* and 1.50 (20)° in molecule *C*]. The butene groups which attached to atom C14 in each molecule (*A*, *B* and *C*) are disordered over two positions with a refined site-occupancy ratio of 0.695 (6): 0.305 (6).

In the crystal packing (Fig. 2), two adjacent molecules are linked into inversion dimers, forming $R^2_2(8)$ graph-set motifs (Bernstein *et al.* 1995) by a pair of intermolecular O2—H···O1 hydrogen bond (Table 1). These dimers are linked into chain along the *a* axis *via* intermolecular C5—H5···O2 and C6—H6···O1 hydrogen bonds. The crystal structure is further stabilized by a weak intermolecular C17B—H17C···*Cg*1 interaction (*Cg*1 is the centroid of the C4C—C9,*C* Table 1).

### S2. Experimental

The title compound is synthesized according to the literature (Gopalakrishnan & Sadashiva 1998). Pure and suitable single crystals were obtained on slow evaporation of ethyl alcohol at room temperature. The compound melts at 419 K to nematic phase, then it goes to isotropic state at 461 K. It returns to nematic phase at 486 K and then crystallizes at 410 K when it was cooled from isotropic state.

### S3. Refinement

The butene group and hydrogen atoms which are attached to atom C14 in each molecule (*A*, *B* and *C*) are disordered over two positions with a refined site-occupancy ratio of 0.695 (6): 0.305 (6). All C-bound H atoms were positioned geometrically [C—H = 0.95–0.97 Å] and refined using a riding model with $U_{iso}$(H) = 1.2 or 1.5 $U_{eq}$(C). All O-bound H

atoms were located from difference Fourier map and were fixed to their parent atoms with $U_{iso}$(H) = 1.5 $U_{eq}$(O). The restraints of same geometries were applied to all disordered components. Three outliners, (1 - 3 2), (-3 2 0) and (0 3 3), were omitted.

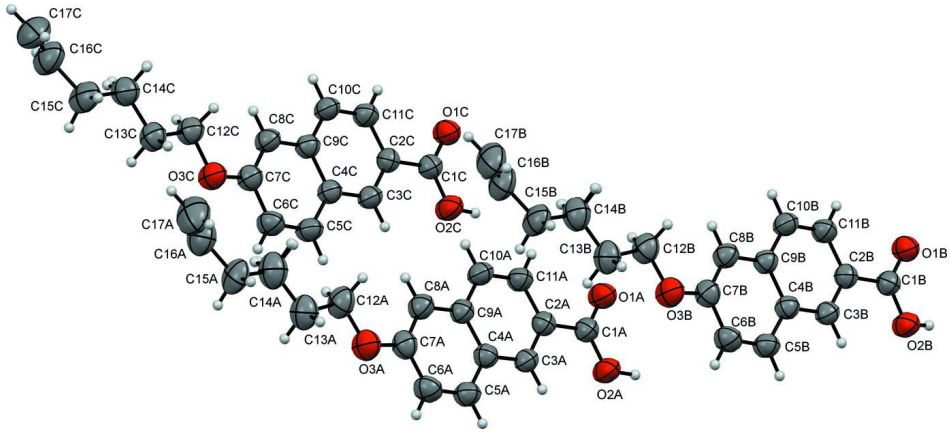


**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids. Disordered butene groups (molecules A, B and C) with higher population components are shown.

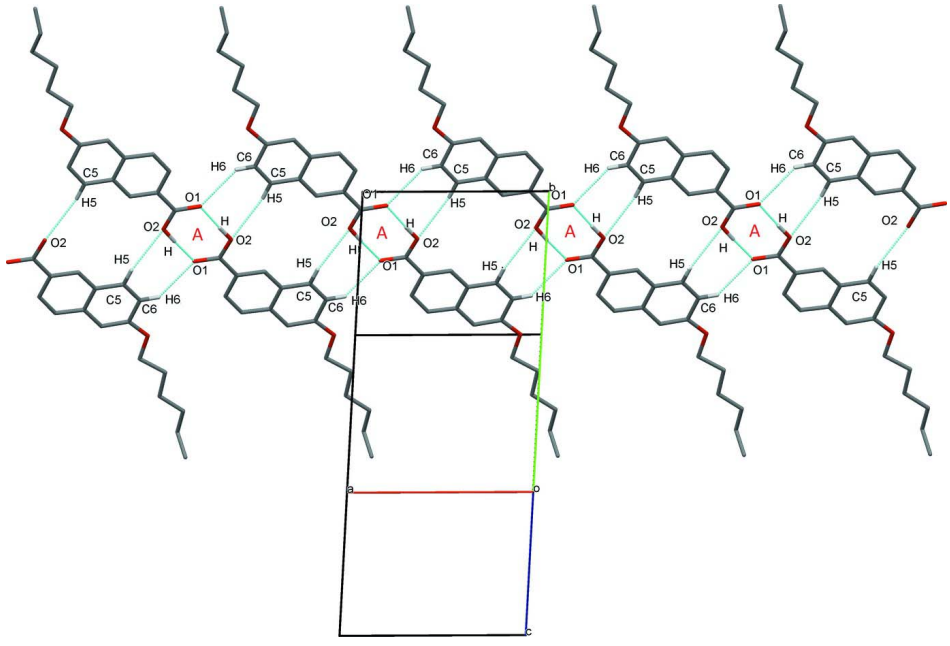


**Figure 2**

Part of the crystal packing of the title compound. Blue dashed lines represent the intermolecular hydrogen bonds and atoms involved in interactions are labelled. Disordered butene groups (in all molecules of asymmetric unit) with higher population components are shown. The symbol A represent the $R^2_2(8)$ graph-set motifs.

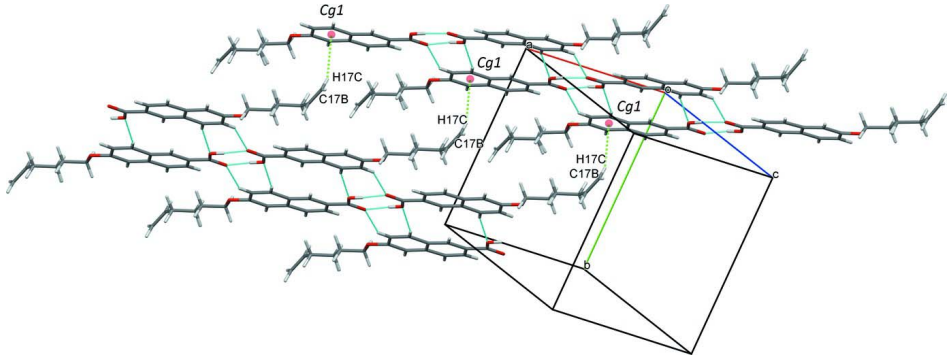


**Figure 3**

Part of the crystal packing of the title compound. Blue dashed lines represent the intermolecular hydrogen bonds within a layer and the green dashed lines represent the weak intermolecular C17B—H17C···*Cg*1 interaction (*Cg1* is the centroid of the C4C—C9C).

### 6-(Hex-5-enyloxy)naphthalene-2-carboxylic acid

*Crystal data*

$C_{17}H_{18}O_3$
$M_r = 270.31$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.5018$ (2) Å
$b = 14.8695$ (2) Å
$c = 17.6757$ (3) Å
$\alpha = 113.638$ (1)°
$\beta = 102.188$ (1)°
$\gamma = 93.127$ (1)°
$V = 2209.06$ (7) Å$^3$
$Z = 6$
$F(000) = 864$
$D_x = 1.219$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 9936 reflections
$\theta = 2.8$–$69.4°$
$\mu = 0.67$ mm$^{-1}$
$T = 298$ K
Block, colourless
0.53 × 0.21 × 0.18 mm

*Data collection*

Bruker APEX DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.719$, $T_{max} = 0.890$
25536 measured reflections
6763 independent reflections
5768 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 62.5°$, $\theta_{min} = 2.8°$
$h = -10\rightarrow10$
$k = -17\rightarrow17$
$l = -20\rightarrow17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.152$
$S = 1.06$
6763 reflections
580 parameters
12 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0897P)^2 + 0.1917P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å$^{-3}$
$\Delta\rho_{min} = -0.17$ e Å$^{-3}$

*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.

**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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C11C | 0.95456 (14) | 0.84092 (10) | 0.81731 (8) | 0.0590 (3) | |
| H11A | 1.0541 | 0.8394 | 0.8316 | 0.071* | |
| O1A | 0.88492 (10) | 0.95388 (8) | 0.38257 (7) | 0.0761 (3) | |
| O2A | 0.69392 (11) | 0.99235 (8) | 0.31169 (7) | 0.0755 (3) | |
| H1 | 0.7582 | 1.0190 | 0.2870 | 0.113* | |
| C2B | 1.27582 (13) | 0.89459 (9) | 0.07820 (8) | 0.0514 (3) | |
| C11B | 1.33200 (14) | 0.84821 (10) | 0.13154 (8) | 0.0575 (3) | |
| H11B | 1.4315 | 0.8462 | 0.1453 | 0.069* | |
| O1B | 1.50686 (10) | 0.93180 (7) | 0.05874 (7) | 0.0686 (3) | |
| O2B | 1.31640 (10) | 0.98007 (7) | −0.00396 (7) | 0.0720 (3) | |
| H2 | 1.3830 | 1.0058 | −0.0179 | 0.108* | |
| C9B | 1.08934 (13) | 0.80896 (9) | 0.14448 (8) | 0.0511 (3) | |
| O1C | 1.13044 (10) | 0.92441 (8) | 0.74563 (7) | 0.0702 (3) | |
| C2A | 0.65249 (14) | 0.91504 (9) | 0.39971 (8) | 0.0533 (3) | |
| C9C | 0.71133 (13) | 0.80165 (9) | 0.82925 (8) | 0.0526 (3) | |
| O2C | 0.94033 (10) | 0.96819 (8) | 0.67871 (7) | 0.0754 (3) | |
| H3 | 1.0014 | 0.9978 | 0.6580 | 0.113* | |
| C4B | 1.03382 (13) | 0.85815 (9) | 0.09276 (8) | 0.0512 (3) | |
| C7C | 0.46924 (14) | 0.76419 (10) | 0.84158 (9) | 0.0585 (3) | |
| C2C | 0.89811 (13) | 0.88579 (9) | 0.76267 (8) | 0.0523 (3) | |
| C14A | 0.0353 (2) | 0.62196 (14) | 0.62674 (12) | 0.0919 (5) | |
| H14A | 0.0887 | 0.5681 | 0.6030 | 0.110* | 0.664 (6) |
| H14B | 0.0969 | 0.6683 | 0.6817 | 0.110* | 0.664 (6) |
| H14G | 0.0882 | 0.6670 | 0.6844 | 0.110* | 0.336 (6) |
| H14H | 0.0870 | 0.5663 | 0.6055 | 0.110* | 0.336 (6) |
| C4A | 0.40916 (14) | 0.87883 (9) | 0.41207 (8) | 0.0527 (3) | |
| C11A | 0.70786 (14) | 0.87345 (10) | 0.45694 (8) | 0.0599 (3) | |
| H11C | 0.8074 | 0.8723 | 0.4721 | 0.072* | |
| C7B | 0.84757 (15) | 0.77311 (10) | 0.15801 (9) | 0.0596 (3) | |
| C4C | 0.65552 (13) | 0.84871 (9) | 0.77598 (8) | 0.0520 (3) | |
| C7A | 0.22020 (15) | 0.80107 (10) | 0.47998 (9) | 0.0625 (3) | |
| C6B | 0.79310 (15) | 0.82404 (10) | 0.10851 (9) | 0.0644 (4) | |
| H6BA | 0.6946 | 0.8296 | 0.0976 | 0.077* | |
| C6C | 0.41426 (14) | 0.81381 (10) | 0.79116 (9) | 0.0643 (3) | |
| H6CA | 0.3156 | 0.8188 | 0.7799 | 0.077* | |

| | | | | |
|---|---|---|---|---|
| O3B | 0.74330 (11) | 0.73435 (8) | 0.18358 (7) | 0.0750 (3) |
| C6A | 0.16638 (15) | 0.84526 (11) | 0.42473 (9) | 0.0664 (4) |
| H6AA | 0.0674 | 0.8487 | 0.4109 | 0.080* |
| C3C | 0.75144 (14) | 0.88935 (9) | 0.74318 (8) | 0.0537 (3) |
| H3CA | 0.7148 | 0.9193 | 0.7075 | 0.064* |
| O3C | 0.36603 (10) | 0.72389 (8) | 0.86688 (7) | 0.0695 (3) |
| C3B | 1.12942 (14) | 0.89931 (9) | 0.06024 (8) | 0.0526 (3) |
| H3BA | 1.0926 | 0.9305 | 0.0257 | 0.063* |
| C13C | 0.27997 (15) | 0.62535 (11) | 0.93018 (9) | 0.0655 (4) |
| H13A | 0.2178 | 0.5782 | 0.8757 | 0.079* |
| H13B | 0.2252 | 0.6776 | 0.9557 | 0.079* |
| C13B | 0.64881 (17) | 0.64431 (12) | 0.25026 (10) | 0.0746 (4) |
| H13C | 0.5856 | 0.5976 | 0.1960 | 0.090* |
| H13D | 0.5976 | 0.6994 | 0.2744 | 0.090* |
| C3A | 0.50620 (14) | 0.91728 (9) | 0.37867 (8) | 0.0537 (3) |
| H3AA | 0.4700 | 0.9450 | 0.3412 | 0.064* |
| C10B | 1.24113 (14) | 0.80637 (10) | 0.16294 (8) | 0.0580 (3) |
| H10A | 1.2798 | 0.7754 | 0.1973 | 0.070* |
| O3A | 0.11378 (11) | 0.76599 (8) | 0.50651 (7) | 0.0789 (3) |
| C10C | 0.86334 (14) | 0.79986 (10) | 0.84898 (8) | 0.0598 (3) |
| H10B | 0.9018 | 0.7700 | 0.8843 | 0.072* |
| C10A | 0.61622 (15) | 0.83494 (10) | 0.49016 (9) | 0.0610 (3) |
| H10C | 0.6544 | 0.8077 | 0.5276 | 0.073* |
| C5B | 0.88300 (14) | 0.86486 (10) | 0.07668 (9) | 0.0603 (3) |
| H5BA | 0.8453 | 0.8978 | 0.0438 | 0.072* |
| C5C | 0.50437 (14) | 0.85437 (10) | 0.75895 (9) | 0.0616 (3) |
| H5CA | 0.4664 | 0.8863 | 0.7253 | 0.074* |
| C13A | 0.01091 (18) | 0.67434 (12) | 0.56904 (11) | 0.0807 (4) |
| H13E | −0.0417 | 0.7289 | 0.5923 | 0.097* |
| H13F | −0.0493 | 0.6284 | 0.5134 | 0.097* |
| C1A | 0.75063 (14) | 0.95599 (9) | 0.36308 (8) | 0.0573 (3) |
| C1C | 0.99664 (14) | 0.92866 (9) | 0.72752 (8) | 0.0560 (3) |
| C8B | 0.99318 (15) | 0.76624 (10) | 0.17631 (8) | 0.0575 (3) |
| H8BA | 1.0286 | 0.7334 | 0.2097 | 0.069* |
| C5A | 0.25799 (14) | 0.88260 (10) | 0.39172 (9) | 0.0620 (3) |
| H5AA | 0.2211 | 0.9112 | 0.3551 | 0.074* |
| C1B | 1.37349 (14) | 0.93781 (9) | 0.04264 (8) | 0.0550 (3) |
| C8C | 0.61515 (14) | 0.75945 (10) | 0.86145 (8) | 0.0577 (3) |
| H8CA | 0.6510 | 0.7283 | 0.8962 | 0.069* |
| C9A | 0.46405 (14) | 0.83562 (9) | 0.46872 (8) | 0.0535 (3) |
| C12C | 0.41192 (15) | 0.66930 (11) | 0.91581 (10) | 0.0650 (4) |
| H12A | 0.4781 | 0.7130 | 0.9702 | 0.078* |
| H12B | 0.4626 | 0.6169 | 0.8854 | 0.078* |
| C12A | 0.15113 (17) | 0.71425 (12) | 0.55827 (10) | 0.0759 (4) |
| H12C | 0.2142 | 0.7588 | 0.6134 | 0.091* |
| H12D | 0.2019 | 0.6602 | 0.5311 | 0.091* |
| C12B | 0.78511 (16) | 0.68236 (11) | 0.23525 (10) | 0.0698 (4) |
| H12E | 0.8519 | 0.7266 | 0.2892 | 0.084* |

| | | | | | |
|---|---|---|---|---|---|
| H12F | 0.8333 | 0.6275 | 0.2064 | 0.084* | |
| C8A | 0.36617 (15) | 0.79645 (10) | 0.50215 (9) | 0.0610 (3) | |
| H8AA | 0.4006 | 0.7677 | 0.5390 | 0.073* | |
| C14C | 0.32087 (17) | 0.57320 (12) | 0.98788 (11) | 0.0754 (4) | |
| H14E | 0.3880 | 0.6194 | 1.0409 | 0.090* | 0.664 (6) |
| H14F | 0.3706 | 0.5185 | 0.9606 | 0.090* | 0.664 (6) |
| H14K | 0.3715 | 0.6223 | 1.0446 | 0.090* | 0.336 (6) |
| H14L | 0.3877 | 0.5281 | 0.9665 | 0.090* | 0.336 (6) |
| C14B | 0.67968 (19) | 0.59356 (13) | 0.30987 (11) | 0.0828 (5) | |
| H14C | 0.7294 | 0.5380 | 0.2847 | 0.099* | 0.664 (6) |
| H14D | 0.7460 | 0.6401 | 0.3631 | 0.099* | 0.664 (6) |
| H14I | 0.7411 | 0.6387 | 0.3653 | 0.099* | 0.336 (6) |
| H14J | 0.7261 | 0.5357 | 0.2862 | 0.099* | 0.336 (6) |
| C15A | −0.0974 (6) | 0.5802 (3) | 0.6415 (3) | 0.0832 (11) | 0.664 (6) |
| H15A | −0.1574 | 0.6319 | 0.6583 | 0.100* | 0.664 (6) |
| H15B | −0.1530 | 0.5274 | 0.5878 | 0.100* | 0.664 (6) |
| C16A | −0.0708 (5) | 0.5402 (2) | 0.7067 (3) | 0.0916 (10) | 0.664 (6) |
| H16A | −0.0137 | 0.5813 | 0.7610 | 0.110* | 0.664 (6) |
| C17A | −0.1241 (6) | 0.4492 (3) | 0.6915 (3) | 0.1266 (16) | 0.664 (6) |
| H17A | −0.1816 | 0.4066 | 0.6376 | 0.152* | 0.664 (6) |
| H17B | −0.1042 | 0.4275 | 0.7346 | 0.152* | 0.664 (6) |
| C15B | 0.5494 (6) | 0.5560 (4) | 0.3299 (3) | 0.0813 (11) | 0.664 (6) |
| H15C | 0.4917 | 0.6092 | 0.3460 | 0.098* | 0.664 (6) |
| H15D | 0.4909 | 0.5025 | 0.2776 | 0.098* | 0.664 (6) |
| C16B | 0.5729 (5) | 0.5199 (3) | 0.3958 (3) | 0.0875 (11) | 0.664 (6) |
| H16B | 0.6295 | 0.5635 | 0.4496 | 0.105* | 0.664 (6) |
| C17B | 0.5219 (6) | 0.4323 (3) | 0.3865 (3) | 0.1046 (13) | 0.664 (6) |
| H17C | 0.4648 | 0.3863 | 0.3338 | 0.126* | 0.664 (6) |
| H17D | 0.5426 | 0.4154 | 0.4325 | 0.126* | 0.664 (6) |
| C15C | 0.1867 (6) | 0.5328 (5) | 1.0080 (4) | 0.0738 (19) | 0.664 (6) |
| H15E | 0.1222 | 0.5823 | 1.0194 | 0.089* | 0.664 (6) |
| H15F | 0.1341 | 0.4739 | 0.9581 | 0.089* | 0.664 (6) |
| C16C | 0.2253 (3) | 0.5076 (3) | 1.0819 (3) | 0.0928 (11) | 0.664 (6) |
| H16C | 0.2837 | 0.5577 | 1.1321 | 0.111* | 0.664 (6) |
| C17C | 0.1892 (4) | 0.4272 (3) | 1.0857 (3) | 0.1042 (12) | 0.664 (6) |
| H17E | 0.1308 | 0.3743 | 1.0377 | 0.125* | 0.664 (6) |
| H17F | 0.2208 | 0.4207 | 1.1365 | 0.125* | 0.664 (6) |
| C15X | −0.1273 (16) | 0.5851 (10) | 0.6242 (9) | 0.114 (4)* | 0.336 (6) |
| H15G | −0.1746 | 0.6422 | 0.6491 | 0.137* | 0.336 (6) |
| H15H | −0.1822 | 0.5467 | 0.5654 | 0.137* | 0.336 (6) |
| C16X | −0.1261 (15) | 0.5260 (9) | 0.6701 (8) | 0.154 (5)* | 0.336 (6) |
| H16D | −0.2039 | 0.5362 | 0.6953 | 0.185* | 0.336 (6) |
| C17X | −0.0641 (15) | 0.4698 (11) | 0.6878 (9) | 0.164 (5)* | 0.336 (6) |
| H17G | 0.0176 | 0.4509 | 0.6679 | 0.196* | 0.336 (6) |
| H17H | −0.0957 | 0.4434 | 0.7220 | 0.196* | 0.336 (6) |
| C15Y | 0.5194 (14) | 0.5626 (10) | 0.3175 (9) | 0.096 (4)* | 0.336 (6) |
| H15I | 0.4718 | 0.6205 | 0.3384 | 0.116* | 0.336 (6) |
| H15J | 0.4590 | 0.5154 | 0.2625 | 0.116* | 0.336 (6) |

| | | | | | |
|---|---|---|---|---|---|
| C16Y | 0.544 (2) | 0.5186 (13) | 0.3768 (11) | 0.210 (10)* | 0.336 (6) |
| H16E | 0.5448 | 0.5665 | 0.4307 | 0.252* | 0.336 (6) |
| C17Y | 0.563 (2) | 0.4435 (13) | 0.3816 (13) | 0.203 (9)* | 0.336 (6) |
| H17I | 0.5645 | 0.3875 | 0.3331 | 0.244* | 0.336 (6) |
| H17J | 0.5755 | 0.4401 | 0.4340 | 0.244* | 0.336 (6) |
| C15Z | 0.1984 (19) | 0.5311 (13) | 1.0046 (12) | 0.112 (7)* | 0.336 (6) |
| H15K | 0.1227 | 0.4989 | 0.9516 | 0.135* | 0.336 (6) |
| H15L | 0.1603 | 0.5844 | 1.0440 | 0.135* | 0.336 (6) |
| C16Z | 0.2317 (7) | 0.4548 (5) | 1.0422 (4) | 0.0839 (19)* | 0.336 (6) |
| H16F | 0.2543 | 0.3923 | 1.0122 | 0.101* | 0.336 (6) |
| C17Z | 0.2239 (9) | 0.4900 (8) | 1.1239 (5) | 0.121 (3)* | 0.336 (6) |
| H17K | 0.2007 | 0.5533 | 1.1503 | 0.145* | 0.336 (6) |
| H17L | 0.2416 | 0.4511 | 1.1540 | 0.145* | 0.336 (6) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C11C | 0.0464 (7) | 0.0740 (8) | 0.0662 (8) | 0.0126 (6) | 0.0140 (6) | 0.0389 (6) |
| O1A | 0.0526 (6) | 0.1063 (8) | 0.1005 (8) | 0.0207 (5) | 0.0269 (5) | 0.0701 (6) |
| O2A | 0.0641 (6) | 0.1051 (7) | 0.0933 (7) | 0.0256 (5) | 0.0294 (5) | 0.0716 (6) |
| C2B | 0.0504 (7) | 0.0533 (7) | 0.0531 (7) | 0.0082 (5) | 0.0148 (5) | 0.0243 (5) |
| C11B | 0.0450 (7) | 0.0713 (8) | 0.0639 (8) | 0.0115 (6) | 0.0135 (6) | 0.0360 (6) |
| O1B | 0.0514 (6) | 0.0867 (7) | 0.0895 (7) | 0.0153 (5) | 0.0243 (5) | 0.0552 (5) |
| O2B | 0.0612 (6) | 0.0923 (7) | 0.0952 (7) | 0.0218 (5) | 0.0299 (5) | 0.0662 (6) |
| C9B | 0.0483 (7) | 0.0538 (6) | 0.0512 (7) | 0.0060 (5) | 0.0110 (5) | 0.0233 (5) |
| O1C | 0.0527 (6) | 0.0904 (7) | 0.0918 (7) | 0.0181 (5) | 0.0251 (5) | 0.0586 (6) |
| C2A | 0.0515 (7) | 0.0572 (7) | 0.0561 (7) | 0.0110 (5) | 0.0159 (6) | 0.0274 (6) |
| C9C | 0.0489 (7) | 0.0572 (7) | 0.0532 (7) | 0.0076 (5) | 0.0100 (5) | 0.0265 (5) |
| O2C | 0.0613 (6) | 0.1042 (7) | 0.0961 (7) | 0.0216 (5) | 0.0281 (5) | 0.0726 (6) |
| C4B | 0.0491 (7) | 0.0527 (6) | 0.0519 (7) | 0.0066 (5) | 0.0112 (5) | 0.0232 (5) |
| C7C | 0.0497 (7) | 0.0647 (7) | 0.0644 (8) | 0.0047 (6) | 0.0140 (6) | 0.0315 (6) |
| C2C | 0.0522 (7) | 0.0551 (7) | 0.0543 (7) | 0.0098 (5) | 0.0165 (5) | 0.0263 (5) |
| C14A | 0.0899 (12) | 0.0975 (12) | 0.0974 (12) | −0.0029 (9) | 0.0364 (10) | 0.0463 (10) |
| C4A | 0.0503 (7) | 0.0539 (7) | 0.0543 (7) | 0.0084 (5) | 0.0127 (5) | 0.0235 (5) |
| C11A | 0.0485 (7) | 0.0746 (8) | 0.0672 (8) | 0.0139 (6) | 0.0149 (6) | 0.0400 (6) |
| C7B | 0.0500 (7) | 0.0644 (7) | 0.0662 (8) | 0.0015 (6) | 0.0156 (6) | 0.0298 (6) |
| C4C | 0.0492 (7) | 0.0549 (7) | 0.0543 (7) | 0.0074 (5) | 0.0114 (5) | 0.0265 (5) |
| C7A | 0.0559 (7) | 0.0644 (8) | 0.0701 (8) | 0.0028 (6) | 0.0219 (6) | 0.0292 (6) |
| C6B | 0.0464 (7) | 0.0758 (9) | 0.0763 (9) | 0.0090 (6) | 0.0140 (6) | 0.0382 (7) |
| C6C | 0.0464 (7) | 0.0784 (9) | 0.0780 (9) | 0.0105 (6) | 0.0139 (6) | 0.0439 (7) |
| O3B | 0.0539 (5) | 0.0939 (7) | 0.0946 (7) | 0.0026 (5) | 0.0226 (5) | 0.0564 (6) |
| C6A | 0.0494 (7) | 0.0750 (9) | 0.0782 (9) | 0.0097 (6) | 0.0144 (6) | 0.0367 (7) |
| C3C | 0.0550 (7) | 0.0572 (7) | 0.0552 (7) | 0.0113 (5) | 0.0125 (6) | 0.0304 (6) |
| O3C | 0.0497 (5) | 0.0889 (7) | 0.0882 (7) | 0.0051 (4) | 0.0189 (5) | 0.0557 (5) |
| C3B | 0.0533 (7) | 0.0545 (7) | 0.0550 (7) | 0.0097 (5) | 0.0132 (5) | 0.0284 (5) |
| C13C | 0.0582 (8) | 0.0710 (8) | 0.0728 (9) | 0.0030 (6) | 0.0192 (6) | 0.0354 (7) |
| C13B | 0.0701 (9) | 0.0762 (9) | 0.0803 (10) | −0.0026 (7) | 0.0272 (8) | 0.0335 (8) |
| C3A | 0.0553 (7) | 0.0581 (7) | 0.0545 (7) | 0.0113 (5) | 0.0135 (5) | 0.0307 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10B | 0.0527 (7) | 0.0715 (8) | 0.0612 (7) | 0.0126 (6) | 0.0125 (6) | 0.0400 (6) |
| O3A | 0.0627 (6) | 0.0947 (7) | 0.0978 (8) | 0.0065 (5) | 0.0291 (5) | 0.0555 (6) |
| C10C | 0.0522 (7) | 0.0753 (8) | 0.0656 (8) | 0.0127 (6) | 0.0133 (6) | 0.0440 (6) |
| C10A | 0.0574 (7) | 0.0743 (8) | 0.0644 (8) | 0.0156 (6) | 0.0137 (6) | 0.0429 (6) |
| C5B | 0.0506 (7) | 0.0696 (8) | 0.0682 (8) | 0.0118 (6) | 0.0120 (6) | 0.0379 (6) |
| C5C | 0.0519 (7) | 0.0726 (8) | 0.0710 (8) | 0.0132 (6) | 0.0107 (6) | 0.0429 (7) |
| C13A | 0.0756 (10) | 0.0819 (10) | 0.0853 (10) | −0.0057 (8) | 0.0282 (8) | 0.0344 (8) |
| C1A | 0.0553 (7) | 0.0648 (7) | 0.0633 (8) | 0.0150 (6) | 0.0196 (6) | 0.0356 (6) |
| C1C | 0.0548 (7) | 0.0600 (7) | 0.0594 (7) | 0.0128 (6) | 0.0174 (6) | 0.0297 (6) |
| C8B | 0.0549 (7) | 0.0636 (7) | 0.0611 (7) | 0.0059 (6) | 0.0138 (6) | 0.0343 (6) |
| C5A | 0.0535 (7) | 0.0709 (8) | 0.0693 (8) | 0.0118 (6) | 0.0132 (6) | 0.0383 (6) |
| C1B | 0.0533 (7) | 0.0573 (7) | 0.0612 (7) | 0.0114 (6) | 0.0182 (6) | 0.0297 (6) |
| C8C | 0.0525 (7) | 0.0674 (8) | 0.0634 (8) | 0.0079 (6) | 0.0126 (6) | 0.0390 (6) |
| C9A | 0.0537 (7) | 0.0551 (7) | 0.0553 (7) | 0.0083 (5) | 0.0146 (5) | 0.0265 (5) |
| C12C | 0.0577 (8) | 0.0719 (8) | 0.0743 (9) | 0.0054 (6) | 0.0172 (6) | 0.0401 (7) |
| C12A | 0.0738 (9) | 0.0840 (10) | 0.0780 (9) | 0.0006 (8) | 0.0248 (8) | 0.0412 (8) |
| C12B | 0.0651 (8) | 0.0748 (9) | 0.0764 (9) | 0.0007 (7) | 0.0213 (7) | 0.0384 (7) |
| C8A | 0.0620 (8) | 0.0654 (8) | 0.0634 (8) | 0.0083 (6) | 0.0166 (6) | 0.0350 (6) |
| C14C | 0.0631 (8) | 0.0874 (10) | 0.0939 (11) | 0.0102 (7) | 0.0261 (8) | 0.0536 (9) |
| C14B | 0.0829 (11) | 0.0878 (11) | 0.0914 (11) | 0.0055 (8) | 0.0365 (9) | 0.0454 (9) |
| C15A | 0.084 (2) | 0.090 (2) | 0.089 (2) | −0.0152 (17) | 0.031 (2) | 0.0489 (18) |
| C16A | 0.095 (2) | 0.098 (2) | 0.092 (2) | −0.0039 (17) | 0.032 (2) | 0.0482 (17) |
| C17A | 0.160 (4) | 0.110 (3) | 0.161 (4) | 0.027 (3) | 0.088 (3) | 0.085 (2) |
| C15B | 0.074 (2) | 0.104 (2) | 0.091 (3) | 0.0020 (19) | 0.030 (2) | 0.063 (2) |
| C16B | 0.089 (2) | 0.105 (3) | 0.0872 (19) | −0.0023 (15) | 0.0335 (16) | 0.0553 (16) |
| C17B | 0.127 (3) | 0.106 (2) | 0.127 (3) | 0.0277 (19) | 0.069 (2) | 0.076 (2) |
| C15C | 0.0571 (18) | 0.094 (3) | 0.096 (3) | 0.0009 (11) | 0.0241 (15) | 0.065 (2) |
| C16C | 0.0880 (18) | 0.121 (3) | 0.098 (2) | 0.0082 (16) | 0.0299 (16) | 0.072 (2) |
| C17C | 0.122 (3) | 0.110 (3) | 0.118 (3) | 0.028 (2) | 0.042 (2) | 0.079 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C11C—C10C | 1.3634 (18) | C10C—H10B | 0.9300 |
| C11C—C2C | 1.4151 (18) | C10A—C9A | 1.4169 (19) |
| C11C—H11A | 0.9300 | C10A—H10C | 0.9300 |
| O1A—C1A | 1.2551 (16) | C5B—H5BA | 0.9300 |
| O2A—C1A | 1.2755 (15) | C5C—H5CA | 0.9300 |
| O2A—H1 | 0.9728 | C13A—C12A | 1.508 (2) |
| C2B—C3B | 1.3722 (18) | C13A—H13E | 0.9700 |
| C2B—C11B | 1.4138 (18) | C13A—H13F | 0.9700 |
| C2B—C1B | 1.4746 (17) | C8B—H8BA | 0.9300 |
| C11B—C10B | 1.3643 (18) | C5A—H5AA | 0.9300 |
| C11B—H11B | 0.9300 | C8C—H8CA | 0.9300 |
| O1B—C1B | 1.2551 (16) | C9A—C8A | 1.4149 (19) |
| O2B—C1B | 1.2773 (15) | C12C—H12A | 0.9700 |
| O2B—H2 | 0.8501 | C12C—H12B | 0.9700 |
| C9B—C8B | 1.4125 (19) | C12A—H12C | 0.9700 |
| C9B—C10B | 1.4162 (18) | C12A—H12D | 0.9700 |

| | | | |
|---|---|---|---|
| C9B—C4B | 1.4224 (18) | C12B—H12E | 0.9700 |
| O1C—C1C | 1.2554 (16) | C12B—H12F | 0.9700 |
| C2A—C3A | 1.3669 (18) | C8A—H8AA | 0.9300 |
| C2A—C11A | 1.4124 (18) | C14C—C15Z | 1.430 (16) |
| C2A—C1A | 1.4726 (18) | C14C—C15C | 1.546 (5) |
| C9C—C8C | 1.4129 (18) | C14C—H14E | 0.9700 |
| C9C—C10C | 1.4169 (18) | C14C—H14F | 0.9700 |
| C9C—C4C | 1.4197 (17) | C14C—H14K | 0.9699 |
| O2C—C1C | 1.2736 (15) | C14C—H14L | 0.9700 |
| O2C—H3 | 0.9243 | C14B—C15B | 1.496 (4) |
| C4B—C3B | 1.4043 (18) | C14B—C15Y | 1.616 (14) |
| C4B—C5B | 1.4180 (18) | C14B—H14C | 0.9700 |
| C7C—O3C | 1.3628 (16) | C14B—H14D | 0.9700 |
| C7C—C8C | 1.3695 (19) | C14B—H14I | 0.9700 |
| C7C—C6C | 1.4085 (19) | C14B—H14J | 0.9700 |
| C2C—C3C | 1.3724 (18) | C15A—C16A | 1.478 (6) |
| C2C—C1C | 1.4721 (18) | C15A—H15A | 0.9700 |
| C14A—C15A | 1.493 (4) | C15A—H15B | 0.9700 |
| C14A—C13A | 1.502 (2) | C16A—C17A | 1.318 (6) |
| C14A—C15X | 1.596 (14) | C16A—H16A | 0.9300 |
| C14A—H14A | 0.9700 | C17A—H17A | 0.9300 |
| C14A—H14B | 0.9700 | C17A—H17B | 0.9300 |
| C14A—H14G | 0.9700 | C15B—C16B | 1.448 (5) |
| C14A—H14H | 0.9700 | C15B—H15C | 0.9700 |
| C4A—C3A | 1.4032 (18) | C15B—H15D | 0.9700 |
| C4A—C5A | 1.4151 (18) | C16B—C17B | 1.299 (5) |
| C4A—C9A | 1.4211 (18) | C16B—H16B | 0.9300 |
| C11A—C10A | 1.3645 (19) | C17B—H17C | 0.9300 |
| C11A—H11C | 0.9300 | C17B—H17D | 0.9300 |
| C7B—O3B | 1.3614 (17) | C15C—C16C | 1.480 (5) |
| C7B—C8B | 1.372 (2) | C15C—H15E | 0.9700 |
| C7B—C6B | 1.411 (2) | C15C—H15F | 0.9700 |
| C4C—C3C | 1.4056 (18) | C16C—C17C | 1.257 (5) |
| C4C—C5C | 1.4182 (18) | C16C—H16C | 0.9300 |
| C7A—O3A | 1.3615 (17) | C17C—H17E | 0.9300 |
| C7A—C8A | 1.373 (2) | C17C—H17F | 0.9300 |
| C7A—C6A | 1.410 (2) | C15X—C16X | 1.414 (12) |
| C6B—C5B | 1.355 (2) | C15X—H15G | 0.9700 |
| C6B—H6BA | 0.9300 | C15X—H15H | 0.9700 |
| C6C—C5C | 1.3585 (19) | C16X—C17X | 1.152 (13) |
| C6C—H6CA | 0.9300 | C16X—H16D | 0.9300 |
| O3B—C12B | 1.4269 (18) | C17X—H17G | 0.9300 |
| C6A—C5A | 1.352 (2) | C17X—H17H | 0.9300 |
| C6A—H6AA | 0.9300 | C15Y—C16Y | 1.429 (11) |
| C3C—H3CA | 0.9300 | C15Y—H15I | 0.9700 |
| O3C—C12C | 1.4280 (16) | C15Y—H15J | 0.9700 |
| C3B—H3BA | 0.9300 | C16Y—C17Y | 1.174 (12) |
| C13C—C12C | 1.4972 (19) | C16Y—H16E | 0.9300 |

| | | | |
|---|---|---|---|
| C13C—C14C | 1.514 (2) | C17Y—H17I | 0.9300 |
| C13C—H13A | 0.9700 | C17Y—H17J | 0.9300 |
| C13C—H13B | 0.9700 | C15Z—C16Z | 1.545 (12) |
| C13B—C12B | 1.501 (2) | C15Z—H15K | 0.9700 |
| C13B—C14B | 1.516 (2) | C15Z—H15L | 0.9700 |
| C13B—H13C | 0.9700 | C16Z—C17Z | 1.344 (10) |
| C13B—H13D | 0.9700 | C16Z—H16F | 0.9300 |
| C3A—H3AA | 0.9300 | C17Z—H17K | 0.9300 |
| C10B—H10A | 0.9300 | C17Z—H17L | 0.9300 |
| O3A—C12A | 1.4183 (18) | | |

| | | | |
|---|---|---|---|
| C10C—C11C—C2C | 120.14 (12) | C8A—C9A—C10A | 122.75 (12) |
| C10C—C11C—H11A | 119.9 | C8A—C9A—C4A | 119.25 (12) |
| C2C—C11C—H11A | 119.9 | C10A—C9A—C4A | 117.99 (12) |
| C1A—O2A—H1 | 118.0 | O3C—C12C—C13C | 108.49 (11) |
| C3B—C2B—C11B | 119.20 (11) | O3C—C12C—H12A | 110.0 |
| C3B—C2B—C1B | 120.41 (12) | C13C—C12C—H12A | 110.0 |
| C11B—C2B—C1B | 120.40 (11) | O3C—C12C—H12B | 110.0 |
| C10B—C11B—C2B | 120.37 (12) | C13C—C12C—H12B | 110.0 |
| C10B—C11B—H11B | 119.8 | H12A—C12C—H12B | 108.4 |
| C2B—C11B—H11B | 119.8 | O3A—C12A—C13A | 107.21 (13) |
| C1B—O2B—H2 | 109.4 | O3A—C12A—H12C | 110.3 |
| C8B—C9B—C10B | 122.61 (12) | C13A—C12A—H12C | 110.3 |
| C8B—C9B—C4B | 119.53 (12) | O3A—C12A—H12D | 110.3 |
| C10B—C9B—C4B | 117.86 (12) | C13A—C12A—H12D | 110.3 |
| C3A—C2A—C11A | 119.26 (12) | H12C—C12A—H12D | 108.5 |
| C3A—C2A—C1A | 120.05 (12) | O3B—C12B—C13B | 107.38 (13) |
| C11A—C2A—C1A | 120.69 (11) | O3B—C12B—H12E | 110.2 |
| C8C—C9C—C10C | 122.28 (12) | C13B—C12B—H12E | 110.2 |
| C8C—C9C—C4C | 119.52 (12) | O3B—C12B—H12F | 110.2 |
| C10C—C9C—C4C | 118.20 (11) | C13B—C12B—H12F | 110.2 |
| C1C—O2C—H3 | 118.4 | H12E—C12B—H12F | 108.5 |
| C3B—C4B—C5B | 122.20 (12) | C7A—C8A—C9A | 119.82 (13) |
| C3B—C4B—C9B | 119.36 (12) | C7A—C8A—H8AA | 120.1 |
| C5B—C4B—C9B | 118.44 (12) | C9A—C8A—H8AA | 120.1 |
| O3C—C7C—C8C | 125.36 (12) | C15Z—C14C—C13C | 113.8 (6) |
| O3C—C7C—C6C | 114.22 (11) | C15Z—C14C—C15C | 2.8 (10) |
| C8C—C7C—C6C | 120.42 (12) | C13C—C14C—C15C | 112.4 (2) |
| C3C—C2C—C11C | 119.53 (12) | C15Z—C14C—H14E | 110.5 |
| C3C—C2C—C1C | 120.48 (12) | C13C—C14C—H14E | 109.1 |
| C11C—C2C—C1C | 119.99 (11) | C15C—C14C—H14E | 109.1 |
| C15A—C14A—C13A | 116.7 (3) | C15Z—C14C—H14F | 106.3 |
| C15A—C14A—C15X | 14.5 (6) | C13C—C14C—H14F | 109.1 |
| C13A—C14A—C15X | 102.3 (5) | C15C—C14C—H14F | 109.1 |
| C15A—C14A—H14A | 108.1 | H14E—C14C—H14F | 107.9 |
| C13A—C14A—H14A | 108.1 | C15Z—C14C—H14K | 101.5 |
| C15X—C14A—H14A | 113.5 | C13C—C14C—H14K | 108.9 |
| C15A—C14A—H14B | 108.1 | C15C—C14C—H14K | 99.9 |

| | | | |
|---|---|---|---|
| C13A—C14A—H14B | 108.1 | H14E—C14C—H14K | 10.8 |
| C15X—C14A—H14B | 117.0 | H14F—C14C—H14K | 117.2 |
| H14A—C14A—H14B | 107.3 | C15Z—C14C—H14L | 115.5 |
| C15A—C14A—H14G | 101.7 | C13C—C14C—H14L | 108.9 |
| C13A—C14A—H14G | 111.5 | C15C—C14C—H14L | 118.3 |
| C15X—C14A—H14G | 110.6 | H14E—C14C—H14L | 97.9 |
| H14A—C14A—H14G | 110.6 | H14F—C14C—H14L | 11.2 |
| H14B—C14A—H14G | 6.5 | H14K—C14C—H14L | 107.7 |
| C15A—C14A—H14H | 105.1 | C15B—C14B—C13B | 115.8 (2) |
| C13A—C14A—H14H | 111.8 | C15B—C14B—C15Y | 12.7 (5) |
| C15X—C14A—H14H | 111.2 | C13B—C14B—C15Y | 103.1 (4) |
| H14A—C14A—H14H | 3.8 | C15B—C14B—H14C | 108.3 |
| H14B—C14A—H14H | 106.5 | C13B—C14B—H14C | 108.3 |
| H14G—C14A—H14H | 109.4 | C15Y—C14B—H14C | 114.5 |
| C3A—C4A—C5A | 121.96 (12) | C15B—C14B—H14D | 108.3 |
| C3A—C4A—C9A | 119.21 (12) | C13B—C14B—H14D | 108.3 |
| C5A—C4A—C9A | 118.82 (12) | C15Y—C14B—H14D | 114.8 |
| C10A—C11A—C2A | 120.41 (12) | H14C—C14B—H14D | 107.4 |
| C10A—C11A—H11C | 119.8 | C15B—C14B—H14I | 104.0 |
| C2A—C11A—H11C | 119.8 | C13B—C14B—H14I | 111.3 |
| O3B—C7B—C8B | 126.05 (13) | C15Y—C14B—H14I | 110.6 |
| O3B—C7B—C6B | 113.55 (12) | H14C—C14B—H14I | 108.9 |
| C8B—C7B—C6B | 120.40 (13) | H14D—C14B—H14I | 4.4 |
| C3C—C4C—C5C | 122.33 (12) | C15B—C14B—H14J | 104.8 |
| C3C—C4C—C9C | 119.25 (11) | C13B—C14B—H14J | 111.3 |
| C5C—C4C—C9C | 118.42 (12) | C15Y—C14B—H14J | 111.3 |
| O3A—C7A—C8A | 126.28 (14) | H14C—C14B—H14J | 3.7 |
| O3A—C7A—C6A | 112.93 (12) | H14D—C14B—H14J | 107.9 |
| C8A—C7A—C6A | 120.79 (13) | H14I—C14B—H14J | 109.2 |
| C5B—C6B—C7B | 120.57 (13) | C16A—C15A—C14A | 115.8 (4) |
| C5B—C6B—H6BA | 119.7 | C16A—C15A—H15A | 108.3 |
| C7B—C6B—H6BA | 119.7 | C14A—C15A—H15A | 108.3 |
| C5C—C6C—C7C | 120.46 (12) | C16A—C15A—H15B | 108.3 |
| C5C—C6C—H6CA | 119.8 | C14A—C15A—H15B | 108.3 |
| C7C—C6C—H6CA | 119.8 | H15A—C15A—H15B | 107.4 |
| C7B—O3B—C12B | 118.92 (11) | C17A—C16A—C15A | 123.2 (4) |
| C5A—C6A—C7A | 120.29 (13) | C17A—C16A—H16A | 118.4 |
| C5A—C6A—H6AA | 119.9 | C15A—C16A—H16A | 118.4 |
| C7A—C6A—H6AA | 119.9 | C16A—C17A—H17A | 120.0 |
| C2C—C3C—C4C | 121.35 (12) | C16A—C17A—H17B | 120.0 |
| C2C—C3C—H3CA | 119.3 | H17A—C17A—H17B | 120.0 |
| C4C—C3C—H3CA | 119.3 | C16B—C15B—C14B | 118.4 (4) |
| C7C—O3C—C12C | 117.80 (10) | C16B—C15B—H15C | 107.7 |
| C2B—C3B—C4B | 121.58 (12) | C14B—C15B—H15C | 107.7 |
| C2B—C3B—H3BA | 119.2 | C16B—C15B—H15D | 107.7 |
| C4B—C3B—H3BA | 119.2 | C14B—C15B—H15D | 107.7 |
| C12C—C13C—C14C | 111.61 (12) | H15C—C15B—H15D | 107.1 |
| C12C—C13C—H13A | 109.3 | C17B—C16B—C15B | 125.8 (5) |

| | | | |
|---|---|---|---|
| C14C—C13C—H13A | 109.3 | C17B—C16B—H16B | 117.1 |
| C12C—C13C—H13B | 109.3 | C15B—C16B—H16B | 117.1 |
| C14C—C13C—H13B | 109.3 | C16B—C17B—H17C | 120.0 |
| H13A—C13C—H13B | 108.0 | C16B—C17B—H17D | 120.0 |
| C12B—C13B—C14B | 112.58 (14) | H17C—C17B—H17D | 120.0 |
| C12B—C13B—H13C | 109.1 | C16C—C15C—C14C | 113.2 (4) |
| C14B—C13B—H13C | 109.1 | C16C—C15C—H15E | 108.9 |
| C12B—C13B—H13D | 109.1 | C14C—C15C—H15E | 108.9 |
| C14B—C13B—H13D | 109.1 | C16C—C15C—H15F | 108.9 |
| H13C—C13B—H13D | 107.8 | C14C—C15C—H15F | 108.9 |
| C2A—C3A—C4A | 121.75 (12) | H15E—C15C—H15F | 107.8 |
| C2A—C3A—H3AA | 119.1 | C17C—C16C—C15C | 128.3 (5) |
| C4A—C3A—H3AA | 119.1 | C17C—C16C—H16C | 115.9 |
| C11B—C10B—C9B | 121.60 (12) | C15C—C16C—H16C | 115.9 |
| C11B—C10B—H10A | 119.2 | C16C—C17C—H17E | 120.0 |
| C9B—C10B—H10A | 119.2 | C16C—C17C—H17F | 120.0 |
| C7A—O3A—C12A | 118.97 (12) | H17E—C17C—H17F | 120.0 |
| C11C—C10C—C9C | 121.49 (12) | C16X—C15X—C14A | 110.2 (10) |
| C11C—C10C—H10B | 119.3 | C16X—C15X—H15G | 109.6 |
| C9C—C10C—H10B | 119.3 | C14A—C15X—H15G | 109.6 |
| C11A—C10A—C9A | 121.37 (13) | C16X—C15X—H15H | 109.6 |
| C11A—C10A—H10C | 119.3 | C14A—C15X—H15H | 109.6 |
| C9A—C10A—H10C | 119.3 | H15G—C15X—H15H | 108.1 |
| C6B—C5B—C4B | 120.96 (13) | C17X—C16X—C15X | 143.1 (16) |
| C6B—C5B—H5BA | 119.5 | C17X—C16X—H16D | 108.4 |
| C4B—C5B—H5BA | 119.5 | C15X—C16X—H16D | 108.4 |
| C6C—C5C—C4C | 120.94 (13) | C16X—C17X—H17G | 120.0 |
| C6C—C5C—H5CA | 119.5 | C16X—C17X—H17H | 120.0 |
| C4C—C5C—H5CA | 119.5 | H17G—C17X—H17H | 120.0 |
| C14A—C13A—C12A | 112.81 (14) | C16Y—C15Y—C14B | 105.1 (11) |
| C14A—C13A—H13E | 109.0 | C16Y—C15Y—H15I | 110.7 |
| C12A—C13A—H13E | 109.0 | C14B—C15Y—H15I | 110.7 |
| C14A—C13A—H13F | 109.0 | C16Y—C15Y—H15J | 110.7 |
| C12A—C13A—H13F | 109.0 | C14B—C15Y—H15J | 110.7 |
| H13E—C13A—H13F | 107.8 | H15I—C15Y—H15J | 108.8 |
| O1A—C1A—O2A | 122.42 (12) | C17Y—C16Y—C15Y | 142 (2) |
| O1A—C1A—C2A | 119.90 (12) | C17Y—C16Y—H16E | 108.8 |
| O2A—C1A—C2A | 117.68 (11) | C15Y—C16Y—H16E | 108.8 |
| O1C—C1C—O2C | 122.79 (12) | C16Y—C17Y—H17I | 120.0 |
| O1C—C1C—C2C | 119.71 (12) | C16Y—C17Y—H17J | 120.0 |
| O2C—C1C—C2C | 117.50 (11) | H17I—C17Y—H17J | 120.0 |
| C7B—C8B—C9B | 120.08 (13) | C14C—C15Z—C16Z | 114.7 (11) |
| C7B—C8B—H8BA | 120.0 | C14C—C15Z—H15K | 108.6 |
| C9B—C8B—H8BA | 120.0 | C16Z—C15Z—H15K | 108.6 |
| C6A—C5A—C4A | 121.02 (13) | C14C—C15Z—H15L | 108.6 |
| C6A—C5A—H5AA | 119.5 | C16Z—C15Z—H15L | 108.6 |
| C4A—C5A—H5AA | 119.5 | H15K—C15Z—H15L | 107.6 |
| O1B—C1B—O2B | 122.96 (11) | C17Z—C16Z—C15Z | 111.5 (10) |

| | | | |
|---|---|---|---|
| O1B—C1B—C2B | 119.68 (12) | C17Z—C16Z—H16F | 124.3 |
| O2B—C1B—C2B | 117.36 (11) | C15Z—C16Z—H16F | 124.3 |
| C7C—C8C—C9C | 120.19 (12) | C16Z—C17Z—H17K | 120.0 |
| C7C—C8C—H8CA | 119.9 | C16Z—C17Z—H17L | 120.0 |
| C9C—C8C—H8CA | 119.9 | H17K—C17Z—H17L | 120.0 |
| | | | |
| C3B—C2B—C11B—C10B | 1.7 (2) | C3C—C2C—C1C—O1C | −179.67 (11) |
| C1B—C2B—C11B—C10B | −178.59 (11) | C11C—C2C—C1C—O1C | 0.63 (19) |
| C8B—C9B—C4B—C3B | −179.12 (10) | C3C—C2C—C1C—O2C | −0.28 (19) |
| C10B—C9B—C4B—C3B | 1.80 (19) | C11C—C2C—C1C—O2C | −179.98 (11) |
| C8B—C9B—C4B—C5B | 1.64 (19) | O3B—C7B—C8B—C9B | 179.10 (12) |
| C10B—C9B—C4B—C5B | −177.44 (11) | C6B—C7B—C8B—C9B | −1.0 (2) |
| C10C—C11C—C2C—C3C | 1.3 (2) | C10B—C9B—C8B—C7B | 178.42 (12) |
| C10C—C11C—C2C—C1C | −179.04 (12) | C4B—C9B—C8B—C7B | −0.6 (2) |
| C3A—C2A—C11A—C10A | 0.7 (2) | C7A—C6A—C5A—C4A | −0.4 (2) |
| C1A—C2A—C11A—C10A | −179.50 (12) | C3A—C4A—C5A—C6A | −179.89 (12) |
| C8C—C9C—C4C—C3C | −179.12 (11) | C9A—C4A—C5A—C6A | −0.5 (2) |
| C10C—C9C—C4C—C3C | 1.57 (18) | C3B—C2B—C1B—O1B | −179.09 (11) |
| C8C—C9C—C4C—C5C | 1.91 (19) | C11B—C2B—C1B—O1B | 1.21 (19) |
| C10C—C9C—C4C—C5C | −177.40 (11) | C3B—C2B—C1B—O2B | 0.80 (19) |
| O3B—C7B—C6B—C5B | −178.51 (12) | C11B—C2B—C1B—O2B | −178.90 (11) |
| C8B—C7B—C6B—C5B | 1.5 (2) | O3C—C7C—C8C—C9C | 178.08 (11) |
| O3C—C7C—C6C—C5C | −177.60 (12) | C6C—C7C—C8C—C9C | −2.0 (2) |
| C8C—C7C—C6C—C5C | 2.5 (2) | C10C—C9C—C8C—C7C | 179.09 (12) |
| C8B—C7B—O3B—C12B | 0.9 (2) | C4C—C9C—C8C—C7C | −0.2 (2) |
| C6B—C7B—O3B—C12B | −179.03 (12) | C11A—C10A—C9A—C8A | −179.90 (12) |
| O3A—C7A—C6A—C5A | −179.09 (12) | C11A—C10A—C9A—C4A | −0.7 (2) |
| C8A—C7A—C6A—C5A | 0.9 (2) | C3A—C4A—C9A—C8A | −179.73 (11) |
| C11C—C2C—C3C—C4C | −0.40 (19) | C5A—C4A—C9A—C8A | 0.88 (19) |
| C1C—C2C—C3C—C4C | 179.90 (10) | C3A—C4A—C9A—C10A | 1.07 (18) |
| C5C—C4C—C3C—C2C | 177.91 (12) | C5A—C4A—C9A—C10A | −178.32 (11) |
| C9C—C4C—C3C—C2C | −1.01 (19) | C7C—O3C—C12C—C13C | −175.46 (11) |
| C8C—C7C—O3C—C12C | −2.2 (2) | C14C—C13C—C12C—O3C | −175.34 (12) |
| C6C—C7C—O3C—C12C | 177.91 (12) | C7A—O3A—C12A—C13A | −173.54 (12) |
| C11B—C2B—C3B—C4B | −0.8 (2) | C14A—C13A—C12A—O3A | −177.02 (13) |
| C1B—C2B—C3B—C4B | 179.53 (10) | C7B—O3B—C12B—C13B | −177.49 (12) |
| C5B—C4B—C3B—C2B | 178.22 (11) | C14B—C13B—C12B—O3B | −175.95 (12) |
| C9B—C4B—C3B—C2B | −1.00 (19) | O3A—C7A—C8A—C9A | 179.48 (12) |
| C11A—C2A—C3A—C4A | −0.34 (19) | C6A—C7A—C8A—C9A | −0.6 (2) |
| C1A—C2A—C3A—C4A | 179.86 (11) | C10A—C9A—C8A—C7A | 178.81 (12) |
| C5A—C4A—C3A—C2A | 178.82 (11) | C4A—C9A—C8A—C7A | −0.3 (2) |
| C9A—C4A—C3A—C2A | −0.55 (19) | C12C—C13C—C14C—C15Z | 179.2 (9) |
| C2B—C11B—C10B—C9B | −0.9 (2) | C12C—C13C—C14C—C15C | 176.5 (3) |
| C8B—C9B—C10B—C11B | −179.95 (12) | C12B—C13B—C14B—C15B | 178.4 (3) |
| C4B—C9B—C10B—C11B | −0.9 (2) | C12B—C13B—C14B—C15Y | 178.6 (5) |
| C8A—C7A—O3A—C12A | −3.8 (2) | C13A—C14A—C15A—C16A | −172.6 (3) |
| C6A—C7A—O3A—C12A | 176.22 (12) | C15X—C14A—C15A—C16A | 180 (3) |
| C2C—C11C—C10C—C9C | −0.7 (2) | C14A—C15A—C16A—C17A | −125.5 (5) |

| | | | |
|---|---|---|---|
| C8C—C9C—C10C—C11C | 179.97 (12) | C13B—C14B—C15B—C16B | −171.1 (3) |
| C4C—C9C—C10C—C11C | −0.7 (2) | C15Y—C14B—C15B—C16B | −172 (4) |
| C2A—C11A—C10A—C9A | −0.2 (2) | C14B—C15B—C16B—C17B | −123.6 (5) |
| C7B—C6B—C5B—C4B | −0.5 (2) | C15Z—C14C—C15C—C16C | 77 (17) |
| C3B—C4B—C5B—C6B | 179.68 (12) | C13C—C14C—C15C—C16C | −163.7 (4) |
| C9B—C4B—C5B—C6B | −1.1 (2) | C14C—C15C—C16C—C17C | −126.8 (5) |
| C7C—C6C—C5C—C4C | −0.7 (2) | C15A—C14A—C15X—C16X | −12 (2) |
| C3C—C4C—C5C—C6C | 179.59 (12) | C13A—C14A—C15X—C16X | 175.0 (9) |
| C9C—C4C—C5C—C6C | −1.5 (2) | C14A—C15X—C16X—C17X | −33 (3) |
| C15A—C14A—C13A—C12A | 179.8 (2) | C15B—C14B—C15Y—C16Y | 2 (3) |
| C15X—C14A—C13A—C12A | −178.2 (6) | C13B—C14B—C15Y—C16Y | −177.2 (10) |
| C3A—C2A—C1A—O1A | 179.96 (12) | C14B—C15Y—C16Y—C17Y | −83 (4) |
| C11A—C2A—C1A—O1A | 0.2 (2) | C13C—C14C—C15Z—C16Z | 164.4 (9) |
| C3A—C2A—C1A—O2A | −0.32 (19) | C15C—C14C—C15Z—C16Z | −134 (18) |
| C11A—C2A—C1A—O2A | 179.88 (11) | C14C—C15Z—C16Z—C17Z | 110.9 (13) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2*A*—H1···O1*C*$^{i}$ | 0.97 | 1.65 | 2.6150 (16) | 174 |
| O2*B*—H2···O1*B*$^{ii}$ | 0.85 | 1.80 | 2.6342 (15) | 168 |
| O2*C*—H3···O1*A*$^{i}$ | 0.93 | 1.69 | 2.6133 (16) | 177 |
| C6*A*—H6*AA*···O1*A*$^{iii}$ | 0.93 | 2.50 | 3.3032 (19) | 144 |
| C6*B*—H6*BA*···O1*B*$^{iii}$ | 0.93 | 2.56 | 3.3666 (19) | 145 |
| C6*C*—H6*CA*···O1*C*$^{iii}$ | 0.93 | 2.56 | 3.3547 (18) | 144 |
| C5*A*—H5*AA*···O2*C*$^{iv}$ | 0.93 | 2.59 | 3.421 (2) | 149 |
| C5*B*—H5*BA*···O2*B*$^{v}$ | 0.93 | 2.65 | 3.520 (2) | 156 |
| C5*C*—H5*CA*···O2*A*$^{iv}$ | 0.93 | 2.61 | 3.472 (2) | 154 |
| C17*B*—H17*C*···*Cg*1$^{vi}$ | 0.93 | 2.93 | 3.736 (5) | 146 |

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+1; (ii) −*x*+3, −*y*+2, −*z*; (iii) *x*−1, *y*, *z*; (iv) −*x*+1, −*y*+2, −*z*+1; (v) −*x*+2, −*y*+2, −*z*; (vi) −*x*+1, −*y*+1, −*z*+1.