

(1*E*,4*E*)-1,5-Bis(2,4,6-trimethoxyphenyl)-penta-1,4-dien-3-onePumsak Ruanwas,^a Suchada Chantrapromma^{b*‡} and Hoong-Kun Fun^{c§}^aCrystal Materials Research Unit, Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand, ^bDepartment of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand, and ^cX-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

Correspondence e-mail: suchada.c@psu.ac.th

Received 5 November 2010; accepted 25 November 2010

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.002$ Å; R factor = 0.052; wR factor = 0.139; data-to-parameter ratio = 19.7.

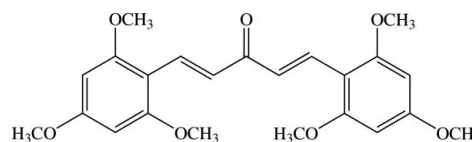
There are two crystallographically independent molecules in the asymmetric unit of the title bischalcone derivative, $C_{23}H_{26}O_7$. The molecules are unsymmetrical and almost planar: the dihedral angle between two benzene rings is 1.04 (7)° in one molecule and 2.31 (7)° in the other. The central penta-1,4-dien-3-one fragment makes dihedral angles of 7.61 (7) and 6.82 (7)° with the two adjacent benzene rings in one molecule, while the corresponding values are 7.85 (7) and 9.42 (6)° in the other. In both molecules, the three methoxy groups of the two 2,4,6-trimethoxyphenyl units are coplanar with the attached benzene rings [C—O—C—C—torsion angles of -1.5 (2), -7.2 (2) and 4.1 (2)° in one molecule and -0.7 (2), -5.5 (2) and -0.6 (2)° in the other]. The molecular conformations are stabilized by weak intramolecular C—H...O interactions generating two $S(6)$ ring motifs. In the crystal, molecules are linked by weak intermolecular C—H...O interactions into zigzag chains parallel to the c axis. The crystal structure is further stabilized by C—H... π interactions and π — π interactions with centroid—centroid distances of 3.6433 (8) Å.

Related literature

For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For related structures, see: Fun *et al.* (2010); Harrison *et al.* (2006). For background to and applications of bischalcones, see: Gomes *et al.* (2009); Lee *et al.* (2009); Quincoces *et al.* (2008); Uchida *et al.* (1998). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).

‡ Thomson Reuters ResearcherID: A-5085-2009.

§ Additional correspondence author, e-mail: hkfun@usm.my. Thomson Reuters ResearcherID: A-3561-2009.

**Experimental***Crystal data*

$C_{23}H_{26}O_7$
 $M_r = 414.44$
 Monoclinic, $P2_1/c$
 $a = 15.7417$ (2) Å
 $b = 15.1192$ (2) Å
 $c = 19.4803$ (3) Å
 $\beta = 117.827$ (1)°

$V = 4100.21$ (11) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 100$ K
 $0.39 \times 0.32 \times 0.17$ mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\min} = 0.963$, $T_{\max} = 0.983$

50384 measured reflections
 10908 independent reflections
 7903 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.139$
 $S = 1.04$
 10908 reflections

553 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.36$ e Å⁻³
 $\Delta\rho_{\min} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$Cg1$, $Cg2$ and $Cg3$ are the centroids of the $C1A-C6A$, $C12A-C17A$ and $C12B-C17B$ rings, respectively

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C7A-H7AA\cdots O1A$	0.93	2.42	2.787 (2)	104
$C7A-H7AA\cdots O2A$	0.93	2.29	2.704 (2)	106
$C8A-H8AA\cdots O4A$	0.93	2.18	2.7844 (17)	121
$C7B-H7BA\cdots O1B$	0.93	2.49	2.8351 (19)	102
$C7B-H7BA\cdots O2B$	0.93	2.33	2.704 (2)	104
$C8B-H8BA\cdots O4B$	0.93	2.16	2.7643 (18)	121
$C10A-H10A\cdots O5A$	0.93	2.26	2.852 (2)	121
$C10B-H10B\cdots O5B$	0.93	2.26	2.855 (2)	121
$C11A-H11A\cdots O7A$	0.93	2.23	2.6599 (17)	108
$C11B-H11B\cdots O7B$	0.93	2.23	2.6700 (17)	108
$C20A-H20C\cdots O1B$	0.96	2.47	3.339 (2)	151
$C20B-H20E\cdots O1A^i$	0.96	2.37	3.0238 (19)	125
$C23A-H23C\cdots O1A^{ii}$	0.96	2.39	3.319 (2)	162
$C23B-H23D\cdots O1B^{ii}$	0.96	2.41	3.262 (2)	148
$C18A-H18C\cdots Cg1^{iii}$	0.96	2.65	3.4503 (17)	141
$C21A-H21C\cdots Cg2^{iv}$	0.96	2.94	3.5813 (18)	126
$C21B-H21E\cdots Cg3^v$	0.96	2.72	3.5809 (16)	150

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

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).

PR thanks the Center of Excellence for Innovation in Chemistry (PERCH-CIC), Commission on Higher Education, Ministry of Education, and the Graduate School, Prince of

Songkla University, for financial support. The authors thank the Prince of Songkla University and Universiti Sains Malaysia for the Research University Golden Goose grant No. 1001/PFIZIK/811160.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2523).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Bernstein, J., Davis, R. E., Shimon, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Bruker (2005). *APEX2, SAINT and SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
- Fun, H.-K., Ruanwas, P. & Chantrapromma, S. (2010). *Acta Cryst.* **E66**, o307–o308.
- Gomes, A., Neuwirth, O., Freitas, M., Couto, D., Ribeiro, D., Figueiredo, A. G. P. R., Silva, A. M. S., Seixas, R. S. G. R., Pinto, D. C. G. A., Tomé, A. C., Cavaleiro, J. A. S., Fernandes, E. & Lima, J. L. F. C. (2009). *Bioorg. Med. Chem.* **17**, 7218–7226.
- Harrison, W. T. A., Sarojini, B. K., Vijaya Raj, K. K., Yathirajan, H. S. & Narayana, B. (2006). *Acta Cryst.* **E62**, o1522–o1523.
- Lee, K.-H., Ab Aziz, F. H., Syahida, A., Abas, F., Shaari, K., Israf, D. A. & Iajis, N. H. (2009). *Eur. J. Med. Chem.* **44**, 3195–3200.
- Quincoces, J., Peseke, K., Kordian, M., Carvalho, J., Brunhari, H., Kohn, L. & António, M. (2008). US Patent No. 7 432 401 B2.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Uchida, T., Kozawa, K., Sakai, T., Aoki, M., Yoguchi, H., Abduryim, A. & Watanabe, Y. (1998). *Mol. Cryst. Liq. Cryst.* **315**, 135–140.

supplementary materials

Acta Cryst. (2011). E67, o33-o34 [doi:10.1107/S1600536810049299]

(1*E*,4*E*)-1,5-Bis(2,4,6-trimethoxyphenyl)penta-1,4-dien-3-one

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

Comment

Bis(chalcone) is an important class of compounds due to their variety of properties such as non-linear optical (Uchida *et al.*, 1998) and fluorescence properties (Gomes *et al.*, 2009) and activities involving anti-inflammatory, antioxidant and anti-tyrosinase activities (Lee *et al.*, 2009) and cytotoxic activities (Quincoces *et al.*, 2008). We have previously reported the crystal structure of (1*E*,4*E*)-1,5-bis(2,4,5-trimethoxyphenyl)penta-1,4-dien-3-one (I) (Fun *et al.*, 2010). The title bis(chalcone) (II) was synthesized in order to study the effect of the positions of the trimethoxy substituents to its fluorescence property and anti-tyrosinase activity. Our anti-tyrosinase activity testing showed that the title bis(chalcone) possesses anti-tyrosinase activity. We report herein the crystal structure of (II).

There are two crystallographically independent molecules (*A* and *B*) in the asymmetric unit of (II) (Fig. 1) with the same conformation but with slight differences in bond angles. The molecular structure of (II) is unsymmetrical and almost planar. The dihedral angle between the C1–C6 and C12–C17 benzene rings is 1.04 (7)° in molecule *A* whereas it is 2.31 (7)° in molecule *B*. The central penta-1,4-dien-3-one unit (C7–C11/O1) is planar with *r.m.s.* of 0.0124 (1) and 0.0433 (1) Å for molecule *A* and *B*, respectively. This unit makes dihedral angles of 7.61 (7) and 6.82 (7)° with the two adjacent C1–C6 and C12–C17 benzene rings, respectively, in molecule *A* whereas the corresponding values are 7.85 (7) and 9.42 (6)° in molecule *B*. The three methoxy groups on the C1–C6 benzene ring are planarly attached, with the C18–O2–C1–C2, C19–O3–C3–C2 and C20–O4–C5–C4 torsion angles of -1.5 (2), -7.2 (2) and 4.1 (2)° in molecule *A* and -0.7 (2), -5.5 (2) and -0.6 (2)° in molecule *B*. The same orientation is observed for the three methoxy groups on the C12–C17 benzene ring as indicated by the torsion angles C21–O5–C13–C14, C22–O6–C15–C14 and C23–O7–C17–C16 of -0.1 (2), -0.7 (2) and 0.8 (2)°, respectively, for molecule *A* and the corresponding values of -0.9 (2), 1.6 (2) and -4.9 (2)° for molecule *B*. In each molecule, intramolecular C8A—H8AA···O4A and C10A—H10A···O5A [in molecule *A*]; C8B—H8BA···O4B and C10B—H10B···O5B [in molecule *B*] weak interactions (Table 1, Fig. 1) generate S(6) ring motifs (Bernstein *et al.*, 1995). The bond distances are in normal ranges (Allen *et al.*, 1987) and are comparable with those of related structures (Fun *et al.*, 2010; Harrison *et al.*, 2006). However there are less C—H···O weak interactions but more C—H··· π interactions in (II) than in (I).

In the crystal packing (Fig. 2), the molecules are linked by intermolecular C—H···O weak interactions (Table 1) into zigzag chains along the *c* axis. The crystal is stabilized by intermolecular C—H···O weak interactions and C—H··· π interactions (Table 1). π – π interactions are observed with $Cg_1 \cdots Cg_3^i = 3.6433$ (8) Å (symmetry code: (i) $x, 1/2 - y, -1/2 + z$; Cg_1 and Cg_3 are the centroids of the C1A–C6A and C12B–C17B rings, respectively).

Experimental

The title compound was synthesized by dissolving the 2,4,6-trimethoxybenzaldehyde (0.5 g, 2.55 mmol) in acetone (50 ml). A NaOH 50% aqueous solution (2 ml) was then added and, after stirring at room temperature for 1 h, the resulting yellow solid was collected by filtration, washed with distilled water and dried. Pale yellow block-shaped single crystals of the title

supplementary materials

compound suitable for *x*-ray structure determination were recrystallized from ethanol by the slow evaporation of the solvent at room temperature after a week. M. p. 494–495 K.

Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with $d(\text{C—H}) = 0.93 \text{ \AA}$ for aromatic and 0.96 \AA for CH_3 atoms. The U_{iso} values were constrained to be $1.5U_{\text{eq}}$ of the carrier atom for methyl H atoms and $1.2U_{\text{eq}}$ for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual electron density peak is located at 0.70 \AA from C12B and the deepest hole is located at 1.24 \AA from C13B.

Figures

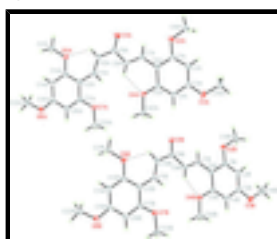


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme. Intramolecular C—H...O interactions are shown as dashed lines.

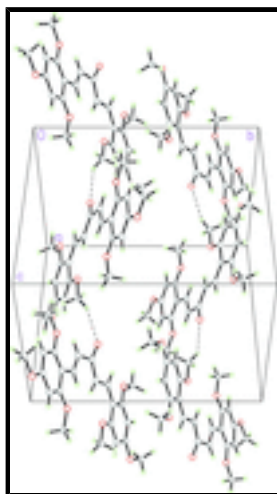


Fig. 2. The crystal packing of the title compound showing the zigzag chains along the *c* axis. Hydrogen bonds are shown as dashed lines.

(1*E*,4*E*)-1,5-Bis(2,4,6-trimethoxyphenyl)penta-1,4-dien-3-one

Crystal data

$\text{C}_{23}\text{H}_{26}\text{O}_7$

$M_r = 414.44$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 15.7417(2) \text{ \AA}$

$b = 15.1192(2) \text{ \AA}$

$c = 19.4803(3) \text{ \AA}$

$\beta = 117.827(1)^\circ$

$F(000) = 1760$

$D_x = 1.343 \text{ Mg m}^{-3}$

Melting point = 494–495 K

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 10908 reflections

$\theta = 2.1\text{--}29.0^\circ$

$\mu = 0.10 \text{ mm}^{-1}$

$T = 100 \text{ K}$

$V = 4100.21 (11) \text{ \AA}^3$
 $Z = 8$

Block, pale yellow
 $0.39 \times 0.32 \times 0.17 \text{ mm}$

Data collection

Bruker APEXII DUO CCD area-detector
 diffractometer
 Radiation source: sealed tube
 graphite
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2005)
 $T_{\min} = 0.963$, $T_{\max} = 0.983$
 50384 measured reflections

10908 independent reflections
 7903 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$
 $\theta_{\max} = 29.0^\circ$, $\theta_{\min} = 2.1^\circ$
 $h = -20 \rightarrow 21$
 $k = -20 \rightarrow 18$
 $l = -26 \rightarrow 26$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.139$
 $S = 1.04$
 10908 reflections
 553 parameters
 0 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
 $w = 1/[\sigma^2(F_o^2) + (0.0631P)^2 + 1.5299P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.36 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.24 \text{ e \AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1A	0.17578 (9)	0.23957 (10)	-0.12657 (6)	0.0395 (3)
O2A	0.45629 (7)	0.37966 (7)	-0.07200 (6)	0.0219 (2)

supplementary materials

O3A	0.72990 (7)	0.41499 (7)	0.18177 (6)	0.0257 (2)
O4A	0.43772 (7)	0.29181 (7)	0.15211 (5)	0.0209 (2)
O5A	-0.05667 (7)	0.12267 (7)	-0.05942 (6)	0.0218 (2)
O6A	-0.07167 (8)	0.03212 (8)	0.17332 (6)	0.0287 (3)
O7A	0.20935 (7)	0.16050 (7)	0.18551 (6)	0.0233 (2)
C1A	0.50181 (11)	0.37297 (9)	0.00690 (8)	0.0176 (3)
C2A	0.59599 (11)	0.40105 (9)	0.05208 (9)	0.0196 (3)
H2AA	0.6305	0.4261	0.0292	0.023*
C3A	0.63756 (10)	0.39085 (10)	0.13221 (9)	0.0199 (3)
C4A	0.58625 (10)	0.35517 (10)	0.16765 (8)	0.0200 (3)
H4AA	0.6148	0.3497	0.2214	0.024*
C5A	0.49247 (10)	0.32789 (9)	0.12218 (8)	0.0180 (3)
C6A	0.44650 (10)	0.33541 (9)	0.03973 (8)	0.0169 (3)
C7A	0.35023 (10)	0.30407 (9)	-0.01164 (8)	0.0180 (3)
H7AA	0.3314	0.3105	-0.0643	0.022*
C8A	0.28416 (10)	0.26743 (10)	0.00458 (8)	0.0191 (3)
H8AA	0.2963	0.2625	0.0559	0.023*
C9A	0.19240 (11)	0.23482 (10)	-0.05818 (8)	0.0209 (3)
C10A	0.12089 (11)	0.19400 (10)	-0.04001 (8)	0.0204 (3)
H10A	0.0631	0.1753	-0.0809	0.024*
C11A	0.13474 (10)	0.18232 (9)	0.03281 (8)	0.0175 (3)
H11A	0.1931	0.2040	0.0708	0.021*
C12A	0.07555 (10)	0.14215 (9)	0.06315 (8)	0.0177 (3)
C13A	-0.01944 (10)	0.11210 (9)	0.01869 (8)	0.0183 (3)
C14A	-0.07145 (11)	0.07451 (10)	0.05295 (8)	0.0202 (3)
H14A	-0.1340	0.0547	0.0226	0.024*
C15A	-0.02790 (11)	0.06729 (10)	0.13332 (9)	0.0221 (3)
C16A	0.06571 (11)	0.09625 (10)	0.17972 (9)	0.0224 (3)
H16A	0.0937	0.0912	0.2334	0.027*
C17A	0.11655 (10)	0.13254 (10)	0.14487 (8)	0.0193 (3)
C18A	0.50745 (11)	0.41912 (10)	-0.10866 (9)	0.0235 (3)
H18A	0.4664	0.4221	-0.1637	0.035*
H18B	0.5630	0.3840	-0.0983	0.035*
H18C	0.5273	0.4777	-0.0886	0.035*
C19A	0.78857 (12)	0.44273 (12)	0.14764 (10)	0.0325 (4)
H19A	0.8528	0.4535	0.1878	0.049*
H19B	0.7627	0.4961	0.1185	0.049*
H19C	0.7896	0.3973	0.1136	0.049*
C20A	0.47734 (12)	0.28718 (12)	0.23484 (8)	0.0264 (3)
H20A	0.4308	0.2620	0.2480	0.040*
H20B	0.4938	0.3456	0.2564	0.040*
H20C	0.5339	0.2509	0.2556	0.040*
C21A	-0.15303 (11)	0.09395 (10)	-0.10841 (9)	0.0229 (3)
H21A	-0.1695	0.1054	-0.1616	0.034*
H21B	-0.1962	0.1255	-0.0951	0.034*
H21C	-0.1580	0.0317	-0.1013	0.034*
C22A	-0.16834 (11)	0.00175 (11)	0.13032 (10)	0.0271 (3)
H22A	-0.1905	-0.0197	0.1655	0.041*
H22B	-0.1710	-0.0451	0.0962	0.041*

H22C	-0.2085	0.0497	0.1004	0.041*
C23A	0.25648 (12)	0.15076 (12)	0.26804 (8)	0.0272 (4)
H23A	0.3190	0.1774	0.2894	0.041*
H23B	0.2629	0.0890	0.2811	0.041*
H23C	0.2192	0.1793	0.2890	0.041*
O1B	0.68800 (7)	0.20303 (8)	0.36386 (6)	0.0241 (2)
O2B	0.99141 (7)	0.09844 (7)	0.41753 (6)	0.0225 (2)
O3B	1.26319 (8)	0.06825 (8)	0.67341 (6)	0.0287 (3)
O4B	0.96545 (7)	0.18131 (7)	0.63905 (6)	0.0223 (2)
O5B	0.48221 (7)	0.36335 (7)	0.43616 (6)	0.0209 (2)
O6B	0.47137 (8)	0.44271 (8)	0.67297 (6)	0.0260 (2)
O7B	0.75115 (7)	0.31918 (7)	0.67890 (6)	0.0211 (2)
C1B	1.03565 (10)	0.10545 (10)	0.49647 (8)	0.0185 (3)
C2B	1.13074 (10)	0.07922 (10)	0.54267 (9)	0.0206 (3)
H2BA	1.1665	0.0549	0.5205	0.025*
C3B	1.17063 (10)	0.09028 (10)	0.62243 (9)	0.0213 (3)
C4B	1.11777 (11)	0.12564 (10)	0.65642 (8)	0.0220 (3)
H4BA	1.1457	0.1329	0.7100	0.026*
C5B	1.02313 (10)	0.14997 (9)	0.60976 (8)	0.0184 (3)
C6B	0.97838 (10)	0.14116 (9)	0.52777 (8)	0.0172 (3)
C7B	0.87935 (10)	0.16500 (9)	0.47616 (8)	0.0169 (3)
H7BA	0.8555	0.1456	0.4252	0.020*
C8B	0.81720 (10)	0.21120 (9)	0.49162 (8)	0.0174 (3)
H8BA	0.8372	0.2320	0.5418	0.021*
C9B	0.71850 (10)	0.22977 (9)	0.43148 (8)	0.0164 (3)
C10B	0.65299 (10)	0.28005 (9)	0.45157 (8)	0.0174 (3)
H10B	0.5947	0.2990	0.4115	0.021*
C11B	0.67345 (10)	0.29988 (9)	0.52518 (8)	0.0163 (3)
H11B	0.7353	0.2846	0.5620	0.020*
C12B	0.61648 (10)	0.34076 (9)	0.55742 (8)	0.0162 (3)
C13B	0.52085 (10)	0.37092 (9)	0.51463 (8)	0.0169 (3)
C14B	0.46987 (10)	0.40590 (9)	0.55087 (8)	0.0190 (3)
H14B	0.4072	0.4259	0.5217	0.023*
C15B	0.51478 (11)	0.41016 (9)	0.63141 (9)	0.0195 (3)
C16B	0.60879 (11)	0.38162 (10)	0.67653 (8)	0.0194 (3)
H16B	0.6376	0.3849	0.7304	0.023*
C17B	0.65853 (10)	0.34824 (9)	0.63965 (8)	0.0171 (3)
C18B	1.04507 (11)	0.06389 (11)	0.38133 (9)	0.0248 (3)
H18D	1.0042	0.0593	0.3264	0.037*
H18E	1.0694	0.0064	0.4021	0.037*
H18F	1.0978	0.1027	0.3911	0.037*
C19B	1.31903 (11)	0.02436 (11)	0.64289 (10)	0.0280 (4)
H19D	1.3822	0.0125	0.6843	0.042*
H19E	1.3238	0.0615	0.6049	0.042*
H19F	1.2885	-0.0303	0.6191	0.042*
C20B	1.00518 (12)	0.18825 (12)	0.72165 (8)	0.0293 (4)
H20D	0.9576	0.2116	0.7344	0.044*
H20E	1.0597	0.2271	0.7413	0.044*
H20F	1.0249	0.1308	0.7446	0.044*

supplementary materials

C21B	0.38459 (10)	0.39154 (10)	0.38923 (8)	0.0226 (3)
H21D	0.3672	0.3838	0.3354	0.034*
H21E	0.3787	0.4528	0.3992	0.034*
H21G	0.3427	0.3568	0.4018	0.034*
C22B	0.37374 (12)	0.47159 (12)	0.63068 (10)	0.0315 (4)
H22D	0.3517	0.4916	0.6664	0.047*
H22G	0.3344	0.4233	0.6006	0.047*
H22E	0.3697	0.5192	0.5967	0.047*
C23B	0.80039 (12)	0.33050 (12)	0.76164 (8)	0.0273 (4)
H23G	0.8652	0.3097	0.7818	0.041*
H23D	0.7680	0.2974	0.7845	0.041*
H23E	0.8009	0.3920	0.7740	0.041*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0300 (7)	0.0677 (9)	0.0156 (5)	-0.0216 (6)	0.0063 (5)	0.0002 (6)
O2A	0.0209 (6)	0.0262 (6)	0.0191 (5)	-0.0032 (4)	0.0099 (4)	0.0011 (4)
O3A	0.0156 (5)	0.0298 (6)	0.0281 (6)	-0.0049 (4)	0.0072 (5)	-0.0042 (5)
O4A	0.0176 (5)	0.0289 (6)	0.0148 (5)	-0.0008 (4)	0.0064 (4)	0.0027 (4)
O5A	0.0171 (5)	0.0276 (6)	0.0170 (5)	-0.0012 (4)	0.0049 (4)	-0.0006 (4)
O6A	0.0247 (6)	0.0382 (7)	0.0270 (6)	-0.0021 (5)	0.0151 (5)	0.0055 (5)
O7A	0.0178 (5)	0.0333 (6)	0.0154 (5)	-0.0011 (4)	0.0049 (4)	0.0006 (4)
C1A	0.0195 (7)	0.0141 (7)	0.0196 (7)	0.0018 (5)	0.0094 (6)	-0.0001 (5)
C2A	0.0194 (7)	0.0167 (7)	0.0258 (7)	0.0003 (6)	0.0133 (6)	-0.0008 (6)
C3A	0.0143 (7)	0.0175 (7)	0.0252 (7)	0.0003 (6)	0.0069 (6)	-0.0035 (6)
C4A	0.0179 (7)	0.0214 (7)	0.0174 (7)	0.0017 (6)	0.0055 (6)	-0.0003 (5)
C5A	0.0173 (7)	0.0162 (7)	0.0197 (7)	0.0024 (5)	0.0080 (6)	0.0006 (5)
C6A	0.0155 (7)	0.0161 (7)	0.0175 (7)	0.0012 (5)	0.0065 (6)	-0.0002 (5)
C7A	0.0185 (7)	0.0174 (7)	0.0153 (6)	0.0021 (6)	0.0056 (6)	0.0005 (5)
C8A	0.0183 (7)	0.0208 (7)	0.0147 (6)	-0.0002 (6)	0.0047 (6)	-0.0002 (5)
C9A	0.0208 (8)	0.0220 (7)	0.0164 (7)	-0.0005 (6)	0.0058 (6)	0.0019 (6)
C10A	0.0166 (7)	0.0217 (7)	0.0202 (7)	-0.0015 (6)	0.0064 (6)	-0.0011 (6)
C11A	0.0162 (7)	0.0155 (7)	0.0185 (7)	0.0015 (5)	0.0061 (6)	-0.0007 (5)
C12A	0.0171 (7)	0.0157 (7)	0.0193 (7)	0.0023 (5)	0.0078 (6)	0.0000 (5)
C13A	0.0190 (7)	0.0160 (7)	0.0185 (7)	0.0042 (6)	0.0076 (6)	-0.0001 (5)
C14A	0.0172 (7)	0.0190 (7)	0.0236 (7)	0.0002 (6)	0.0088 (6)	-0.0010 (6)
C15A	0.0226 (8)	0.0208 (8)	0.0264 (8)	0.0029 (6)	0.0145 (7)	0.0024 (6)
C16A	0.0235 (8)	0.0252 (8)	0.0184 (7)	0.0038 (6)	0.0099 (6)	0.0014 (6)
C17A	0.0177 (7)	0.0184 (7)	0.0200 (7)	0.0027 (6)	0.0074 (6)	-0.0008 (5)
C18A	0.0253 (8)	0.0243 (8)	0.0257 (8)	0.0001 (6)	0.0158 (7)	0.0025 (6)
C19A	0.0198 (8)	0.0420 (10)	0.0378 (9)	-0.0093 (7)	0.0152 (7)	-0.0138 (8)
C20A	0.0226 (8)	0.0380 (9)	0.0156 (7)	-0.0009 (7)	0.0064 (6)	0.0028 (6)
C21A	0.0188 (8)	0.0230 (8)	0.0218 (7)	-0.0007 (6)	0.0052 (6)	-0.0039 (6)
C22A	0.0235 (8)	0.0286 (8)	0.0330 (8)	-0.0006 (7)	0.0162 (7)	0.0025 (7)
C23A	0.0224 (8)	0.0403 (10)	0.0166 (7)	-0.0001 (7)	0.0072 (6)	0.0002 (6)
O1B	0.0171 (5)	0.0371 (6)	0.0154 (5)	0.0035 (5)	0.0053 (4)	-0.0032 (4)
O2B	0.0181 (5)	0.0317 (6)	0.0179 (5)	0.0030 (4)	0.0085 (4)	-0.0004 (4)

O3B	0.0161 (5)	0.0345 (7)	0.0276 (6)	0.0042 (5)	0.0036 (5)	0.0039 (5)
O4B	0.0188 (5)	0.0312 (6)	0.0133 (5)	0.0019 (4)	0.0044 (4)	-0.0025 (4)
O5B	0.0158 (5)	0.0258 (6)	0.0169 (5)	0.0038 (4)	0.0042 (4)	0.0001 (4)
O6B	0.0224 (6)	0.0326 (6)	0.0266 (6)	0.0046 (5)	0.0144 (5)	-0.0028 (5)
O7B	0.0169 (5)	0.0304 (6)	0.0142 (5)	0.0040 (4)	0.0059 (4)	0.0000 (4)
C1B	0.0180 (7)	0.0176 (7)	0.0190 (7)	-0.0025 (6)	0.0081 (6)	0.0008 (5)
C2B	0.0165 (7)	0.0186 (7)	0.0267 (8)	-0.0001 (6)	0.0101 (6)	0.0022 (6)
C3B	0.0137 (7)	0.0190 (7)	0.0259 (8)	-0.0006 (6)	0.0046 (6)	0.0042 (6)
C4B	0.0190 (8)	0.0229 (8)	0.0172 (7)	-0.0018 (6)	0.0026 (6)	0.0009 (6)
C5B	0.0171 (7)	0.0170 (7)	0.0191 (7)	-0.0017 (6)	0.0070 (6)	-0.0001 (5)
C6B	0.0153 (7)	0.0158 (7)	0.0179 (7)	-0.0023 (5)	0.0057 (6)	0.0007 (5)
C7B	0.0155 (7)	0.0194 (7)	0.0141 (6)	-0.0038 (5)	0.0054 (5)	0.0006 (5)
C8B	0.0176 (7)	0.0185 (7)	0.0138 (6)	-0.0021 (6)	0.0054 (6)	-0.0005 (5)
C9B	0.0170 (7)	0.0174 (7)	0.0151 (6)	-0.0026 (5)	0.0079 (6)	0.0008 (5)
C10B	0.0144 (7)	0.0186 (7)	0.0170 (6)	0.0006 (5)	0.0055 (6)	0.0015 (5)
C11B	0.0150 (7)	0.0147 (7)	0.0183 (7)	0.0000 (5)	0.0070 (6)	0.0015 (5)
C12B	0.0178 (7)	0.0145 (7)	0.0172 (6)	-0.0008 (5)	0.0089 (6)	-0.0001 (5)
C13B	0.0180 (7)	0.0143 (7)	0.0167 (6)	-0.0014 (5)	0.0066 (6)	-0.0005 (5)
C14B	0.0151 (7)	0.0168 (7)	0.0245 (7)	0.0006 (5)	0.0089 (6)	-0.0006 (6)
C15B	0.0218 (8)	0.0167 (7)	0.0258 (7)	-0.0012 (6)	0.0159 (6)	-0.0017 (6)
C16B	0.0212 (8)	0.0206 (7)	0.0175 (7)	-0.0001 (6)	0.0098 (6)	-0.0006 (5)
C17B	0.0169 (7)	0.0166 (7)	0.0173 (6)	-0.0006 (5)	0.0076 (6)	0.0006 (5)
C18B	0.0238 (8)	0.0286 (8)	0.0273 (8)	0.0000 (6)	0.0164 (7)	-0.0014 (6)
C19B	0.0163 (8)	0.0273 (9)	0.0360 (9)	0.0032 (6)	0.0084 (7)	0.0064 (7)
C20B	0.0307 (9)	0.0356 (9)	0.0151 (7)	0.0042 (7)	0.0053 (7)	-0.0030 (6)
C21B	0.0168 (7)	0.0251 (8)	0.0208 (7)	0.0016 (6)	0.0045 (6)	0.0028 (6)
C22B	0.0232 (9)	0.0388 (10)	0.0357 (9)	0.0053 (7)	0.0165 (7)	-0.0035 (7)
C23B	0.0224 (8)	0.0412 (10)	0.0152 (7)	0.0045 (7)	0.0063 (6)	-0.0010 (6)

Geometric parameters (Å, °)

O1A—C9A	1.2341 (17)	O1B—C9B	1.2404 (16)
O2A—C1A	1.3631 (17)	O2B—C1B	1.3643 (17)
O2A—C18A	1.4324 (17)	O2B—C18B	1.4282 (18)
O3A—C3A	1.3668 (17)	O3B—C3B	1.3672 (18)
O3A—C19A	1.430 (2)	O3B—C19B	1.433 (2)
O4A—C5A	1.3600 (17)	O4B—C5B	1.3631 (18)
O4A—C20A	1.4327 (16)	O4B—C20B	1.4324 (17)
O5A—C13A	1.3607 (16)	O5B—C13B	1.3607 (16)
O5A—C21A	1.4314 (17)	O5B—C21B	1.4379 (17)
O6A—C15A	1.3661 (18)	O6B—C15B	1.3716 (17)
O6A—C22A	1.4277 (19)	O6B—C22B	1.4316 (19)
O7A—C17A	1.3637 (17)	O7B—C17B	1.3648 (17)
O7A—C23A	1.4294 (17)	O7B—C23B	1.4357 (17)
C1A—C2A	1.391 (2)	C1B—C2B	1.396 (2)
C1A—C6A	1.418 (2)	C1B—C6B	1.410 (2)
C2A—C3A	1.391 (2)	C2B—C3B	1.388 (2)
C2A—H2AA	0.9300	C2B—H2BA	0.9300
C3A—C4A	1.393 (2)	C3B—C4B	1.390 (2)

supplementary materials

C4A—C5A	1.383 (2)	C4B—C5B	1.384 (2)
C4A—H4AA	0.9300	C4B—H4BA	0.9300
C5A—C6A	1.4250 (19)	C5B—C6B	1.4194 (19)
C6A—C7A	1.451 (2)	C6B—C7B	1.4518 (19)
C7A—C8A	1.340 (2)	C7B—C8B	1.346 (2)
C7A—H7AA	0.9300	C7B—H7BA	0.9300
C8A—C9A	1.475 (2)	C8B—C9B	1.4717 (19)
C8A—H8AA	0.9300	C8B—H8BA	0.9300
C9A—C10A	1.465 (2)	C9B—C10B	1.474 (2)
C10A—C11A	1.342 (2)	C10B—C11B	1.3484 (19)
C10A—H10A	0.9300	C10B—H10B	0.9300
C11A—C12A	1.449 (2)	C11B—C12B	1.4514 (19)
C11A—H11A	0.9300	C11B—H11B	0.9300
C12A—C13A	1.408 (2)	C12B—C13B	1.413 (2)
C12A—C17A	1.4186 (19)	C12B—C17B	1.4238 (19)
C13A—C14A	1.396 (2)	C13B—C14B	1.397 (2)
C14A—C15A	1.390 (2)	C14B—C15B	1.389 (2)
C14A—H14A	0.9300	C14B—H14B	0.9300
C15A—C16A	1.392 (2)	C15B—C16B	1.391 (2)
C16A—C17A	1.382 (2)	C16B—C17B	1.382 (2)
C16A—H16A	0.9300	C16B—H16B	0.9300
C18A—H18A	0.9600	C18B—H18D	0.9600
C18A—H18B	0.9600	C18B—H18E	0.9600
C18A—H18C	0.9600	C18B—H18F	0.9600
C19A—H19A	0.9600	C19B—H19D	0.9600
C19A—H19B	0.9600	C19B—H19E	0.9600
C19A—H19C	0.9600	C19B—H19F	0.9600
C20A—H20A	0.9600	C20B—H20D	0.9600
C20A—H20B	0.9600	C20B—H20E	0.9600
C20A—H20C	0.9600	C20B—H20F	0.9600
C21A—H21A	0.9600	C21B—H21D	0.9600
C21A—H21B	0.9600	C21B—H21E	0.9600
C21A—H21C	0.9600	C21B—H21G	0.9600
C22A—H22A	0.9600	C22B—H22D	0.9600
C22A—H22B	0.9600	C22B—H22G	0.9600
C22A—H22C	0.9600	C22B—H22E	0.9600
C23A—H23A	0.9600	C23B—H23G	0.9600
C23A—H23B	0.9600	C23B—H23D	0.9600
C23A—H23C	0.9600	C23B—H23E	0.9600
C1A—O2A—C18A	118.11 (11)	C1B—O2B—C18B	118.46 (12)
C3A—O3A—C19A	117.06 (12)	C3B—O3B—C19B	117.61 (12)
C5A—O4A—C20A	118.13 (11)	C5B—O4B—C20B	117.96 (12)
C13A—O5A—C21A	118.64 (11)	C13B—O5B—C21B	118.29 (11)
C15A—O6A—C22A	118.28 (12)	C15B—O6B—C22B	117.81 (12)
C17A—O7A—C23A	118.30 (12)	C17B—O7B—C23B	117.80 (11)
O2A—C1A—C2A	122.34 (13)	O2B—C1B—C2B	122.27 (13)
O2A—C1A—C6A	115.35 (12)	O2B—C1B—C6B	115.09 (12)
C2A—C1A—C6A	122.31 (13)	C2B—C1B—C6B	122.64 (13)
C1A—C2A—C3A	118.70 (13)	C3B—C2B—C1B	118.43 (14)

C1A—C2A—H2AA	120.6	C3B—C2B—H2BA	120.8
C3A—C2A—H2AA	120.6	C1B—C2B—H2BA	120.8
O3A—C3A—C2A	123.44 (13)	O3B—C3B—C2B	123.77 (14)
O3A—C3A—C4A	115.15 (13)	O3B—C3B—C4B	114.82 (13)
C2A—C3A—C4A	121.41 (13)	C2B—C3B—C4B	121.41 (13)
C5A—C4A—C3A	119.37 (13)	C5B—C4B—C3B	119.32 (13)
C5A—C4A—H4AA	120.3	C5B—C4B—H4BA	120.3
C3A—C4A—H4AA	120.3	C3B—C4B—H4BA	120.3
O4A—C5A—C4A	123.06 (13)	O4B—C5B—C4B	122.72 (13)
O4A—C5A—C6A	115.16 (12)	O4B—C5B—C6B	115.21 (12)
C4A—C5A—C6A	121.78 (13)	C4B—C5B—C6B	122.04 (13)
C1A—C6A—C5A	116.41 (13)	C1B—C6B—C5B	116.16 (13)
C1A—C6A—C7A	118.89 (12)	C1B—C6B—C7B	119.47 (13)
C5A—C6A—C7A	124.64 (13)	C5B—C6B—C7B	124.37 (13)
C8A—C7A—C6A	130.38 (13)	C8B—C7B—C6B	129.17 (13)
C8A—C7A—H7AA	114.8	C8B—C7B—H7BA	115.4
C6A—C7A—H7AA	114.8	C6B—C7B—H7BA	115.4
C7A—C8A—C9A	120.69 (13)	C7B—C8B—C9B	121.91 (13)
C7A—C8A—H8AA	119.7	C7B—C8B—H8BA	119.0
C9A—C8A—H8AA	119.7	C9B—C8B—H8BA	119.0
O1A—C9A—C10A	119.07 (13)	O1B—C9B—C8B	121.64 (13)
O1A—C9A—C8A	120.49 (14)	O1B—C9B—C10B	118.57 (12)
C10A—C9A—C8A	120.42 (12)	C8B—C9B—C10B	119.77 (12)
C11A—C10A—C9A	123.14 (13)	C11B—C10B—C9B	123.21 (13)
C11A—C10A—H10A	118.4	C11B—C10B—H10B	118.4
C9A—C10A—H10A	118.4	C9B—C10B—H10B	118.4
C10A—C11A—C12A	131.90 (14)	C10B—C11B—C12B	131.73 (13)
C10A—C11A—H11A	114.0	C10B—C11B—H11B	114.1
C12A—C11A—H11A	114.0	C12B—C11B—H11B	114.1
C13A—C12A—C17A	116.96 (13)	C13B—C12B—C17B	116.47 (12)
C13A—C12A—C11A	125.77 (13)	C13B—C12B—C11B	125.83 (12)
C17A—C12A—C11A	117.27 (13)	C17B—C12B—C11B	117.65 (12)
O5A—C13A—C14A	122.67 (13)	O5B—C13B—C14B	122.59 (13)
O5A—C13A—C12A	115.42 (13)	O5B—C13B—C12B	115.46 (12)
C14A—C13A—C12A	121.91 (13)	C14B—C13B—C12B	121.95 (13)
C15A—C14A—C13A	118.66 (14)	C15B—C14B—C13B	118.61 (13)
C15A—C14A—H14A	120.7	C15B—C14B—H14B	120.7
C13A—C14A—H14A	120.7	C13B—C14B—H14B	120.7
O6A—C15A—C14A	123.94 (14)	O6B—C15B—C14B	123.52 (13)
O6A—C15A—C16A	114.52 (13)	O6B—C15B—C16B	114.49 (13)
C14A—C15A—C16A	121.54 (14)	C14B—C15B—C16B	121.99 (13)
C17A—C16A—C15A	119.10 (14)	C17B—C16B—C15B	118.61 (13)
C17A—C16A—H16A	120.5	C17B—C16B—H16B	120.7
C15A—C16A—H16A	120.5	C15B—C16B—H16B	120.7
O7A—C17A—C16A	123.15 (13)	O7B—C17B—C16B	122.87 (12)
O7A—C17A—C12A	115.01 (13)	O7B—C17B—C12B	114.76 (12)
C16A—C17A—C12A	121.83 (14)	C16B—C17B—C12B	122.37 (13)
O2A—C18A—H18A	109.5	O2B—C18B—H18D	109.5
O2A—C18A—H18B	109.5	O2B—C18B—H18E	109.5

supplementary materials

H18A—C18A—H18B	109.5	H18D—C18B—H18E	109.5
O2A—C18A—H18C	109.5	O2B—C18B—H18F	109.5
H18A—C18A—H18C	109.5	H18D—C18B—H18F	109.5
H18B—C18A—H18C	109.5	H18E—C18B—H18F	109.5
O3A—C19A—H19A	109.5	O3B—C19B—H19D	109.5
O3A—C19A—H19B	109.5	O3B—C19B—H19E	109.5
H19A—C19A—H19B	109.5	H19D—C19B—H19E	109.5
O3A—C19A—H19C	109.5	O3B—C19B—H19F	109.5
H19A—C19A—H19C	109.5	H19D—C19B—H19F	109.5
H19B—C19A—H19C	109.5	H19E—C19B—H19F	109.5
O4A—C20A—H20A	109.5	O4B—C20B—H20D	109.5
O4A—C20A—H20B	109.5	O4B—C20B—H20E	109.5
H20A—C20A—H20B	109.5	H20D—C20B—H20E	109.5
O4A—C20A—H20C	109.5	O4B—C20B—H20F	109.5
H20A—C20A—H20C	109.5	H20D—C20B—H20F	109.5
H20B—C20A—H20C	109.5	H20E—C20B—H20F	109.5
O5A—C21A—H21A	109.5	O5B—C21B—H21D	109.5
O5A—C21A—H21B	109.5	O5B—C21B—H21E	109.5
H21A—C21A—H21B	109.5	H21D—C21B—H21E	109.5
O5A—C21A—H21C	109.5	O5B—C21B—H21G	109.5
H21A—C21A—H21C	109.5	H21D—C21B—H21G	109.5
H21B—C21A—H21C	109.5	H21E—C21B—H21G	109.5
O6A—C22A—H22A	109.5	O6B—C22B—H22D	109.5
O6A—C22A—H22B	109.5	O6B—C22B—H22G	109.5
H22A—C22A—H22B	109.5	H22D—C22B—H22G	109.5
O6A—C22A—H22C	109.5	O6B—C22B—H22E	109.5
H22A—C22A—H22C	109.5	H22D—C22B—H22E	109.5
H22B—C22A—H22C	109.5	H22G—C22B—H22E	109.5
O7A—C23A—H23A	109.5	O7B—C23B—H23G	109.5
O7A—C23A—H23B	109.5	O7B—C23B—H23D	109.5
H23A—C23A—H23B	109.5	H23G—C23B—H23D	109.5
O7A—C23A—H23C	109.5	O7B—C23B—H23E	109.5
H23A—C23A—H23C	109.5	H23G—C23B—H23E	109.5
H23B—C23A—H23C	109.5	H23D—C23B—H23E	109.5
C18A—O2A—C1A—C2A	-1.5 (2)	C18B—O2B—C1B—C2B	-0.7 (2)
C18A—O2A—C1A—C6A	178.45 (12)	C18B—O2B—C1B—C6B	179.23 (13)
O2A—C1A—C2A—C3A	-179.22 (13)	O2B—C1B—C2B—C3B	178.78 (13)
C6A—C1A—C2A—C3A	0.8 (2)	C6B—C1B—C2B—C3B	-1.1 (2)
C19A—O3A—C3A—C2A	-7.2 (2)	C19B—O3B—C3B—C2B	-5.5 (2)
C19A—O3A—C3A—C4A	173.26 (13)	C19B—O3B—C3B—C4B	174.68 (13)
C1A—C2A—C3A—O3A	179.02 (13)	C1B—C2B—C3B—O3B	-179.09 (14)
C1A—C2A—C3A—C4A	-1.4 (2)	C1B—C2B—C3B—C4B	0.7 (2)
O3A—C3A—C4A—C5A	-179.30 (13)	O3B—C3B—C4B—C5B	-179.89 (13)
C2A—C3A—C4A—C5A	1.1 (2)	C2B—C3B—C4B—C5B	0.3 (2)
C20A—O4A—C5A—C4A	4.1 (2)	C20B—O4B—C5B—C4B	-0.6 (2)
C20A—O4A—C5A—C6A	-176.28 (13)	C20B—O4B—C5B—C6B	177.44 (13)
C3A—C4A—C5A—O4A	179.50 (13)	C3B—C4B—C5B—O4B	176.94 (13)
C3A—C4A—C5A—C6A	-0.1 (2)	C3B—C4B—C5B—C6B	-0.9 (2)
O2A—C1A—C6A—C5A	-179.87 (12)	O2B—C1B—C6B—C5B	-179.37 (12)

C2A—C1A—C6A—C5A	0.1 (2)	C2B—C1B—C6B—C5B	0.5 (2)
O2A—C1A—C6A—C7A	2.78 (19)	O2B—C1B—C6B—C7B	1.53 (19)
C2A—C1A—C6A—C7A	-177.23 (13)	C2B—C1B—C6B—C7B	-178.56 (13)
O4A—C5A—C6A—C1A	179.88 (12)	O4B—C5B—C6B—C1B	-177.51 (12)
C4A—C5A—C6A—C1A	-0.5 (2)	C4B—C5B—C6B—C1B	0.5 (2)
O4A—C5A—C6A—C7A	-2.9 (2)	O4B—C5B—C6B—C7B	1.5 (2)
C4A—C5A—C6A—C7A	176.72 (14)	C4B—C5B—C6B—C7B	179.55 (14)
C1A—C6A—C7A—C8A	-179.23 (15)	C1B—C6B—C7B—C8B	-169.16 (14)
C5A—C6A—C7A—C8A	3.7 (2)	C5B—C6B—C7B—C8B	11.8 (2)
C6A—C7A—C8A—C9A	-175.78 (14)	C6B—C7B—C8B—C9B	179.71 (13)
C7A—C8A—C9A—O1A	1.1 (2)	C7B—C8B—C9B—O1B	0.5 (2)
C7A—C8A—C9A—C10A	179.37 (14)	C7B—C8B—C9B—C10B	179.49 (13)
O1A—C9A—C10A—C11A	176.83 (15)	O1B—C9B—C10B—C11B	169.13 (14)
C8A—C9A—C10A—C11A	-1.4 (2)	C8B—C9B—C10B—C11B	-9.9 (2)
C9A—C10A—C11A—C12A	-178.22 (15)	C9B—C10B—C11B—C12B	-173.57 (14)
C10A—C11A—C12A—C13A	-6.6 (3)	C10B—C11B—C12B—C13B	-0.5 (3)
C10A—C11A—C12A—C17A	173.70 (15)	C10B—C11B—C12B—C17B	176.71 (15)
C21A—O5A—C13A—C14A	-0.1 (2)	C21B—O5B—C13B—C14B	-0.9 (2)
C21A—O5A—C13A—C12A	-179.80 (12)	C21B—O5B—C13B—C12B	179.03 (12)
C17A—C12A—C13A—O5A	179.72 (12)	C17B—C12B—C13B—O5B	179.84 (12)
C11A—C12A—C13A—O5A	0.1 (2)	C11B—C12B—C13B—O5B	-2.9 (2)
C17A—C12A—C13A—C14A	0.0 (2)	C17B—C12B—C13B—C14B	-0.3 (2)
C11A—C12A—C13A—C14A	-179.66 (14)	C11B—C12B—C13B—C14B	177.01 (13)
O5A—C13A—C14A—C15A	-179.28 (13)	O5B—C13B—C14B—C15B	179.29 (13)
C12A—C13A—C14A—C15A	0.4 (2)	C12B—C13B—C14B—C15B	-0.6 (2)
C22A—O6A—C15A—C14A	-0.7 (2)	C22B—O6B—C15B—C14B	1.6 (2)
C22A—O6A—C15A—C16A	179.22 (13)	C22B—O6B—C15B—C16B	-178.63 (14)
C13A—C14A—C15A—O6A	179.70 (14)	C13B—C14B—C15B—O6B	-179.60 (13)
C13A—C14A—C15A—C16A	-0.2 (2)	C13B—C14B—C15B—C16B	0.7 (2)
O6A—C15A—C16A—C17A	179.69 (13)	O6B—C15B—C16B—C17B	-179.62 (13)
C14A—C15A—C16A—C17A	-0.4 (2)	C14B—C15B—C16B—C17B	0.1 (2)
C23A—O7A—C17A—C16A	0.8 (2)	C23B—O7B—C17B—C16B	-4.9 (2)
C23A—O7A—C17A—C12A	-178.34 (13)	C23B—O7B—C17B—C12B	175.67 (13)
C15A—C16A—C17A—O7A	-178.23 (14)	C15B—C16B—C17B—O7B	179.56 (13)
C15A—C16A—C17A—C12A	0.8 (2)	C15B—C16B—C17B—C12B	-1.0 (2)
C13A—C12A—C17A—O7A	178.48 (12)	C13B—C12B—C17B—O7B	-179.45 (12)
C11A—C12A—C17A—O7A	-1.82 (19)	C11B—C12B—C17B—O7B	3.04 (18)
C13A—C12A—C17A—C16A	-0.6 (2)	C13B—C12B—C17B—C16B	1.1 (2)
C11A—C12A—C17A—C16A	179.06 (13)	C11B—C12B—C17B—C16B	-176.40 (13)

Hydrogen-bond geometry (Å, °)

Cg1, Cg2 and Cg3 are the centroids of the C1A—C6A, C12A—C17A and C12B—C17B rings, respectively

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C7A—H7AA...O1A	0.93	2.42	2.787 (2)	104
C7A—H7AA...O2A	0.93	2.29	2.704 (2)	106
C8A—H8AA...O4A	0.93	2.18	2.7844 (17)	121
C7B—H7BA...O1B	0.93	2.49	2.8351 (19)	102
C7B—H7BA...O2B	0.93	2.33	2.704 (2)	104

supplementary materials

C8B—H8BA…O4B	0.93	2.16	2.7643 (18)	121
C10A—H10A…O5A	0.93	2.26	2.852 (2)	121
C10B—H10B…O5B	0.93	2.26	2.855 (2)	121
C11A—H11A…O7A	0.93	2.23	2.6599 (17)	108
C11B—H11B…O7B	0.93	2.23	2.6700 (17)	108
C20A—H20C…O1B	0.96	2.47	3.339 (2)	151
C20B—H20E…O1A ⁱ	0.96	2.37	3.0238 (19)	125
C23A—H23C…O1A ⁱⁱ	0.96	2.39	3.319 (2)	162
C23B—H23D…O1B ⁱⁱ	0.96	2.41	3.262 (2)	148
C18A—H18C…Cg1 ⁱⁱⁱ	0.96	2.65	3.4503 (17)	141
C21A—H21C…Cg2 ^{iv}	0.96	2.94	3.5813 (18)	126
C21B—H21E…Cg3 ^v	0.96	2.72	3.5809 (16)	150

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

Fig. 1

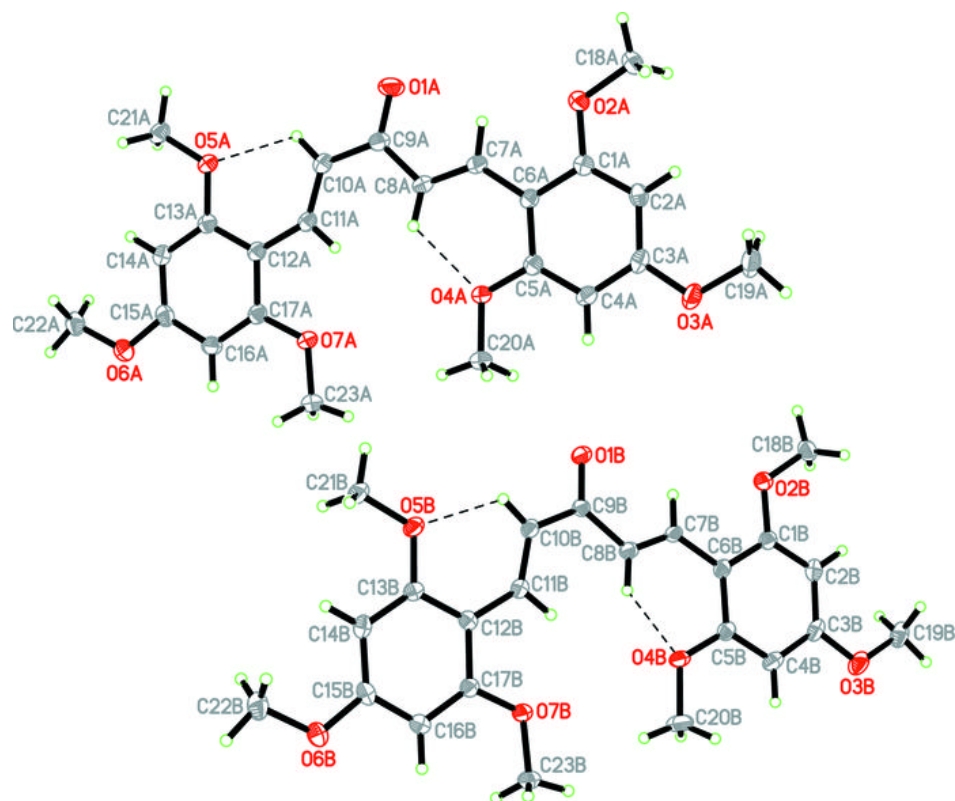


Fig. 2

