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# (1*E*,4*E*)-1,5-Bis(2,4,5-trimethoxyphenyl)-penta-1,4-dien-3-one[1]

**Hoong-Kun Fun,[a]*§ Pumsak Ruanwas[b] and Suchada Chantrapromma[b]¶**

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [b]Crystal Materials Research Unit, Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand
Correspondence e-mail: hkfun@usm.my

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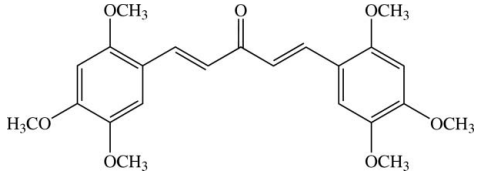
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.067; $wR$ factor = 0.150; data-to-parameter ratio = 22.2.

There are three molecules in the asymmetric unit of the title compound, $C_{23}H_{26}O_7$, in which the dihedral angles between two benzene rings are 4.34 (9), 18.11 (8) and 8.54 (8)°. The central penta-1,4-dien-3-one fragment makes dihedral angles of 3.95 (9) and 3.32 (16)° with the two adjacent benzene rings in one molecule, whereas the corresponding pairs of angles in the other two molecules are 10.34 (9)/17.46 (8)° and 7.87 (8)/13.33 (8)°. In the crystal, molecules are linked by intermolecular C—H···O and C—H···$\pi$ weak interactions into a three-dimensional network. Finally, $\pi$–$\pi$ interactions [centroid···centroid distances = 3.5984 (10) and 3.5545 (10) Å] are observed.

## Related literature

For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For a related structure, see: Harrison *et al.* (2006). For background to and applications of chalcones, see: Baeyer & von Villiger (1902); Gomes *et al.* (2009); Gould *et al.* (1995); Masuda *et al.* (1993); Quincoces *et al.* (2002; 2003; 2008); Uchida *et al.* (1998). For the stability of the temperature controller, see: Cosier & Glazer, (1986).




## Experimental

### Crystal data

$C_{23}H_{26}O_7$
$M_r$ = 414.44
Monoclinic, $P2_1/c$
$a$ = 9.4157 (1) Å
$b$ = 36.8613 (5) Å
$c$ = 19.1226 (3) Å
$\beta$ = 107.737 (1)°
$V$ = 6321.49 (15) Å$^3$
$Z$ = 12
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 100 K
0.37 × 0.22 × 0.13 mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.965, $T_{max}$ = 0.988
81495 measured reflections
18387 independent reflections
12498 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.046

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.150
$S$ = 1.06
18387 reflections
829 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

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

*Cg*3 and *Cg*4 are the centroids of the C1*C*–C6*C* and C12*C*–C17*C* rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C10*B*—H10*B*···O1*C*$^{i}$ | 0.93 | 2.29 | 3.149 (2) | 153 |
| C10*C*—H10*C*···O1*B* | 0.93 | 2.33 | 3.195 (2) | 155 |
| C14*B*—H14*B*···O1*A*$^{ii}$ | 0.93 | 2.52 | 3.353 (2) | 149 |
| C21*A*—H21*B*···O3*A*$^{iii}$ | 0.96 | 2.49 | 3.301 (2) | 142 |
| C22*A*—H22*C*···O7*C*$^{iv}$ | 0.96 | 2.50 | 3.435 (2) | 165 |
| C22*B*—H22*D*···O2*A*$^{v}$ | 0.96 | 2.50 | 3.407 (2) | 158 |
| C22*B*—H22*F*···O1*A*$^{ii}$ | 0.96 | 2.58 | 3.227 (2) | 125 |
| C23*A*—H23*A*···O5*A*$^{i}$ | 0.96 | 2.52 | 3.308 (2) | 140 |
| C23*A*—H23*C*···O3*C* | 0.96 | 2.53 | 3.452 (2) | 161 |
| C23*C*—H23*G*···O5*C*$^{i}$ | 0.96 | 2.54 | 3.305 (2) | 136 |
| C18*C*—H18*H*···*Cg*4$^{ii}$ | 0.96 | 2.80 | 3.678 (2) | 152 |
| C20*A*—H20*B*···*Cg*3$^{vi}$ | 0.96 | 2.94 | 3.855 (2) | 159 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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[1] This paper is dedicated to His Majesty King Bhumibol Adulyadej of Thailand (King Rama IX) for his sustainable development of the country.
§ Thomson Reuters ResearcherID: A-3561-2009.
¶ Additional correspondence author, e-mail: suchada.c@psu.ac.th. Thomson Reuters ResearcherID: A-5085-2009.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5282).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, o307-o308 [ **doi:10.1107/S1600536809055421** ]

# (1*E*,4*E*)-1,5-Bis(2,4,5-trimethoxyphenyl)penta-1,4-dien-3-one

**H.-K. Fun, P. Ruanwas and S. Chantrapromma**

## Comment

Bischalcones with the general formula Ar—CH=CH—CO—CH=CH—Ar (Baeyer & Villiger, 1902) are an important class of compounds because they are widely used in many fields such as in organic solid-state photochemistry (Gould *et al.*, 1995), anti-oxidative and anti-inflammatory activities (Masuda *et al.*, 1993), cytotoxicity (Quincoces *et al.*, 2002; 2003; 2008) and activities involving their non-linear optical (Uchida *et al.*, 1998) and fluorescence properties (Gomes *et al.*, 2009). However not much crystal structures of this type of compound were reported. The title bischalcone (I) was synthesized on the account of its fluorescence property which will be reported elsewhere together with the other bichalcone derivatives. We reported herein the crystal structure of (I).

There are three crystallographic independent molecules *A*, *B* and *C* in the asymmetric unit of (I) (Fig. 1) with slight differences in bond angles. The molecular structure of (I), $C_{23}H_{26}O_7$, is not planar. The dihedral angle between the C1–C6 and C12–C17 benzene rings is 4.34 (9)° in molecule *A* whereas its is 18.11 (8) and 8.54 (8)° in molecules *B* and *C*, respectively. The central penta-1,4-dien-3-one fragment (C7–C11/O1) is planar with the r.m.s. 0.0204 (2) Å for molecule *A* [0.0227 (2) and 0.0252 (2) Å for molecule *B* and *C*, respectively]. This fragment makes the dihedral angles of 3.95 (9) and 3.32 (16)° with the two adjacent C1–C6 and C12–C17 benzene rings, respectively in molecule *A* whereas the corresponding values are 10.34 (9) and 17.46 (8)° in molecule *B*; and 7.87 (8) and 13.33 (8)° in the molecule *C*. The three methoxy groups on C1–C6 benzene ring are essentially planarly attached [C18–O2–C1–C2, C19–O3–C3–C2 and C20–O4–C4–C5 torsion angles of -3.7 (2), 1.4 (3) and -3.9 (2)° in molecule *A*; -0.2 (3), 3.5 (3) and -1.7 (2)° in molecule *B*; 3.8 (3), 4.4 (3) and -4.3 (3)° in molecule *C*]. The middle methoxy group of the 2,4,5-trimethoxyphenyl moeity is co-planar with the C12–C17 benzene ring, with the C22–O6–C15–C14 torsion angle being 1.1 (3)° whereas the other two methoxy groups are twisted with the torsion angles C21–O5–C13–C14 and C23–O7–C16–C17 being -111.48 (18) and -14.4 (3)°, respectively in molecule *A* [the three corresponding values are -7.6 (3), -30.2 (2) and 9.6 (2)° in molecule *B* and 0.4 (3), 73.5 (2) and -8.2 (3)° in molecule *C*]. Intramolecular C—H···O weak interactions (Table 1) generate S(5) ring motifs (Bernstein *et al.*, 1995). The bond distances agree with the literature values (Allen *et al.*, 1987) and are comparable with the related structure (Harrison *et al.*, 2006).

In the crystal packing (Fig. 2), the molecules are linked by intermolecular C—H···O weak interactions (Table 1) into a supramolecular three-dimensional network. The crystal is stabilized by intra- and intermolecular C—H···O weak interactions and C—H···π interactions (Table 1). π–π interactions were observed with the distances of $Cg_1\cdots Cg_4$ = 3.5984 (10) Å (symmetry code: *x*, *y*, *z*) and $Cg_2\cdots Cg_5$ = 3.5984 (10) Å (symmetry code: 1 + *x*, 3/2 - *y*, 1/2 + *z*); $Cg_1$, $Cg_2$, $Cg_3$, $Cg_4$ and $Cg_5$ are the centroids of C12A–C17A, C1B–C6B, C12B–C17B, C1C–C6C and C12C–C17B rings, respectively.

## Experimental

The title compound was synthesized by dissolving 2,4,5-trimethoxybenzaldehyde (0.5 g, 4.85 mmol) in acetone (50 ml). NaOH 50% aqueous solution (2 ml) was then added. After stirring at room temperature for 1 hr, the resulting orange solid

was collected by filtration, washed with distilled water and dried. Pale yellow blocks of (I) were recrystalized from acetone/ethanol (1:1 *v*/*v*) by the slow evaporation of the solvent at room temperature after a week, Mp. 441–442 K.

### Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å for aromatic and CH; 0.96 Å for $CH_3$ atoms. The $U_{iso}$ values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual electron density peak is 0.71 Å from C12C and the deepest hole is 0.45 Å from C9A.

### Figures

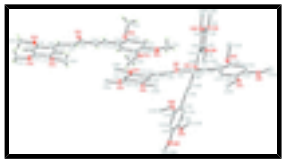

Fig. 1. The molecular structure of (I) showing 50% probability displacement ellipsoids. H atoms of molecules *B* and *C* are omitted for clarity.

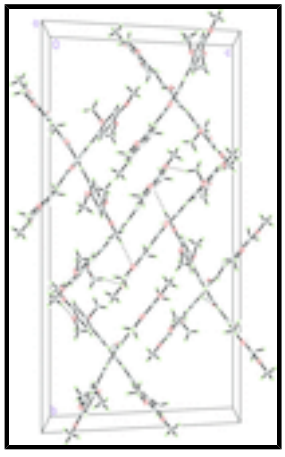

Fig. 2. The crystal packing of (I) viewed along the *a* axis, showing the three-dimensional network. Hydrogen bonds are shown as dashed lines.

### (1*E*,4*E*)-1,5-Bis(2,4,5-trimethoxyphenyl)penta-1,4-dien-3-one

*Crystal data*

| | |
|---|---|
| $C_{23}H_{26}O_7$ | $F(000) = 2640$ |
| $M_r = 414.44$ | $D_x = 1.306$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Melting point = 441–442 K |
| Hall symbol: -P 2ybc | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 9.4157$ (1) Å | Cell parameters from 18387 reflections |
| $b = 36.8613$ (5) Å | $\theta = 1.1$–$30.0°$ |
| $c = 19.1226$ (3) Å | $\mu = 0.10$ mm$^{-1}$ |
| $\beta = 107.737$ (1)° | $T = 100$ K |
| $V = 6321.49$ (15) Å$^3$ | Block, colorless |
| $Z = 12$ | 0.37 × 0.22 × 0.13 mm |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 18387 independent reflections |
| Radiation source: sealed tube | 12498 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.046$ |
| phi and ω scans | $\theta_{max} = 30.0°$, $\theta_{min} = 1.1°$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2005) | $h = -13\rightarrow13$ |
| $T_{min} = 0.965$, $T_{max} = 0.988$ | $k = -45\rightarrow51$ |
| 81495 measured reflections | $l = -26\rightarrow26$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.067$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.150$ | H-atom parameters constrained |
| $S = 1.06$ | $w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 4.2947P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 18387 reflections | $(\Delta/\sigma)_{max} = 0.002$ |
| 829 parameters | $\Delta\rho_{max} = 0.38$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.25$ e Å$^{-3}$ |

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1A | 0.61853 (14) | 0.99343 (4) | 0.88798 (8) | 0.0259 (3) |
| O2A | 0.77349 (15) | 1.09843 (4) | 1.05130 (7) | 0.0262 (3) |
| O3A | 1.27431 (15) | 1.14769 (4) | 1.10886 (7) | 0.0279 (3) |
| O4A | 1.34759 (15) | 1.09825 (4) | 1.03136 (7) | 0.0274 (3) |

| | | | | |
|---|---|---|---|---|
| O5A | 0.47925 (14) | 0.89473 (3) | 0.70474 (7) | 0.0242 (3) |
| O6A | 0.83737 (14) | 0.84534 (3) | 0.59545 (7) | 0.0238 (3) |
| O7A | 1.03708 (14) | 0.89136 (4) | 0.66503 (8) | 0.0257 (3) |
| C1A | 0.9167 (2) | 1.09853 (5) | 1.04751 (10) | 0.0203 (4) |
| C2A | 1.0225 (2) | 1.12410 (5) | 1.08416 (10) | 0.0225 (4) |
| H2AA | 0.9977 | 1.1416 | 1.1134 | 0.027* |
| C3A | 1.1646 (2) | 1.12340 (5) | 1.07698 (10) | 0.0218 (4) |
| C4A | 1.2038 (2) | 1.09658 (5) | 1.03338 (10) | 0.0212 (4) |
| C5A | 1.0980 (2) | 1.07165 (5) | 0.99736 (10) | 0.0198 (4) |
| H5AA | 1.1233 | 1.0542 | 0.9681 | 0.024* |
| C6A | 0.95201 (19) | 1.07169 (5) | 1.00345 (9) | 0.0189 (3) |
| C7A | 0.84093 (19) | 1.04502 (5) | 0.96501 (9) | 0.0191 (3) |
| H7AA | 0.7457 | 1.0472 | 0.9695 | 0.023* |
| C8A | 0.86455 (19) | 1.01757 (5) | 0.92372 (9) | 0.0184 (3) |
| H8AA | 0.9607 | 1.0138 | 0.9214 | 0.022* |
| C9A | 0.74500 (19) | 0.99314 (5) | 0.88200 (9) | 0.0182 (3) |
| C10A | 0.78751 (19) | 0.96863 (5) | 0.83046 (10) | 0.0193 (3) |
| H10A | 0.8828 | 0.9706 | 0.8260 | 0.023* |
| C11A | 0.69497 (19) | 0.94367 (5) | 0.78996 (10) | 0.0190 (3) |
| H11A | 0.5998 | 0.9424 | 0.7949 | 0.023* |
| C12A | 0.72921 (19) | 0.91817 (5) | 0.73880 (9) | 0.0180 (3) |
| C13A | 0.62264 (18) | 0.89351 (5) | 0.69924 (10) | 0.0192 (3) |
| C14A | 0.65461 (19) | 0.86840 (5) | 0.65119 (10) | 0.0201 (4) |
| H14A | 0.5822 | 0.8519 | 0.6260 | 0.024* |
| C15A | 0.79434 (19) | 0.86815 (5) | 0.64133 (10) | 0.0191 (3) |
| C16A | 0.90353 (19) | 0.89331 (5) | 0.67985 (10) | 0.0191 (3) |
| C17A | 0.87092 (19) | 0.91748 (5) | 0.72729 (10) | 0.0191 (3) |
| H17A | 0.9437 | 0.9338 | 0.7526 | 0.023* |
| C18A | 0.7343 (2) | 1.12439 (6) | 1.09820 (11) | 0.0297 (4) |
| H18A | 0.6322 | 1.1209 | 1.0964 | 0.045* |
| H18B | 0.7469 | 1.1485 | 1.0819 | 0.045* |
| H18C | 0.7976 | 1.1212 | 1.1477 | 0.045* |
| C19A | 1.2386 (2) | 1.17568 (5) | 1.15221 (11) | 0.0315 (5) |
| H19A | 1.3210 | 1.1922 | 1.1683 | 0.047* |
| H19B | 1.2186 | 1.1651 | 1.1942 | 0.047* |
| H19C | 1.1520 | 1.1886 | 1.1233 | 0.047* |
| C20A | 1.3885 (2) | 1.07307 (6) | 0.98420 (12) | 0.0319 (5) |
| H20A | 1.4908 | 1.0769 | 0.9867 | 0.048* |
| H20B | 1.3260 | 1.0766 | 0.9346 | 0.048* |
| H20C | 1.3762 | 1.0488 | 0.9995 | 0.048* |
| C21A | 0.4405 (2) | 0.86423 (5) | 0.74166 (11) | 0.0258 (4) |
| H21A | 0.3344 | 0.8636 | 0.7323 | 0.039* |
| H21B | 0.4888 | 0.8664 | 0.7935 | 0.039* |
| H21C | 0.4723 | 0.8423 | 0.7239 | 0.039* |
| C22A | 0.7279 (2) | 0.82026 (5) | 0.55365 (11) | 0.0271 (4) |
| H22A | 0.7709 | 0.8055 | 0.5240 | 0.041* |
| H22B | 0.6445 | 0.8334 | 0.5225 | 0.041* |
| H22C | 0.6949 | 0.8051 | 0.5864 | 0.041* |
| C23A | 1.1351 (2) | 0.92146 (5) | 0.68810 (12) | 0.0271 (4) |

| | | | | |
|---|---|---|---|---|
| H23A | 1.2172 | 0.9192 | 0.6685 | 0.041* |
| H23B | 1.1720 | 0.9220 | 0.7407 | 0.041* |
| H23C | 1.0821 | 0.9435 | 0.6706 | 0.041* |
| O1B | 0.67886 (14) | 0.79921 (4) | 0.36869 (8) | 0.0296 (3) |
| O2B | 0.90239 (14) | 0.70489 (4) | 0.53331 (8) | 0.0273 (3) |
| O3B | 1.41632 (14) | 0.66614 (4) | 0.58013 (7) | 0.0267 (3) |
| O4B | 1.45884 (14) | 0.71537 (4) | 0.49398 (8) | 0.0297 (3) |
| O5B | 0.52194 (14) | 0.92198 (3) | 0.26449 (7) | 0.0223 (3) |
| O6B | 0.84488 (14) | 0.99180 (3) | 0.15955 (7) | 0.0236 (3) |
| O7B | 1.04120 (13) | 0.94003 (3) | 0.19064 (7) | 0.0213 (3) |
| C1B | 1.04099 (19) | 0.70706 (5) | 0.52494 (10) | 0.0201 (4) |
| C2B | 1.1587 (2) | 0.68375 (5) | 0.56056 (10) | 0.0202 (4) |
| H2BA | 1.1447 | 0.6659 | 0.5921 | 0.024* |
| C3B | 1.2953 (2) | 0.68751 (5) | 0.54854 (10) | 0.0209 (4) |
| C4B | 1.3190 (2) | 0.71448 (5) | 0.50116 (10) | 0.0220 (4) |
| C5B | 1.20241 (19) | 0.73714 (5) | 0.46616 (10) | 0.0204 (4) |
| H5BA | 1.2170 | 0.7549 | 0.4346 | 0.024* |
| C6B | 1.06154 (19) | 0.73390 (5) | 0.47726 (10) | 0.0191 (3) |
| C7B | 0.93671 (19) | 0.75743 (5) | 0.44029 (10) | 0.0195 (3) |
| H7BA | 0.8464 | 0.7524 | 0.4486 | 0.023* |
| C8B | 0.93721 (19) | 0.78538 (5) | 0.39580 (10) | 0.0201 (4) |
| H8BA | 1.0248 | 0.7913 | 0.3856 | 0.024* |
| C9B | 0.80148 (18) | 0.80706 (5) | 0.36257 (10) | 0.0183 (3) |
| C10B | 0.82631 (19) | 0.83942 (5) | 0.32294 (10) | 0.0199 (4) |
| H10B | 0.9200 | 0.8424 | 0.3169 | 0.024* |
| C11B | 0.72314 (18) | 0.86483 (5) | 0.29492 (9) | 0.0170 (3) |
| H11B | 0.6277 | 0.8612 | 0.2983 | 0.020* |
| C12B | 0.75129 (18) | 0.89799 (4) | 0.25939 (9) | 0.0154 (3) |
| C13B | 0.64957 (18) | 0.92681 (5) | 0.24499 (9) | 0.0164 (3) |
| C14B | 0.67679 (19) | 0.95861 (5) | 0.21126 (10) | 0.0183 (3) |
| H14B | 0.6070 | 0.9773 | 0.2009 | 0.022* |
| C15B | 0.80799 (19) | 0.96226 (5) | 0.19337 (9) | 0.0170 (3) |
| C16B | 0.91373 (18) | 0.93376 (5) | 0.20913 (9) | 0.0169 (3) |
| C17B | 0.88319 (18) | 0.90239 (5) | 0.24028 (9) | 0.0171 (3) |
| H17B | 0.9517 | 0.8835 | 0.2490 | 0.021* |
| C18B | 0.8747 (2) | 0.67823 (5) | 0.58179 (11) | 0.0277 (4) |
| H18D | 0.7715 | 0.6790 | 0.5795 | 0.042* |
| H18E | 0.9356 | 0.6832 | 0.6311 | 0.042* |
| H18F | 0.8985 | 0.6546 | 0.5674 | 0.042* |
| C19B | 1.3972 (2) | 0.63691 (5) | 0.62517 (11) | 0.0271 (4) |
| H19D | 1.4889 | 0.6236 | 0.6429 | 0.041* |
| H19E | 1.3200 | 0.6211 | 0.5969 | 0.041* |
| H19F | 1.3698 | 0.6463 | 0.6660 | 0.041* |
| C20B | 1.4894 (2) | 0.74387 (6) | 0.45006 (13) | 0.0386 (5) |
| H20D | 1.5918 | 0.7426 | 0.4510 | 0.058* |
| H20E | 1.4711 | 0.7669 | 0.4692 | 0.058* |
| H20F | 1.4258 | 0.7413 | 0.4004 | 0.058* |
| C21B | 0.4564 (2) | 0.95365 (5) | 0.28354 (11) | 0.0254 (4) |
| H21D | 0.3852 | 0.9469 | 0.3080 | 0.038* |

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|---|---|---|---|---|
| H21E | 0.4070 | 0.9671 | 0.2398 | 0.038* |
| H21F | 0.5326 | 0.9685 | 0.3157 | 0.038* |
| C22B | 0.7315 (2) | 1.01884 (5) | 0.13343 (12) | 0.0280 (4) |
| H22D | 0.7693 | 1.0381 | 0.1103 | 0.042* |
| H22E | 0.7033 | 1.0284 | 0.1740 | 0.042* |
| H22F | 0.6461 | 1.0081 | 0.0985 | 0.042* |
| C23B | 1.1362 (2) | 0.90947 (5) | 0.19467 (11) | 0.0255 (4) |
| H23D | 1.2174 | 0.9161 | 0.1768 | 0.038* |
| H23E | 1.0804 | 0.8901 | 0.1652 | 0.038* |
| H23F | 1.1747 | 0.9016 | 0.2447 | 0.038* |
| O1C | 0.17116 (13) | 0.85328 (4) | 0.35904 (7) | 0.0250 (3) |
| O2C | 0.36440 (14) | 0.94816 (3) | 0.52907 (7) | 0.0225 (3) |
| O3C | 0.88225 (14) | 0.98683 (3) | 0.59876 (7) | 0.0230 (3) |
| O4C | 0.93952 (13) | 0.93975 (3) | 0.51207 (7) | 0.0228 (3) |
| O5C | 0.00738 (14) | 0.74097 (3) | 0.20661 (7) | 0.0238 (3) |
| O6C | 0.33553 (14) | 0.68688 (3) | 0.08487 (7) | 0.0235 (3) |
| O7C | 0.54343 (14) | 0.73320 (4) | 0.14497 (8) | 0.0269 (3) |
| C1C | 0.50778 (18) | 0.94655 (5) | 0.52632 (9) | 0.0174 (3) |
| C2C | 0.62239 (19) | 0.96902 (5) | 0.56811 (9) | 0.0182 (3) |
| H2CA | 0.6031 | 0.9860 | 0.6000 | 0.022* |
| C3C | 0.76404 (19) | 0.96585 (5) | 0.56170 (9) | 0.0176 (3) |
| C4C | 0.79536 (18) | 0.94012 (5) | 0.51384 (10) | 0.0178 (3) |
| C5C | 0.68220 (18) | 0.91813 (5) | 0.47306 (9) | 0.0168 (3) |
| H5CA | 0.7024 | 0.9012 | 0.4413 | 0.020* |
| C6C | 0.53558 (18) | 0.92067 (4) | 0.47832 (9) | 0.0163 (3) |
| C7C | 0.41633 (18) | 0.89700 (4) | 0.43687 (9) | 0.0165 (3) |
| H7CA | 0.3206 | 0.9029 | 0.4374 | 0.020* |
| C8C | 0.42894 (18) | 0.86764 (4) | 0.39794 (9) | 0.0164 (3) |
| H8CA | 0.5230 | 0.8606 | 0.3967 | 0.020* |
| C9C | 0.29764 (18) | 0.84615 (4) | 0.35702 (9) | 0.0157 (3) |
| C10C | 0.32957 (18) | 0.81622 (5) | 0.31329 (9) | 0.0178 (3) |
| H10C | 0.4278 | 0.8127 | 0.3141 | 0.021* |
| C11C | 0.22491 (18) | 0.79370 (5) | 0.27220 (9) | 0.0168 (3) |
| H11C | 0.1277 | 0.7966 | 0.2735 | 0.020* |
| C12C | 0.25297 (18) | 0.76502 (5) | 0.22576 (9) | 0.0167 (3) |
| C13C | 0.14380 (18) | 0.73940 (5) | 0.19315 (9) | 0.0180 (3) |
| C14C | 0.16725 (19) | 0.71267 (5) | 0.14619 (10) | 0.0197 (3) |
| H14C | 0.0928 | 0.6958 | 0.1254 | 0.024* |
| C15C | 0.30085 (19) | 0.71122 (5) | 0.13060 (10) | 0.0191 (3) |
| C16C | 0.41492 (19) | 0.73680 (5) | 0.16373 (10) | 0.0196 (4) |
| C17C | 0.38995 (19) | 0.76270 (5) | 0.20996 (10) | 0.0196 (4) |
| H17C | 0.4652 | 0.7792 | 0.2316 | 0.023* |
| C18C | 0.3321 (2) | 0.97249 (5) | 0.58045 (10) | 0.0225 (4) |
| H18G | 0.2274 | 0.9717 | 0.5750 | 0.034* |
| H18H | 0.3597 | 0.9967 | 0.5714 | 0.034* |
| H18I | 0.3876 | 0.9654 | 0.6295 | 0.034* |
| C19C | 0.8569 (2) | 1.01450 (5) | 0.64584 (11) | 0.0271 (4) |
| H19G | 0.9477 | 1.0277 | 0.6674 | 0.041* |
| H19H | 0.8244 | 1.0036 | 0.6839 | 0.041* |

| | | | | |
|---|---|---|---|---|
| H19I | 0.7815 | 1.0308 | 0.6178 | 0.041* |
| C20C | 0.9770 (2) | 0.91258 (6) | 0.46759 (12) | 0.0299 (4) |
| H20G | 1.0814 | 0.9141 | 0.4724 | 0.045* |
| H20H | 0.9197 | 0.9163 | 0.4172 | 0.045* |
| H20I | 0.9552 | 0.8890 | 0.4832 | 0.045* |
| C21C | −0.0131 (2) | 0.71272 (6) | 0.25332 (12) | 0.0330 (5) |
| H21G | −0.1110 | 0.7146 | 0.2587 | 0.049* |
| H21H | 0.0604 | 0.7149 | 0.3006 | 0.049* |
| H21I | −0.0026 | 0.6896 | 0.2322 | 0.049* |
| C22C | 0.2219 (2) | 0.66088 (5) | 0.05013 (11) | 0.0283 (4) |
| H22G | 0.2587 | 0.6449 | 0.0200 | 0.042* |
| H22H | 0.1352 | 0.6734 | 0.0202 | 0.042* |
| H22I | 0.1960 | 0.6471 | 0.0870 | 0.042* |
| C23C | 0.6505 (2) | 0.76178 (5) | 0.16901 (12) | 0.0302 (5) |
| H23G | 0.7337 | 0.7574 | 0.1511 | 0.045* |
| H23H | 0.6843 | 0.7625 | 0.2217 | 0.045* |
| H23I | 0.6051 | 0.7845 | 0.1504 | 0.045* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1A | 0.0184 (6) | 0.0268 (7) | 0.0349 (8) | −0.0002 (5) | 0.0116 (5) | −0.0028 (6) |
| O2A | 0.0277 (7) | 0.0229 (7) | 0.0320 (8) | 0.0025 (5) | 0.0152 (6) | −0.0038 (6) |
| O3A | 0.0293 (7) | 0.0241 (7) | 0.0269 (7) | −0.0018 (5) | 0.0033 (6) | −0.0076 (6) |
| O4A | 0.0213 (7) | 0.0316 (8) | 0.0291 (7) | −0.0044 (5) | 0.0072 (5) | −0.0085 (6) |
| O5A | 0.0151 (6) | 0.0236 (7) | 0.0350 (8) | 0.0000 (5) | 0.0092 (5) | 0.0000 (6) |
| O6A | 0.0234 (7) | 0.0235 (7) | 0.0270 (7) | 0.0004 (5) | 0.0112 (5) | −0.0027 (5) |
| O7A | 0.0188 (6) | 0.0252 (7) | 0.0376 (8) | −0.0012 (5) | 0.0155 (6) | −0.0026 (6) |
| C1A | 0.0244 (9) | 0.0181 (9) | 0.0196 (9) | 0.0037 (7) | 0.0084 (7) | 0.0048 (7) |
| C2A | 0.0314 (10) | 0.0172 (9) | 0.0183 (9) | 0.0046 (7) | 0.0069 (7) | 0.0014 (7) |
| C3A | 0.0266 (9) | 0.0181 (9) | 0.0170 (9) | −0.0005 (7) | 0.0010 (7) | 0.0021 (7) |
| C4A | 0.0217 (9) | 0.0228 (9) | 0.0185 (9) | 0.0005 (7) | 0.0054 (7) | 0.0019 (7) |
| C5A | 0.0225 (9) | 0.0186 (9) | 0.0175 (9) | 0.0019 (6) | 0.0051 (7) | 0.0018 (7) |
| C6A | 0.0217 (9) | 0.0173 (9) | 0.0173 (8) | 0.0018 (6) | 0.0054 (7) | 0.0027 (7) |
| C7A | 0.0184 (8) | 0.0195 (9) | 0.0201 (9) | 0.0019 (6) | 0.0071 (7) | 0.0049 (7) |
| C8A | 0.0168 (8) | 0.0174 (8) | 0.0212 (9) | 0.0015 (6) | 0.0060 (6) | 0.0036 (7) |
| C9A | 0.0193 (8) | 0.0154 (8) | 0.0196 (9) | 0.0027 (6) | 0.0058 (6) | 0.0057 (7) |
| C10A | 0.0156 (8) | 0.0211 (9) | 0.0222 (9) | 0.0021 (6) | 0.0072 (6) | 0.0029 (7) |
| C11A | 0.0157 (8) | 0.0190 (9) | 0.0231 (9) | 0.0030 (6) | 0.0070 (6) | 0.0044 (7) |
| C12A | 0.0165 (8) | 0.0181 (9) | 0.0194 (9) | 0.0017 (6) | 0.0053 (6) | 0.0036 (7) |
| C13A | 0.0144 (8) | 0.0190 (9) | 0.0247 (9) | 0.0018 (6) | 0.0065 (6) | 0.0042 (7) |
| C14A | 0.0170 (8) | 0.0200 (9) | 0.0222 (9) | −0.0006 (6) | 0.0045 (7) | 0.0016 (7) |
| C15A | 0.0211 (9) | 0.0180 (9) | 0.0188 (9) | 0.0029 (6) | 0.0069 (7) | 0.0024 (7) |
| C16A | 0.0151 (8) | 0.0199 (9) | 0.0234 (9) | 0.0021 (6) | 0.0076 (6) | 0.0045 (7) |
| C17A | 0.0158 (8) | 0.0183 (9) | 0.0227 (9) | −0.0005 (6) | 0.0052 (6) | 0.0021 (7) |
| C18A | 0.0340 (11) | 0.0280 (11) | 0.0315 (11) | 0.0058 (8) | 0.0165 (9) | −0.0032 (9) |
| C19A | 0.0364 (11) | 0.0216 (10) | 0.0291 (11) | 0.0049 (8) | −0.0010 (8) | −0.0069 (8) |
| C20A | 0.0237 (10) | 0.0398 (12) | 0.0347 (11) | −0.0057 (8) | 0.0124 (8) | −0.0117 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C21A | 0.0184 (9) | 0.0304 (11) | 0.0297 (10) | 0.0001 (7) | 0.0089 (7) | 0.0029 (8) |
| C22A | 0.0307 (10) | 0.0241 (10) | 0.0277 (10) | −0.0030 (8) | 0.0107 (8) | −0.0049 (8) |
| C23A | 0.0157 (9) | 0.0274 (10) | 0.0399 (12) | 0.0005 (7) | 0.0110 (8) | 0.0049 (9) |
| O1B | 0.0167 (6) | 0.0280 (7) | 0.0447 (9) | 0.0014 (5) | 0.0103 (6) | 0.0142 (6) |
| O2B | 0.0206 (7) | 0.0277 (7) | 0.0363 (8) | 0.0024 (5) | 0.0125 (6) | 0.0091 (6) |
| O3B | 0.0198 (6) | 0.0260 (7) | 0.0323 (8) | 0.0043 (5) | 0.0049 (5) | 0.0127 (6) |
| O4B | 0.0185 (7) | 0.0335 (8) | 0.0384 (8) | 0.0035 (5) | 0.0105 (6) | 0.0149 (6) |
| O5B | 0.0175 (6) | 0.0169 (6) | 0.0377 (8) | 0.0012 (5) | 0.0159 (5) | 0.0003 (5) |
| O6B | 0.0194 (6) | 0.0195 (7) | 0.0342 (8) | 0.0009 (5) | 0.0114 (5) | 0.0082 (6) |
| O7B | 0.0169 (6) | 0.0215 (7) | 0.0284 (7) | 0.0008 (5) | 0.0113 (5) | 0.0036 (5) |
| C1B | 0.0194 (8) | 0.0194 (9) | 0.0216 (9) | −0.0014 (6) | 0.0064 (7) | −0.0017 (7) |
| C2B | 0.0233 (9) | 0.0165 (9) | 0.0192 (9) | −0.0012 (6) | 0.0042 (7) | 0.0016 (7) |
| C3B | 0.0201 (9) | 0.0187 (9) | 0.0202 (9) | 0.0022 (6) | 0.0009 (7) | 0.0014 (7) |
| C4B | 0.0174 (8) | 0.0238 (9) | 0.0237 (9) | 0.0004 (7) | 0.0047 (7) | 0.0017 (7) |
| C5B | 0.0208 (9) | 0.0182 (9) | 0.0213 (9) | −0.0011 (6) | 0.0051 (7) | 0.0028 (7) |
| C6B | 0.0188 (8) | 0.0168 (9) | 0.0198 (9) | 0.0007 (6) | 0.0029 (6) | −0.0008 (7) |
| C7B | 0.0158 (8) | 0.0197 (9) | 0.0227 (9) | −0.0006 (6) | 0.0051 (6) | −0.0017 (7) |
| C8B | 0.0150 (8) | 0.0198 (9) | 0.0251 (9) | 0.0013 (6) | 0.0056 (7) | 0.0012 (7) |
| C9B | 0.0154 (8) | 0.0161 (8) | 0.0219 (9) | 0.0005 (6) | 0.0034 (6) | 0.0001 (7) |
| C10B | 0.0118 (8) | 0.0207 (9) | 0.0268 (9) | −0.0015 (6) | 0.0055 (6) | 0.0008 (7) |
| C11B | 0.0131 (8) | 0.0178 (8) | 0.0204 (9) | −0.0025 (6) | 0.0054 (6) | −0.0011 (7) |
| C12B | 0.0143 (8) | 0.0151 (8) | 0.0155 (8) | −0.0016 (6) | 0.0025 (6) | −0.0013 (6) |
| C13B | 0.0126 (7) | 0.0169 (8) | 0.0195 (8) | −0.0030 (6) | 0.0047 (6) | −0.0023 (7) |
| C14B | 0.0169 (8) | 0.0145 (8) | 0.0224 (9) | 0.0011 (6) | 0.0044 (6) | −0.0014 (7) |
| C15B | 0.0179 (8) | 0.0143 (8) | 0.0179 (8) | −0.0024 (6) | 0.0039 (6) | −0.0004 (6) |
| C16B | 0.0132 (8) | 0.0205 (9) | 0.0165 (8) | −0.0018 (6) | 0.0040 (6) | −0.0021 (7) |
| C17B | 0.0139 (8) | 0.0177 (8) | 0.0189 (8) | 0.0010 (6) | 0.0035 (6) | −0.0009 (7) |
| C18B | 0.0292 (10) | 0.0247 (10) | 0.0336 (11) | −0.0028 (8) | 0.0159 (8) | 0.0034 (8) |
| C19B | 0.0267 (10) | 0.0226 (10) | 0.0291 (10) | 0.0047 (7) | 0.0042 (8) | 0.0104 (8) |
| C20B | 0.0231 (10) | 0.0437 (13) | 0.0514 (14) | 0.0011 (9) | 0.0148 (9) | 0.0236 (11) |
| C21B | 0.0282 (10) | 0.0212 (10) | 0.0328 (11) | 0.0048 (7) | 0.0182 (8) | 0.0007 (8) |
| C22B | 0.0249 (10) | 0.0202 (10) | 0.0412 (12) | 0.0035 (7) | 0.0138 (8) | 0.0092 (8) |
| C23B | 0.0186 (9) | 0.0259 (10) | 0.0354 (11) | 0.0047 (7) | 0.0135 (8) | 0.0057 (8) |
| O1C | 0.0131 (6) | 0.0277 (7) | 0.0340 (8) | −0.0007 (5) | 0.0070 (5) | −0.0082 (6) |
| O2C | 0.0175 (6) | 0.0241 (7) | 0.0276 (7) | −0.0011 (5) | 0.0093 (5) | −0.0071 (5) |
| O3C | 0.0173 (6) | 0.0227 (7) | 0.0262 (7) | −0.0032 (5) | 0.0026 (5) | −0.0091 (5) |
| O4C | 0.0134 (6) | 0.0262 (7) | 0.0285 (7) | −0.0025 (5) | 0.0056 (5) | −0.0082 (5) |
| O5C | 0.0167 (6) | 0.0236 (7) | 0.0338 (7) | −0.0039 (5) | 0.0118 (5) | −0.0013 (6) |
| O6C | 0.0228 (7) | 0.0217 (7) | 0.0272 (7) | −0.0021 (5) | 0.0096 (5) | −0.0085 (5) |
| O7C | 0.0189 (6) | 0.0256 (7) | 0.0410 (8) | −0.0032 (5) | 0.0162 (6) | −0.0091 (6) |
| C1C | 0.0152 (8) | 0.0168 (8) | 0.0204 (9) | 0.0004 (6) | 0.0058 (6) | 0.0021 (7) |
| C2C | 0.0189 (8) | 0.0157 (8) | 0.0187 (8) | 0.0002 (6) | 0.0039 (6) | −0.0011 (7) |
| C3C | 0.0181 (8) | 0.0159 (8) | 0.0159 (8) | −0.0013 (6) | 0.0010 (6) | −0.0001 (7) |
| C4C | 0.0139 (8) | 0.0181 (9) | 0.0203 (9) | 0.0001 (6) | 0.0039 (6) | 0.0005 (7) |
| C5C | 0.0148 (8) | 0.0172 (8) | 0.0176 (8) | 0.0000 (6) | 0.0036 (6) | −0.0006 (7) |
| C6C | 0.0156 (8) | 0.0149 (8) | 0.0168 (8) | −0.0009 (6) | 0.0025 (6) | 0.0011 (6) |
| C7C | 0.0137 (7) | 0.0168 (8) | 0.0186 (8) | −0.0001 (6) | 0.0043 (6) | 0.0035 (7) |
| C8C | 0.0118 (7) | 0.0169 (8) | 0.0199 (8) | −0.0004 (6) | 0.0038 (6) | 0.0002 (7) |
| C9C | 0.0149 (8) | 0.0140 (8) | 0.0173 (8) | −0.0008 (6) | 0.0036 (6) | 0.0017 (6) |

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|---|---|---|---|---|---|---|
| C10C | 0.0135 (8) | 0.0174 (8) | 0.0230 (9) | 0.0009 (6) | 0.0062 (6) | 0.0003 (7) |
| C11C | 0.0138 (8) | 0.0171 (8) | 0.0202 (9) | 0.0007 (6) | 0.0060 (6) | 0.0017 (7) |
| C12C | 0.0161 (8) | 0.0158 (8) | 0.0183 (8) | −0.0006 (6) | 0.0054 (6) | 0.0009 (7) |
| C13C | 0.0142 (8) | 0.0191 (9) | 0.0210 (9) | 0.0002 (6) | 0.0058 (6) | 0.0021 (7) |
| C14C | 0.0180 (8) | 0.0167 (9) | 0.0227 (9) | −0.0037 (6) | 0.0035 (7) | −0.0018 (7) |
| C15C | 0.0203 (8) | 0.0175 (9) | 0.0197 (9) | 0.0002 (6) | 0.0063 (7) | −0.0009 (7) |
| C16C | 0.0147 (8) | 0.0199 (9) | 0.0256 (9) | 0.0003 (6) | 0.0081 (7) | 0.0003 (7) |
| C17C | 0.0154 (8) | 0.0188 (9) | 0.0243 (9) | −0.0035 (6) | 0.0057 (7) | −0.0028 (7) |
| C18C | 0.0220 (9) | 0.0237 (10) | 0.0241 (9) | 0.0004 (7) | 0.0107 (7) | −0.0035 (8) |
| C19C | 0.0246 (10) | 0.0252 (10) | 0.0281 (10) | −0.0024 (7) | 0.0028 (8) | −0.0109 (8) |
| C20C | 0.0170 (9) | 0.0371 (12) | 0.0367 (11) | −0.0013 (8) | 0.0096 (8) | −0.0126 (9) |
| C21C | 0.0330 (11) | 0.0345 (12) | 0.0387 (12) | −0.0051 (9) | 0.0217 (9) | 0.0023 (9) |
| C22C | 0.0293 (10) | 0.0265 (10) | 0.0285 (10) | −0.0045 (8) | 0.0079 (8) | −0.0109 (8) |
| C23C | 0.0166 (9) | 0.0306 (11) | 0.0469 (13) | −0.0052 (7) | 0.0150 (8) | −0.0111 (9) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1A—C9A | 1.230 (2) | C11B—C12B | 1.461 (2) |
| O2A—C1A | 1.372 (2) | C11B—H11B | 0.9300 |
| O2A—C18A | 1.435 (2) | C12B—C13B | 1.401 (2) |
| O3A—C3A | 1.363 (2) | C12B—C17B | 1.407 (2) |
| O3A—C19A | 1.427 (2) | C13B—C14B | 1.399 (2) |
| O4A—C4A | 1.367 (2) | C14B—C15B | 1.385 (2) |
| O4A—C20A | 1.426 (2) | C14B—H14B | 0.9300 |
| O5A—C13A | 1.386 (2) | C15B—C16B | 1.415 (2) |
| O5A—C21A | 1.433 (2) | C16B—C17B | 1.371 (2) |
| O6A—C15A | 1.363 (2) | C17B—H17B | 0.9300 |
| O6A—C22A | 1.433 (2) | C18B—H18D | 0.9600 |
| O7A—C16A | 1.373 (2) | C18B—H18E | 0.9600 |
| O7A—C23A | 1.425 (2) | C18B—H18F | 0.9600 |
| C1A—C2A | 1.396 (3) | C19B—H19D | 0.9600 |
| C1A—C6A | 1.403 (2) | C19B—H19E | 0.9600 |
| C2A—C3A | 1.386 (3) | C19B—H19F | 0.9600 |
| C2A—H2AA | 0.9300 | C20B—H20D | 0.9600 |
| C3A—C4A | 1.413 (3) | C20B—H20E | 0.9600 |
| C4A—C5A | 1.376 (2) | C20B—H20F | 0.9600 |
| C5A—C6A | 1.415 (2) | C21B—H21D | 0.9600 |
| C5A—H5AA | 0.9300 | C21B—H21E | 0.9600 |
| C6A—C7A | 1.460 (2) | C21B—H21F | 0.9600 |
| C7A—C8A | 1.343 (2) | C22B—H22D | 0.9600 |
| C7A—H7AA | 0.9300 | C22B—H22E | 0.9600 |
| C8A—C9A | 1.472 (2) | C22B—H22F | 0.9600 |
| C8A—H8AA | 0.9300 | C23B—H23D | 0.9600 |
| C9A—C10A | 1.479 (2) | C23B—H23E | 0.9600 |
| C10A—C11A | 1.340 (2) | C23B—H23F | 0.9600 |
| C10A—H10A | 0.9300 | O1C—C9C | 1.232 (2) |
| C11A—C12A | 1.462 (2) | O2C—C1C | 1.368 (2) |
| C11A—H11A | 0.9300 | O2C—C18C | 1.430 (2) |
| C12A—C13A | 1.394 (2) | O3C—C3C | 1.363 (2) |

| | | | |
|---|---|---|---|
| C12A—C17A | 1.417 (2) | O3C—C19C | 1.428 (2) |
| C13A—C14A | 1.400 (3) | O4C—C4C | 1.368 (2) |
| C14A—C15A | 1.385 (2) | O4C—C20C | 1.426 (2) |
| C14A—H14A | 0.9300 | O5C—C13C | 1.386 (2) |
| C15A—C16A | 1.414 (2) | O5C—C21C | 1.423 (2) |
| C16A—C17A | 1.371 (2) | O6C—C15C | 1.360 (2) |
| C17A—H17A | 0.9300 | O6C—C22C | 1.439 (2) |
| C18A—H18A | 0.9600 | O7C—C16C | 1.369 (2) |
| C18A—H18B | 0.9600 | O7C—C23C | 1.433 (2) |
| C18A—H18C | 0.9600 | C1C—C2C | 1.401 (2) |
| C19A—H19A | 0.9600 | C1C—C6C | 1.403 (2) |
| C19A—H19B | 0.9600 | C2C—C3C | 1.381 (2) |
| C19A—H19C | 0.9600 | C2C—H2CA | 0.9300 |
| C20A—H20A | 0.9600 | C3C—C4C | 1.410 (2) |
| C20A—H20B | 0.9600 | C4C—C5C | 1.376 (2) |
| C20A—H20C | 0.9600 | C5C—C6C | 1.417 (2) |
| C21A—H21A | 0.9600 | C5C—H5CA | 0.9300 |
| C21A—H21B | 0.9600 | C6C—C7C | 1.452 (2) |
| C21A—H21C | 0.9600 | C7C—C8C | 1.339 (2) |
| C22A—H22A | 0.9600 | C7C—H7CA | 0.9300 |
| C22A—H22B | 0.9600 | C8C—C9C | 1.476 (2) |
| C22A—H22C | 0.9600 | C8C—H8CA | 0.9300 |
| C23A—H23A | 0.9600 | C9C—C10C | 1.470 (2) |
| C23A—H23B | 0.9600 | C10C—C11C | 1.344 (2) |
| C23A—H23C | 0.9600 | C10C—H10C | 0.9300 |
| O1B—C9B | 1.230 (2) | C11C—C12C | 1.456 (2) |
| O2B—C1B | 1.365 (2) | C11C—H11C | 0.9300 |
| O2B—C18B | 1.428 (2) | C12C—C13C | 1.395 (2) |
| O3B—C3B | 1.366 (2) | C12C—C17C | 1.414 (2) |
| O3B—C19B | 1.425 (2) | C13C—C14C | 1.395 (2) |
| O4B—C4B | 1.366 (2) | C14C—C15C | 1.379 (2) |
| O4B—C20B | 1.428 (2) | C14C—H14C | 0.9300 |
| O5B—C13B | 1.374 (2) | C15C—C16C | 1.425 (2) |
| O5B—C21B | 1.419 (2) | C16C—C17C | 1.369 (2) |
| O6B—C15B | 1.364 (2) | C17C—H17C | 0.9300 |
| O6B—C22B | 1.435 (2) | C18C—H18G | 0.9600 |
| O7B—C16B | 1.370 (2) | C18C—H18H | 0.9600 |
| O7B—C23B | 1.425 (2) | C18C—H18I | 0.9600 |
| C1B—C6B | 1.398 (2) | C19C—H19G | 0.9600 |
| C1B—C2B | 1.404 (2) | C19C—H19H | 0.9600 |
| C2B—C3B | 1.381 (3) | C19C—H19I | 0.9600 |
| C2B—H2BA | 0.9300 | C20C—H20G | 0.9600 |
| C3B—C4B | 1.408 (3) | C20C—H20H | 0.9600 |
| C4B—C5B | 1.379 (2) | C20C—H20I | 0.9600 |
| C5B—C6B | 1.411 (2) | C21C—H21G | 0.9600 |
| C5B—H5BA | 0.9300 | C21C—H21H | 0.9600 |
| C6B—C7B | 1.459 (2) | C21C—H21I | 0.9600 |
| C7B—C8B | 1.337 (3) | C22C—H22G | 0.9600 |
| C7B—H7BA | 0.9300 | C22C—H22H | 0.9600 |

| | | | |
|---|---|---|---|
| C8B—C9B | 1.477 (2) | C22C—H22I | 0.9600 |
| C8B—H8BA | 0.9300 | C23C—H23G | 0.9600 |
| C9B—C10B | 1.470 (2) | C23C—H23H | 0.9600 |
| C10B—C11B | 1.338 (2) | C23C—H23I | 0.9600 |
| C10B—H10B | 0.9300 | | |
| C1A—O2A—C18A | 118.38 (15) | C13B—C14B—H14B | 120.1 |
| C3A—O3A—C19A | 117.03 (16) | O6B—C15B—C14B | 124.72 (15) |
| C4A—O4A—C20A | 116.68 (15) | O6B—C15B—C16B | 115.41 (15) |
| C13A—O5A—C21A | 114.34 (14) | C14B—C15B—C16B | 119.86 (15) |
| C15A—O6A—C22A | 116.90 (14) | O7B—C16B—C17B | 124.78 (15) |
| C16A—O7A—C23A | 116.30 (14) | O7B—C16B—C15B | 115.77 (15) |
| O2A—C1A—C2A | 122.55 (16) | C17B—C16B—C15B | 119.45 (15) |
| O2A—C1A—C6A | 116.50 (16) | C16B—C17B—C12B | 121.93 (16) |
| C2A—C1A—C6A | 120.95 (17) | C16B—C17B—H17B | 119.0 |
| C3A—C2A—C1A | 120.04 (17) | C12B—C17B—H17B | 119.0 |
| C3A—C2A—H2AA | 120.0 | O2B—C18B—H18D | 109.5 |
| C1A—C2A—H2AA | 120.0 | O2B—C18B—H18E | 109.5 |
| O3A—C3A—C2A | 124.48 (17) | H18D—C18B—H18E | 109.5 |
| O3A—C3A—C4A | 115.16 (17) | O2B—C18B—H18F | 109.5 |
| C2A—C3A—C4A | 120.34 (17) | H18D—C18B—H18F | 109.5 |
| O4A—C4A—C5A | 126.01 (17) | H18E—C18B—H18F | 109.5 |
| O4A—C4A—C3A | 115.09 (16) | O3B—C19B—H19D | 109.5 |
| C5A—C4A—C3A | 118.90 (17) | O3B—C19B—H19E | 109.5 |
| C4A—C5A—C6A | 122.12 (17) | H19D—C19B—H19E | 109.5 |
| C4A—C5A—H5AA | 118.9 | O3B—C19B—H19F | 109.5 |
| C6A—C5A—H5AA | 118.9 | H19D—C19B—H19F | 109.5 |
| C1A—C6A—C5A | 117.64 (16) | H19E—C19B—H19F | 109.5 |
| C1A—C6A—C7A | 120.82 (16) | O4B—C20B—H20D | 109.5 |
| C5A—C6A—C7A | 121.53 (16) | O4B—C20B—H20E | 109.5 |
| C8A—C7A—C6A | 125.57 (16) | H20D—C20B—H20E | 109.5 |
| C8A—C7A—H7AA | 117.2 | O4B—C20B—H20F | 109.5 |
| C6A—C7A—H7AA | 117.2 | H20D—C20B—H20F | 109.5 |
| C7A—C8A—C9A | 122.90 (16) | H20E—C20B—H20F | 109.5 |
| C7A—C8A—H8AA | 118.6 | O5B—C21B—H21D | 109.5 |
| C9A—C8A—H8AA | 118.6 | O5B—C21B—H21E | 109.5 |
| O1A—C9A—C8A | 123.11 (16) | H21D—C21B—H21E | 109.5 |
| O1A—C9A—C10A | 122.22 (16) | O5B—C21B—H21F | 109.5 |
| C8A—C9A—C10A | 114.65 (15) | H21D—C21B—H21F | 109.5 |
| C11A—C10A—C9A | 122.98 (16) | H21E—C21B—H21F | 109.5 |
| C11A—C10A—H10A | 118.5 | O6B—C22B—H22D | 109.5 |
| C9A—C10A—H10A | 118.5 | O6B—C22B—H22E | 109.5 |
| C10A—C11A—C12A | 126.25 (16) | H22D—C22B—H22E | 109.5 |
| C10A—C11A—H11A | 116.9 | O6B—C22B—H22F | 109.5 |
| C12A—C11A—H11A | 116.9 | H22D—C22B—H22F | 109.5 |
| C13A—C12A—C17A | 117.40 (16) | H22E—C22B—H22F | 109.5 |
| C13A—C12A—C11A | 120.89 (16) | O7B—C23B—H23D | 109.5 |
| C17A—C12A—C11A | 121.71 (16) | O7B—C23B—H23E | 109.5 |
| O5A—C13A—C12A | 119.63 (16) | H23D—C23B—H23E | 109.5 |
| O5A—C13A—C14A | 118.70 (16) | O7B—C23B—H23F | 109.5 |

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|---|---|---|---|
| C12A—C13A—C14A | 121.61 (16) | H23D—C23B—H23F | 109.5 |
| C15A—C14A—C13A | 119.79 (16) | H23E—C23B—H23F | 109.5 |
| C15A—C14A—H14A | 120.1 | C1C—O2C—C18C | 118.19 (14) |
| C13A—C14A—H14A | 120.1 | C3C—O3C—C19C | 117.77 (14) |
| O6A—C15A—C14A | 124.94 (16) | C4C—O4C—C20C | 116.72 (14) |
| O6A—C15A—C16A | 115.38 (15) | C13C—O5C—C21C | 113.38 (14) |
| C14A—C15A—C16A | 119.68 (16) | C15C—O6C—C22C | 116.48 (14) |
| C17A—C16A—O7A | 125.07 (16) | C16C—O7C—C23C | 115.83 (14) |
| C17A—C16A—C15A | 119.80 (16) | O2C—C1C—C2C | 123.35 (15) |
| O7A—C16A—C15A | 115.13 (15) | O2C—C1C—C6C | 115.95 (15) |
| C16A—C17A—C12A | 121.71 (16) | C2C—C1C—C6C | 120.70 (15) |
| C16A—C17A—H17A | 119.1 | C3C—C2C—C1C | 119.73 (16) |
| C12A—C17A—H17A | 119.1 | C3C—C2C—H2CA | 120.1 |
| O2A—C18A—H18A | 109.5 | C1C—C2C—H2CA | 120.1 |
| O2A—C18A—H18B | 109.5 | O3C—C3C—C2C | 124.29 (16) |
| H18A—C18A—H18B | 109.5 | O3C—C3C—C4C | 114.83 (15) |
| O2A—C18A—H18C | 109.5 | C2C—C3C—C4C | 120.88 (15) |
| H18A—C18A—H18C | 109.5 | O4C—C4C—C5C | 125.64 (16) |
| H18B—C18A—H18C | 109.5 | O4C—C4C—C3C | 115.35 (15) |
| O3A—C19A—H19A | 109.5 | C5C—C4C—C3C | 119.01 (16) |
| O3A—C19A—H19B | 109.5 | C4C—C5C—C6C | 121.57 (16) |
| H19A—C19A—H19B | 109.5 | C4C—C5C—H5CA | 119.2 |
| O3A—C19A—H19C | 109.5 | C6C—C5C—H5CA | 119.2 |
| H19A—C19A—H19C | 109.5 | C1C—C6C—C5C | 118.11 (15) |
| H19B—C19A—H19C | 109.5 | C1C—C6C—C7C | 119.90 (15) |
| O4A—C20A—H20A | 109.5 | C5C—C6C—C7C | 121.98 (15) |
| O4A—C20A—H20B | 109.5 | C8C—C7C—C6C | 127.18 (16) |
| H20A—C20A—H20B | 109.5 | C8C—C7C—H7CA | 116.4 |
| O4A—C20A—H20C | 109.5 | C6C—C7C—H7CA | 116.4 |
| H20A—C20A—H20C | 109.5 | C7C—C8C—C9C | 121.77 (15) |
| H20B—C20A—H20C | 109.5 | C7C—C8C—H8CA | 119.1 |
| O5A—C21A—H21A | 109.5 | C9C—C8C—H8CA | 119.1 |
| O5A—C21A—H21B | 109.5 | O1C—C9C—C10C | 123.05 (15) |
| H21A—C21A—H21B | 109.5 | O1C—C9C—C8C | 122.05 (15) |
| O5A—C21A—H21C | 109.5 | C10C—C9C—C8C | 114.90 (14) |
| H21A—C21A—H21C | 109.5 | C11C—C10C—C9C | 123.76 (15) |
| H21B—C21A—H21C | 109.5 | C11C—C10C—H10C | 118.1 |
| O6A—C22A—H22A | 109.5 | C9C—C10C—H10C | 118.1 |
| O6A—C22A—H22B | 109.5 | C10C—C11C—C12C | 124.63 (15) |
| H22A—C22A—H22B | 109.5 | C10C—C11C—H11C | 117.7 |
| O6A—C22A—H22C | 109.5 | C12C—C11C—H11C | 117.7 |
| H22A—C22A—H22C | 109.5 | C13C—C12C—C17C | 117.36 (15) |
| H22B—C22A—H22C | 109.5 | C13C—C12C—C11C | 121.21 (15) |
| O7A—C23A—H23A | 109.5 | C17C—C12C—C11C | 121.40 (15) |
| O7A—C23A—H23B | 109.5 | O5C—C13C—C12C | 119.15 (15) |
| H23A—C23A—H23B | 109.5 | O5C—C13C—C14C | 119.10 (15) |
| O7A—C23A—H23C | 109.5 | C12C—C13C—C14C | 121.74 (15) |
| H23A—C23A—H23C | 109.5 | C15C—C14C—C13C | 120.00 (16) |
| H23B—C23A—H23C | 109.5 | C15C—C14C—H14C | 120.0 |

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| C1B—O2B—C18B | 119.11 (14) | C13C—C14C—H14C | 120.0 |
| C3B—O3B—C19B | 117.48 (15) | O6C—C15C—C14C | 125.29 (16) |
| C4B—O4B—C20B | 116.76 (15) | O6C—C15C—C16C | 115.24 (15) |
| C13B—O5B—C21B | 116.60 (13) | C14C—C15C—C16C | 119.47 (16) |
| C15B—O6B—C22B | 116.72 (14) | C17C—C16C—O7C | 125.18 (16) |
| C16B—O7B—C23B | 115.94 (14) | C17C—C16C—C15C | 119.61 (16) |
| O2B—C1B—C6B | 116.44 (15) | O7C—C16C—C15C | 115.21 (15) |
| O2B—C1B—C2B | 123.29 (16) | C16C—C17C—C12C | 121.81 (16) |
| C6B—C1B—C2B | 120.27 (16) | C16C—C17C—H17C | 119.1 |
| C3B—C2B—C1B | 119.69 (16) | C12C—C17C—H17C | 119.1 |
| C3B—C2B—H2BA | 120.2 | O2C—C18C—H18G | 109.5 |
| C1B—C2B—H2BA | 120.2 | O2C—C18C—H18H | 109.5 |
| O3B—C3B—C2B | 124.24 (16) | H18G—C18C—H18H | 109.5 |
| O3B—C3B—C4B | 114.66 (16) | O2C—C18C—H18I | 109.5 |
| C2B—C3B—C4B | 121.10 (16) | H18G—C18C—H18I | 109.5 |
| O4B—C4B—C5B | 125.85 (17) | H18H—C18C—H18I | 109.5 |
| O4B—C4B—C3B | 115.39 (16) | O3C—C19C—H19G | 109.5 |
| C5B—C4B—C3B | 118.76 (17) | O3C—C19C—H19H | 109.5 |
| C4B—C5B—C6B | 121.41 (17) | H19G—C19C—H19H | 109.5 |
| C4B—C5B—H5BA | 119.3 | O3C—C19C—H19I | 109.5 |
| C6B—C5B—H5BA | 119.3 | H19G—C19C—H19I | 109.5 |
| C1B—C6B—C5B | 118.77 (16) | H19H—C19C—H19I | 109.5 |
| C1B—C6B—C7B | 119.06 (16) | O4C—C20C—H20G | 109.5 |
| C5B—C6B—C7B | 122.17 (16) | O4C—C20C—H20H | 109.5 |
| C8B—C7B—C6B | 127.45 (16) | H20G—C20C—H20H | 109.5 |
| C8B—C7B—H7BA | 116.3 | O4C—C20C—H20I | 109.5 |
| C6B—C7B—H7BA | 116.3 | H20G—C20C—H20I | 109.5 |
| C7B—C8B—C9B | 121.37 (16) | H20H—C20C—H20I | 109.5 |
| C7B—C8B—H8BA | 119.3 | O5C—C21C—H21G | 109.5 |
| C9B—C8B—H8BA | 119.3 | O5C—C21C—H21H | 109.5 |
| O1B—C9B—C10B | 122.79 (15) | H21G—C21C—H21H | 109.5 |
| O1B—C9B—C8B | 123.08 (16) | O5C—C21C—H21I | 109.5 |
| C10B—C9B—C8B | 114.11 (15) | H21G—C21C—H21I | 109.5 |
| C11B—C10B—C9B | 124.36 (16) | H21H—C21C—H21I | 109.5 |
| C11B—C10B—H10B | 117.8 | O6C—C22C—H22G | 109.5 |
| C9B—C10B—H10B | 117.8 | O6C—C22C—H22H | 109.5 |
| C10B—C11B—C12B | 124.00 (15) | H22G—C22C—H22H | 109.5 |
| C10B—C11B—H11B | 118.0 | O6C—C22C—H22I | 109.5 |
| C12B—C11B—H11B | 118.0 | H22G—C22C—H22I | 109.5 |
| C13B—C12B—C17B | 117.80 (15) | H22H—C22C—H22I | 109.5 |
| C13B—C12B—C11B | 121.06 (15) | O7C—C23C—H23G | 109.5 |
| C17B—C12B—C11B | 121.12 (15) | O7C—C23C—H23H | 109.5 |
| O5B—C13B—C14B | 122.15 (15) | H23G—C23C—H23H | 109.5 |
| O5B—C13B—C12B | 116.78 (14) | O7C—C23C—H23I | 109.5 |
| C14B—C13B—C12B | 121.07 (15) | H23G—C23C—H23I | 109.5 |
| C15B—C14B—C13B | 119.85 (15) | H23H—C23C—H23I | 109.5 |
| C15B—C14B—H14B | 120.1 | | |
| C18A—O2A—C1A—C2A | −3.7 (2) | O1B—C9B—C10B—C11B | 5.5 (3) |
| C18A—O2A—C1A—C6A | 177.34 (16) | C8B—C9B—C10B—C11B | −173.08 (17) |

| | | | |
|---|---|---|---|
| O2A—C1A—C2A—C3A | −178.51 (16) | C9B—C10B—C11B—C12B | 176.23 (16) |
| C6A—C1A—C2A—C3A | 0.4 (3) | C10B—C11B—C12B—C13B | −166.56 (17) |
| C19A—O3A—C3A—C2A | −0.2 (3) | C10B—C11B—C12B—C17B | 11.8 (3) |
| C19A—O3A—C3A—C4A | 178.80 (16) | C21B—O5B—C13B—C14B | −30.2 (2) |
| C1A—C2A—C3A—O3A | 178.18 (16) | C21B—O5B—C13B—C12B | 150.82 (16) |
| C1A—C2A—C3A—C4A | −0.8 (3) | C17B—C12B—C13B—O5B | −179.65 (15) |
| C20A—O4A—C4A—C5A | 3.8 (3) | C11B—C12B—C13B—O5B | −1.3 (2) |
| C20A—O4A—C4A—C3A | −176.10 (17) | C17B—C12B—C13B—C14B | 1.4 (2) |
| O3A—C3A—C4A—O4A | 1.9 (2) | C11B—C12B—C13B—C14B | 179.73 (16) |
| C2A—C3A—C4A—O4A | −179.01 (16) | O5B—C13B—C14B—C15B | 179.36 (15) |
| O3A—C3A—C4A—C5A | −178.01 (16) | C12B—C13B—C14B—C15B | −1.7 (3) |
| C2A—C3A—C4A—C5A | 1.1 (3) | C22B—O6B—C15B—C14B | −7.6 (3) |
| O4A—C4A—C5A—C6A | 179.13 (17) | C22B—O6B—C15B—C16B | 171.36 (16) |
| C3A—C4A—C5A—C6A | −1.0 (3) | C13B—C14B—C15B—O6B | 179.04 (16) |
| O2A—C1A—C6A—C5A | 178.71 (15) | C13B—C14B—C15B—C16B | 0.2 (3) |
| C2A—C1A—C6A—C5A | −0.3 (3) | C23B—O7B—C16B—C17B | 9.6 (2) |
| O2A—C1A—C6A—C7A | −0.8 (2) | C23B—O7B—C16B—C15B | −169.73 (15) |
| C2A—C1A—C6A—C7A | −179.84 (16) | O6B—C15B—C16B—O7B | 2.1 (2) |
| C4A—C5A—C6A—C1A | 0.6 (3) | C14B—C15B—C16B—O7B | −178.93 (15) |
| C4A—C5A—C6A—C7A | −179.88 (16) | O6B—C15B—C16B—C17B | −177.28 (15) |
| C1A—C6A—C7A—C8A | −177.55 (17) | C14B—C15B—C16B—C17B | 1.7 (2) |
| C5A—C6A—C7A—C8A | 2.9 (3) | O7B—C16B—C17B—C12B | 178.63 (15) |
| C6A—C7A—C8A—C9A | −175.45 (16) | C15B—C16B—C17B—C12B | −2.1 (3) |
| C7A—C8A—C9A—O1A | −8.2 (3) | C13B—C12B—C17B—C16B | 0.6 (2) |
| C7A—C8A—C9A—C10A | 170.30 (16) | C11B—C12B—C17B—C16B | −177.81 (16) |
| O1A—C9A—C10A—C11A | −4.0 (3) | C18C—O2C—C1C—C2C | −3.9 (2) |
| C8A—C9A—C10A—C11A | 177.49 (16) | C18C—O2C—C1C—C6C | 176.17 (15) |
| C9A—C10A—C11A—C12A | −179.03 (16) | O2C—C1C—C2C—C3C | −179.51 (16) |
| C10A—C11A—C12A—C13A | −179.58 (17) | C6C—C1C—C2C—C3C | 0.4 (3) |
| C10A—C11A—C12A—C17A | 0.4 (3) | C19C—O3C—C3C—C2C | −1.7 (2) |
| C21A—O5A—C13A—C12A | −111.48 (18) | C19C—O3C—C3C—C4C | 177.40 (16) |
| C21A—O5A—C13A—C14A | 71.4 (2) | C1C—C2C—C3C—O3C | 178.69 (16) |
| C17A—C12A—C13A—O5A | −175.63 (15) | C1C—C2C—C3C—C4C | −0.3 (3) |
| C11A—C12A—C13A—O5A | 4.3 (2) | C20C—O4C—C4C—C5C | −4.3 (3) |
| C17A—C12A—C13A—C14A | 1.4 (3) | C20C—O4C—C4C—C3C | 176.31 (16) |
| C11A—C12A—C13A—C14A | −178.64 (16) | O3C—C3C—C4C—O4C | 0.6 (2) |
| O5A—C13A—C14A—C15A | 176.04 (16) | C2C—C3C—C4C—O4C | 179.66 (15) |
| C12A—C13A—C14A—C15A | −1.0 (3) | O3C—C3C—C4C—C5C | −178.86 (15) |
| C22A—O6A—C15A—C14A | 1.1 (3) | C2C—C3C—C4C—C5C | 0.2 (3) |
| C22A—O6A—C15A—C16A | −177.98 (15) | O4C—C4C—C5C—C6C | −179.61 (16) |
| C13A—C14A—C15A—O6A | −179.14 (16) | C3C—C4C—C5C—C6C | −0.2 (3) |
| C13A—C14A—C15A—C16A | −0.1 (3) | O2C—C1C—C6C—C5C | 179.51 (15) |
| C23A—O7A—C16A—C17A | −14.4 (3) | C2C—C1C—C6C—C5C | −0.4 (2) |
| C23A—O7A—C16A—C15A | 164.98 (16) | O2C—C1C—C6C—C7C | −1.6 (2) |
| O6A—C15A—C16A—C17A | 179.90 (15) | C2C—C1C—C6C—C7C | 178.44 (16) |
| C14A—C15A—C16A—C17A | 0.8 (3) | C4C—C5C—C6C—C1C | 0.3 (3) |
| O6A—C15A—C16A—O7A | 0.5 (2) | C4C—C5C—C6C—C7C | −178.49 (16) |
| C14A—C15A—C16A—O7A | −178.62 (16) | C1C—C6C—C7C—C8C | −168.99 (17) |
| O7A—C16A—C17A—C12A | 178.97 (16) | C5C—C6C—C7C—C8C | 9.8 (3) |

| | | | |
|---|---|---|---|
| C15A—C16A—C17A—C12A | −0.3 (3) | C6C—C7C—C8C—C9C | −178.94 (16) |
| C13A—C12A—C17A—C16A | −0.7 (3) | C7C—C8C—C9C—O1C | −3.0 (3) |
| C11A—C12A—C17A—C16A | 179.33 (16) | C7C—C8C—C9C—C10C | 176.17 (16) |
| C18B—O2B—C1B—C6B | −179.45 (16) | O1C—C9C—C10C—C11C | −0.7 (3) |
| C18B—O2B—C1B—C2B | 1.4 (3) | C8C—C9C—C10C—C11C | −179.82 (16) |
| O2B—C1B—C2B—C3B | 179.33 (17) | C9C—C10C—C11C—C12C | 176.90 (16) |
| C6B—C1B—C2B—C3B | 0.2 (3) | C10C—C11C—C12C—C13C | 170.52 (17) |
| C19B—O3B—C3B—C2B | 3.5 (3) | C10C—C11C—C12C—C17C | −11.6 (3) |
| C19B—O3B—C3B—C4B | −176.27 (16) | C21C—O5C—C13C—C12C | −107.71 (19) |
| C1B—C2B—C3B—O3B | −179.63 (17) | C21C—O5C—C13C—C14C | 73.5 (2) |
| C1B—C2B—C3B—C4B | 0.2 (3) | C17C—C12C—C13C—O5C | −179.32 (15) |
| C20B—O4B—C4B—C5B | 4.4 (3) | C11C—C12C—C13C—O5C | −1.3 (2) |
| C20B—O4B—C4B—C3B | −176.09 (18) | C17C—C12C—C13C—C14C | −0.6 (3) |
| O3B—C3B—C4B—O4B | −0.2 (2) | C11C—C12C—C13C—C14C | 177.38 (16) |
| C2B—C3B—C4B—O4B | 179.97 (17) | O5C—C13C—C14C—C15C | 178.35 (16) |
| O3B—C3B—C4B—C5B | 179.36 (16) | C12C—C13C—C14C—C15C | −0.4 (3) |
| C2B—C3B—C4B—C5B | −0.5 (3) | C22C—O6C—C15C—C14C | 0.4 (3) |
| O4B—C4B—C5B—C6B | 179.85 (17) | C22C—O6C—C15C—C16C | −179.51 (16) |
| C3B—C4B—C5B—C6B | 0.3 (3) | C13C—C14C—C15C—O6C | −178.86 (16) |
| O2B—C1B—C6B—C5B | −179.52 (16) | C13C—C14C—C15C—C16C | 1.0 (3) |
| C2B—C1B—C6B—C5B | −0.4 (3) | C23C—O7C—C16C—C17C | −8.2 (3) |
| O2B—C1B—C6B—C7B | 0.1 (2) | C23C—O7C—C16C—C15C | 171.17 (17) |
| C2B—C1B—C6B—C7B | 179.22 (16) | O6C—C15C—C16C—C17C | 179.22 (16) |
| C4B—C5B—C6B—C1B | 0.1 (3) | C14C—C15C—C16C—C17C | −0.7 (3) |
| C4B—C5B—C6B—C7B | −179.51 (17) | O6C—C15C—C16C—O7C | −0.2 (2) |
| C1B—C6B—C7B—C8B | 176.72 (18) | C14C—C15C—C16C—O7C | 179.96 (16) |
| C5B—C6B—C7B—C8B | −3.7 (3) | O7C—C16C—C17C—C12C | 178.97 (17) |
| C6B—C7B—C8B—C9B | −179.50 (17) | C15C—C16C—C17C—C12C | −0.3 (3) |
| C7B—C8B—C9B—O1B | −6.0 (3) | C13C—C12C—C17C—C16C | 1.0 (3) |
| C7B—C8B—C9B—C10B | 172.61 (17) | C11C—C12C—C17C—C16C | −177.03 (17) |

*Hydrogen-bond geometry (Å, °)*

Cg3 and Cg4 are the centroids of the C1C–C6C and C12C–C17C rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C10B—H10B···O1C$^{i}$ | 0.93 | 2.29 | 3.149 (2) | 153 |
| C10C—H10C···O1B | 0.93 | 2.33 | 3.195 (2) | 155 |
| C14B—H14B···O1A$^{ii}$ | 0.93 | 2.52 | 3.353 (2) | 149 |
| C21A—H21B···O3A$^{iii}$ | 0.96 | 2.49 | 3.301 (2) | 142 |
| C22A—H22C···O7C$^{iv}$ | 0.96 | 2.50 | 3.435 (2) | 165 |
| C22B—H22D···O2A$^{v}$ | 0.96 | 2.50 | 3.407 (2) | 158 |
| C22B—H22F···O1A$^{ii}$ | 0.96 | 2.58 | 3.227 (2) | 125 |
| C23A—H23A···O5A$^{i}$ | 0.96 | 2.52 | 3.308 (2) | 140 |
| C23A—H23C···O3C | 0.96 | 2.53 | 3.452 (2) | 161 |
| C23C—H23G···O5C$^{i}$ | 0.96 | 2.54 | 3.305 (2) | 136 |
| C18C—H18H···Cg4$^{ii}$ | 0.96 | 2.80 | 3.678 (2) | 152 |
| C20A—H20B···Cg3$^{vi}$ | 0.96 | 2.94 | 3.855 (2) | 159 |

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

**Fig. 1**

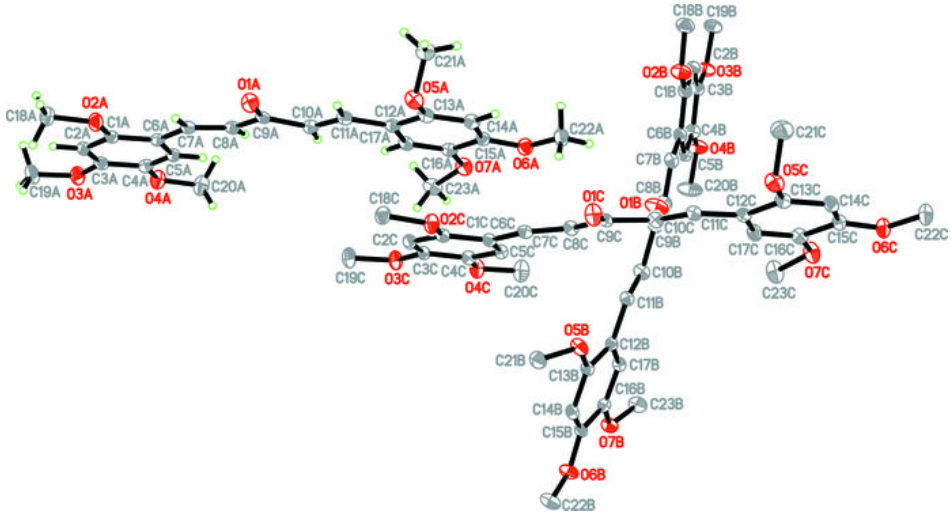

**Fig. 2**