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(E)-Methyl 2-[(2-formyl-6-methoxyphenoxy)methyl]-3-phenylacrylate

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ (C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.137; data-to-parameter ratio = 19.2.

The title compound, C₁₉H₁₈O₅, crystallizes with two independent molecules (A and B) in an asymmetric unit in both of which the two aromatic rings are in a bisectional orientation as evidenced by the dihedral angle between them $[41.7 (1)^{\circ}]$ in molecule A and 35.6 (1)° in molecule B]. Both molecules adopt an E configuration with respect to the C=C bond. An intramolecular C-H···O hydrogen-bond occurs in molecule A. The crystal packing features intermolecular $C-H\cdots O$ interactions.

Related literature

For background to the synthesis, see: Bakthadoss et al. (2009). For related phenyl acrylate compounds, see: Wang et al. (2006); Jones & Jäger (2003). For their biological properties, see: Kim et al. (2004); Zhu et al. (2000).



8303 independent reflections

 $R_{\rm int} = 0.032$

5258 reflections with $I > 2\sigma(I)$

Experimental

Crystal data

$C_{19}H_{18}O_5$	$\gamma = 103.475 \ (3)^{\circ}$
$M_r = 326.33$	V = 1663.33 (16) Å ³
Triclinic, P1	Z = 4
a = 8.4696 (5) Å	Mo $K\alpha$ radiation
b = 12.1662 (7) Å	$\mu = 0.09 \text{ mm}^{-1}$
c = 16.9860 (9) Å	T = 293 K
$\alpha = 94.423 \ (3)^{\circ}$	$0.20 \times 0.20 \times 0.20$ mm
$\beta = 100.038 \ (3)^{\circ}$	

Data collection

Bruker SMART APEXII areadetector diffractometer 30114 measured reflections

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	433 parameters
$vR(F^2) = 0.137$	H-atom parameters constrained
S = 0.93	$\Delta \rho_{\rm max} = 0.17 \ {\rm e} \ {\rm \AA}^{-3}$
3303 reflections	$\Delta \rho_{\rm min} = -0.18 \text{ e } \text{\AA}^{-3}$

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

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$C17A - H17A \cdots O2A$	0.93	2.48	3.354 (2)	156
$C9A - H9A1 \cdots O4B^{i}$	0.97	2.55	3.2215 (16)	126
$C19B - H19D \cdots O5A^{ii}$	0.96	2.43	3.275 (3)	147

Symmetry codes: (i) -x + 1, -y + 2, -z + 2; (ii) -x + 1, -y + 1, -z + 2.

Data collection: APEX2 (Bruker, 2008): cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97, PLATON (Spek, 2009) and publCIF (Westrip, 2010).

The authors thank the TBI X-ray facility, CAS in Crystallography and Biophysics University of Madras, India, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2375).

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supporting information

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(E)-Methyl 2-[(2-formyl-6-methoxyphenoxy)methyl]-3-phenylacrylate

T. Anuradha, G. Sivakumar, P. R. Seshadri and M. Bakthadoss

S1. Comment

Methyl cinnamate is used widely due to its flavour and fragrance in productions of cosmetics, beverages, baked goods, and convenience foods (Kim *et al.*, 2004). Cinnamic acid exhibits higher antifungal activity against *Asperigillus niger*, comparing to that of miconazole and a significant antifungal effect against *A. flavus* and *A. terreus*, while caffeic acid was inactive to the antifungal activity (Zhu *et al.*, 2000). In view of this medicinal importance, the crystal structure determination of the title compound was carried out and the results are presented here.

The asymmetric unit of the title compound contains the two independent molecules, A and B (Fig. 1). The dihedral angle between the C1 – C6 and C10 – C15 benzene rings is 41.7 (1)° in molecule A whereas it is 35.6 (1)° in molecule B. Both the molecules adopt *E* configurations with respect to the C = C bond. The methoxy and formyl group at the *meta* positions of the benzene group are close to being coplanar with the ring (5.7 (1)° and 4.2 (1)° in molecule A and 1.5 (1)° and 2.3 (1)° in molecule B). The central unit(C8/C9/C10/O4) is equatorial with respect to the phenylacrylate and formyl-methoxyphenyoxy (C1- C8/C18/C19/O1/O2 = 78.5 (1)° and C10 – C17/O3/O5 =69.5 (1)° in molecule A and 78.3 (1)° and 61.3 (2)° in molecule B). The acrylate group in molecule A is +*syn* periplanar with respect to central unit (C9/C8/C18/O2 = 2.7 (1)°) whereas in molecule B, the acrylate group is –antiperiplanar with respect to the central unit (C9/C8/C18/O2 = 176.7 (2)°) as evidenced by torsion angles.

The crystal packing is stabilised by intramolecular and intermolecular $C - H^{...} O$ hydrogen bond interactions (Table 1, Fig. 2).

S2. Experimental

A solution of 2-hydroxy-3-methoxybenzaldehyde(1.0 mmol, 0.152 g) and potassium carbonate (2.0 mmol, 0.2293 g) in acetonitrile solvent (5 mL) was stirred for 15 m at room temperature. To this solution, (*Z*)-methyl-2-(bromomethyl)-3-phenylacrylate(1.2 mmol, 0.25 g) was added drop wise. After the completion of the reaction, as indicated by TLC, acetonitrile was evaporated. EtOAc (15 mL) and water (15 mL) were added to the crude mass. The organic layer was dried over anhydrous sodium sulfate. Removal of solvent led to the crude product, which was purified through pad of silica gel (100–200 mesh) using ethylacetate and hexanes (1:9) as solvents. The pure title compound was obtained as a colourless solid (0.31 g, 95% yield). Recrystallization was carried out using ethylacetate as a solvent.

S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.5Ueq(C)$ for methylH atoms and 1.2Ueq(C) for other H atoms.



Figure 1

Molecular structure of the title compound, showing 30% probability displacement ellipsoids.



Fig 2. Packing diagram of the molecule showing hydrogen bonds

Figure 2

Packing of (I) with hydrogen bonds (dashed lines).

(E)-Methyl 2-[(2-formyl-6-methoxyphenoxy)methyl]-3-phenylacrylate

Crystal data

 $\begin{array}{l} C_{19}H_{18}O_5\\ M_r = 326.33\\ \text{Triclinic, }P\overline{1}\\ \text{Hall symbol: -P 1}\\ a = 8.4696 (5) \text{ Å}\\ b = 12.1662 (7) \text{ Å}\\ c = 16.9860 (9) \text{ Å}\\ a = 94.423 (3)^{\circ}\\ \beta = 100.038 (3)^{\circ}\\ \gamma = 103.475 (3)^{\circ}\\ V = 1663.33 (16) \text{ Å}^3 \end{array}$

Data collection

Bruker SMART APEXII area-detector diffractometer Radiation source: fine-focus sealed tube Graphite monochromator ω and φ scans 30114 measured reflections 8303 independent reflections

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier Least-squares matrix: full map $R[F^2 > 2\sigma(F^2)] = 0.044$ Hydrogen site location: inferred from $wR(F^2) = 0.137$ neighbouring sites S = 0.93H-atom parameters constrained 8303 reflections $w = 1/[\sigma^2(F_0^2) + (0.0725P)^2 + 0.2552P]$ 433 parameters where $P = (F_0^2 + 2F_c^2)/3$ 0 restraints $(\Delta/\sigma)_{\rm max} = 0.001$ $\Delta \rho_{\rm max} = 0.17 \text{ e } \text{\AA}^{-3}$ Primary atom site location: structure-invariant $\Delta \rho_{\rm min} = -0.18 \ {\rm e} \ {\rm \AA}^{-3}$ direct methods

Special details

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

Z = 4

F(000) = 688

 $\theta = 1.2 - 28.4^{\circ}$

 $\mu = 0.09 \text{ mm}^{-1}$

T = 293 KBlock, colourless

 $R_{\rm int} = 0.032$

 $h = -11 \rightarrow 11$

 $k = -16 \rightarrow 16$

 $l = -21 \rightarrow 22$

 $D_{\rm x} = 1.303 {\rm Mg} {\rm m}^{-3}$

 $0.20 \times 0.20 \times 0.20$ mm

 $\theta_{\text{max}} = 28.4^{\circ}, \ \theta_{\text{min}} = 1.2^{\circ}$

5258 reflections with $I > 2\sigma(I)$

Mo *K* α radiation, $\lambda = 0.71073$ Å

Cell parameters from 8303 reflections

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	у	Ζ	$U_{ m iso}$ */ $U_{ m eq}$
01A	0.41536 (13)	0.75129 (9)	0.88919 (6)	0.0567 (3)

O2A $0.18473 (14)$ $0.61117 (9)$ $0.85240 (7)$ 0.633 $O3A$ $-0.0529 (15)$ $0.66404 (10)$ $0.52848 (7)$ $0.65973 (6)$ $O4A$ $0.10199 (11)$ $0.59456 (8)$ $0.65973 (6)$ $0.65973 (6)$ $O5A$ $-0.0729 (2)$ $0.29588 (11)$ $0.73737 (9)$ $0.6602 (10)$ $C1A$ $0.2947 (2)$ $0.85775 (14)$ $0.60506 (10)$ $0.6026 (10)$ $C1A$ $0.2947 (2)$ $0.85775 (14)$ $0.60506 (10)$ $0.622 (22)$ $C2A$ $0.2924 (3)$ $0.92180 (17)$ $0.54131 (11)$ $0.621 (22) (22) (22) (23) (23) (23) (23) (23)$		
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C10A $-0.04856(17)$ $0.32761(12)$ $0.61780(8)$ $0.61780(8)$ C11A $-0.11578(19)$ $0.42426(13)$ $0.64278(9)$ $0.61780(8)$ C12A $-0.2642(2)$ $0.35353(15)$ $0.59765(12)$ $0.61780(8)$ H12A -0.3094 0.2836 0.6138 0.6138 C13A $-0.3422(2)$ $0.38740(18)$ $0.53019(12)$ $0.61780(8)$ H13A -0.4405 0.3402 0.5003 $0.61780(8)$ C14A $-0.2767(2)$ $0.49130(17)$ $0.50553(10)$ $0.61780(11)$ H14A -0.3322 0.5136 0.4597 $0.617836(9)$ C15A $-0.12979(19)$ $0.56217(14)$ $0.54836(9)$ $0.617830(11)$ C16A $-0.1390(3)$ $0.71142(19)$ $0.46640(11)$ $0.617830(11)$ H16B -0.2387 0.7232 0.4813 $0.617830(11)$ H16C -0.1667 0.6602 0.4173 $0.617830(11)$ H17A 0.0537 0.4427 $0.7500(11)$ $0.69571(12)$ H19A 0.5496 0.7507 0.9968 0.6284 H19B 0.4553 0.6284 0.9539 0.6284 H19B 0.4553 0.6284 0.9539 $0.62819(7)$ O1B $1.29774(17)$ $1.18987(11)$ $1.37809(7)$ $0.62819(7)$ O2B $1.12347(15)$ $1.32548(10)$ $1.01612(7)$ 0.648	19A2	0.052*
C11A $-0.115/8 (19)$ $0.42426 (13)$ $0.642/8 (9)$ $0.6278 (9)$ C12A $-0.2642 (2)$ $0.35353 (15)$ $0.59765 (12)$ 0.6138 H12A -0.3094 0.2836 0.6138 0.6138 C13A $-0.3422 (2)$ $0.38740 (18)$ $0.53019 (12)$ $0.62767 (2)$ H13A -0.4405 0.3402 0.5003 $0.62767 (2)$ H14A -0.3322 0.5136 0.4597 $0.62767 (2)$ C15A $-0.12979 (19)$ $0.56217 (14)$ $0.54836 (9)$ $0.6640 (11)$ H16A -0.0706 0.7830 0.4586 $0.6640 (11)$ H16B -0.2387 0.7232 0.4813 0.6602 H16B -0.2387 0.7232 0.4813 0.6602 H16C -0.1667 0.6602 0.4173 0.6602 C17A $-0.0340 (2)$ $0.38920 (14)$ $0.71684 (11)$ 0.6602 H17A 0.0537 0.4427 0.7500 0.6602 C18A $0.27580 (17)$ $0.69571 (12)$ $0.83820 (8)$ 0.6284 H19B 0.4553 0.6284 0.9539 0.6284 H19B 0.4553 0.6284 0.9539 $0.6281 (10)$ $0.6673 (10)$ H19B $1.29774 (17)$ $1.18987 (11)$ $1.37809 (7)$ $0.6281 (10)$ $0.62819 (7)$ O1B $1.2947 (15)$ $1.32548 (10)$ $1.01612 (7)$ 0.648	210A	0.0455 (3)
C12A $-0.2642(2)$ $0.35353(15)$ $0.59765(12)$ $0.59765(12)$ H12A -0.3094 0.2836 0.6138 0.6138 C13A $-0.3422(2)$ $0.38740(18)$ $0.53019(12)$ 0.5003 H13A -0.4405 0.3402 0.5003 0.5003 C14A $-0.2767(2)$ $0.49130(17)$ $0.50553(10)$ 0.5136 H14A -0.3322 0.5136 0.4597 $0.54836(9)$ C15A $-0.12979(19)$ $0.56217(14)$ $0.54836(9)$ $0.56217(14)$ C16A $-0.1390(3)$ $0.71142(19)$ $0.46640(11)$ 0.54836 H16B -0.2387 0.7232 0.4813 0.5486 H16B -0.2387 0.7232 0.4813 0.5173 H16C -0.1667 0.6602 0.4173 0.5174 H17A 0.0537 0.4427 0.7500 $0.5184(11)$ H17A $0.5730(17)$ $0.69571(12)$ $0.83820(8)$ 0.5196 C19A $0.4474(2)$ $0.70544(17)$ $0.96434(10)$ 0.5196 H19B 0.4553 0.6284 0.9539 0.5199 H19C 0.3586 0.7067 0.9924 $0.5196(7)$ O1B $1.29774(17)$ $1.18987(11)$ $1.37809(7)$ $0.52819(7)$ O2B $1.12347(15)$ $1.32548(10)$ $1.01612(7)$ $0.512(7)$ O4B $1.04928(12)$ $1.21083(8)$ $1.14210(5)$ $0.512(7)$		0.0512 (4)
H12A -0.3094 0.2836 0.6138 0.6138 C13A $-0.3422 (2)$ $0.38740 (18)$ $0.53019 (12)$ $0.53019 (12)$ H13A -0.4405 0.3402 0.5003 0.5003 C14A $-0.2767 (2)$ $0.49130 (17)$ $0.50553 (10)$ $0.50553 (10)$ H14A -0.3322 0.5136 0.4597 $0.54836 (9)$ C15A $-0.12979 (19)$ $0.56217 (14)$ $0.54836 (9)$ $0.54836 (9)$ C16A $-0.1390 (3)$ $0.71142 (19)$ $0.46640 (11)$ $0.54836 (9)$ H16B -0.2387 0.7232 0.4813 0.4586 H16B -0.2387 0.7232 0.4813 $0.5174 (17)$ H16C -0.1667 0.6602 0.4173 $0.5174 (17)$ H17A 0.0537 0.4427 0.7500 $0.6184 (11)$ H17A 0.0537 0.4427 0.7500 $0.6184 (10)$ H19B 0.4553 0.6284 0.9539 $0.6284 (10)$ H19B 0.4553 0.6284 0.9539 $0.6281 (10)$ H19C 0.3586 0.7067 0.9924 $0.9924 (10)$ O1B $1.29774 (17)$ $1.18987 (11)$ $1.37809 (7)$ $0.6281 (10)$ O2B $1.1832 (2)$ $1.06673 (10)$ $1.26819 (7)$ $0.6481 (10)$ O4B $1.04928 (12)$ $1.21083 (8)$ $1.14210 (5)$ $0.6281 (10)$	212A	0.0664 (5)
C13A $-0.3422 (2)$ $0.38740 (18)$ $0.53019 (12)$ $0.53019 (12)$ H13A -0.4405 0.3402 0.5003 0.5003 C14A $-0.2767 (2)$ $0.49130 (17)$ $0.50553 (10)$ $0.50553 (10)$ H14A -0.3322 0.5136 0.4597 $0.50553 (10)$ C15A $-0.12979 (19)$ $0.56217 (14)$ $0.54836 (9)$ C16A $-0.1390 (3)$ $0.71142 (19)$ $0.46640 (11)$ H16A -0.0706 0.7830 0.4586 H16B -0.2387 0.7232 0.4813 H16C -0.1667 0.6602 0.4173 C17A $-0.0340 (2)$ $0.38920 (14)$ $0.71684 (11)$ H17A 0.0537 0.4427 0.7500 C18A $0.27580 (17)$ $0.69571 (12)$ $0.83820 (8)$ C19A $0.4474 (2)$ $0.70544 (17)$ 0.9968 H19B 0.4553 0.6284 0.9539 H19C 0.3586 0.7067 0.9924 O1B $1.29774 (17)$ $1.18987 (11)$ $1.37809 (7)$ O2B $1.1832 (2)$ $1.06673 (10)$ $1.26819 (7)$ O4B $1.04928 (12)$ $1.21083 (8)$ $1.14210 (5)$	112A	0.080*
H13A -0.4405 0.3402 0.5003 0.5003 C14A $-0.2767 (2)$ $0.49130 (17)$ $0.50553 (10)$ $0.50553 (10)$ H14A -0.3322 0.5136 0.4597 0.5136 C15A $-0.12979 (19)$ $0.56217 (14)$ $0.54836 (9)$ $0.54836 (9)$ C16A $-0.1390 (3)$ $0.71142 (19)$ $0.46640 (11)$ $0.54836 (9)$ H16A -0.0706 0.7830 0.4586 0.4586 H16B -0.2387 0.7232 0.4813 $0.5171 (12)$ H16C -0.1667 0.6602 0.4173 $0.5174 (11)$ H17A 0.0537 0.4427 0.7500 $0.5184 (11)$ H17A 0.0537 0.4427 0.7500 $0.5184 (10)$ H19A $0.27580 (17)$ $0.69571 (12)$ $0.83820 (8)$ $0.5194 (10)$ H19B 0.4553 0.6284 0.9539 0.5239 H19C 0.3586 0.7067 0.9924 $0.52819 (7)$ O1B $1.29774 (17)$ $1.18987 (11)$ $1.37809 (7)$ $0.52819 (7)$ O2B $1.1832 (2)$ $1.06673 (10)$ $1.26819 (7)$ $0.52819 (12)$ O4B $1.04928 (12)$ $1.21083 (8)$ $1.14210 (5)$	C13A	0.0732 (5)
C14A $-0.2767 (2)$ $0.49130 (17)$ $0.50553 (10)$ $0.600000000000000000000000000000000000$	113A	0.088*
H14A -0.3322 0.5136 0.4597 0.65217 C15A -0.12979 (19) 0.56217 (14) 0.54836 (9) 0.6640 (11)C16A -0.1390 (3) 0.71142 (19) 0.46640 (11) 0.6640 H16A -0.0706 0.7830 0.4586 0.6640 H16B -0.2387 0.7232 0.4813 0.6602 H16C -0.1667 0.6602 0.4173 0.6173 C17A -0.0340 (2) 0.38920 (14) 0.71684 (11) 0.6173 H17A 0.0537 0.4427 0.7500 0.602 C18A 0.27580 (17) 0.69571 (12) 0.83820 (8) 0.6284 C19A 0.4474 (2) 0.70544 (17) 0.96434 (10) 0.618820 H19B 0.4553 0.6284 0.9539 0.9924 O1B 1.29774 (17) 1.18987 (11) 1.37809 (7) 0.62819 O2B 1.12347 (15) 1.32548 (10) 1.01612 (7) 0.648 O4B 1.04928 (12) 1.21083 (8) 1.14210 (5) 0.6126	C14A	0.0660 (5)
C15A $-0.12979(19)$ $0.56217(14)$ $0.54836(9)$ $0.6640(11)$ C16A $-0.1390(3)$ $0.71142(19)$ $0.46640(11)$ $0.6640(11)$ H16A -0.0706 0.7830 0.4586 0.4586 H16B -0.2387 0.7232 0.4813 0.6602 H16C -0.1667 0.6602 0.4173 0.6602 C17A $-0.0340(2)$ $0.38920(14)$ $0.71684(11)$ 0.6602 H17A 0.0537 0.4427 0.7500 0.6602 C18A $0.27580(17)$ $0.69571(12)$ $0.83820(8)$ $0.6214(10)$ C19A $0.4474(2)$ $0.70544(17)$ $0.96434(10)$ 0.6624 H19B 0.4553 0.6284 0.9539 0.6284 H19C 0.3586 0.7067 0.9924 0.924 O1B $1.29774(17)$ $1.18987(11)$ $1.37809(7)$ $0.62819(7)$ O2B $1.12347(15)$ $1.32548(10)$ $1.01612(7)$ 0.648 O4B $1.04928(12)$ $1.21083(8)$ $1.14210(5)$ $0.62816(10)$	114A	0.079*
C16A $-0.1390 (3)$ $0.71142 (19)$ $0.46640 (11)$ $0.6640 (11)$ H16A -0.0706 0.7830 0.4586 $0.6640 (11)$ H16B -0.2387 0.7232 0.4813 0.6602 H16C -0.1667 0.6602 0.4173 0.6602 C17A $-0.0340 (2)$ $0.38920 (14)$ $0.71684 (11)$ 0.6602 H17A 0.0537 0.4427 0.7500 0.6602 C18A $0.27580 (17)$ $0.69571 (12)$ $0.83820 (8)$ $0.6214 (10)$ C19A $0.4474 (2)$ $0.70544 (17)$ $0.96434 (10)$ $0.6284 (10)$ H19B 0.4553 0.6284 0.9539 $0.6284 (12)$ H19C 0.3586 $0.7067 (12)$ $0.9924 (12)$ O1B $1.29774 (17)$ $1.18987 (11)$ $1.37809 (7)$ $0.6281 (10)$ O2B $1.12347 (15)$ $1.32548 (10)$ $1.01612 (7)$ $0.648 (12)$ O4B $1.04928 (12)$ $1.21083 (8)$ $1.14210 (5)$	C15A	0.0523 (4)
H16A -0.0706 0.7830 0.4586 0.4586 H16B -0.2387 0.7232 0.4813 0.4813 H16C -0.1667 0.6602 0.4173 0.602 C17A $-0.0340(2)$ $0.38920(14)$ $0.71684(11)$ 0.6602 H17A 0.0537 0.4427 0.7500 $0.69571(12)$ C18A $0.27580(17)$ $0.69571(12)$ $0.83820(8)$ $0.6214(17)$ C19A $0.4474(2)$ $0.70544(17)$ $0.96434(10)$ $0.61414(10)$ H19A 0.5496 0.7507 0.9968 0.9924 H19C 0.3586 0.7067 0.9924 0.9924 O1B $1.29774(17)$ $1.18987(11)$ $1.37809(7)$ $0.62819(7)$ O2B $1.1832(2)$ $1.06673(10)$ $1.26819(7)$ $0.64812(12)$ O4B $1.04928(12)$ $1.21083(8)$ $1.14210(5)$ $0.62812(12)$	C16A	0.0779 (6)
H16B-0.23870.72320.48130H16C-0.16670.66020.41730C17A-0.0340 (2)0.38920 (14)0.71684 (11)0H17A0.05370.44270.75000C18A0.27580 (17)0.69571 (12)0.83820 (8)0C19A0.4474 (2)0.70544 (17)0.96434 (10)0H19B0.54960.75070.99680H19B0.45530.62840.95390H19C0.35860.70670.99240O1B1.29774 (17)1.18987 (11)1.37809 (7)0O2B1.1832 (2)1.06673 (10)1.26819 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	416A	0.117*
H16C-0.16670.66020.41730C17A-0.0340 (2)0.38920 (14)0.71684 (11)0H17A0.05370.44270.75000C18A0.27580 (17)0.69571 (12)0.83820 (8)0C19A0.4474 (2)0.70544 (17)0.96434 (10)0H19A0.54960.75070.99680H19B0.45530.62840.95390H19C0.35860.70670.99240O1B1.29774 (17)1.18987 (11)1.37809 (7)0O2B1.1832 (2)1.06673 (10)1.26819 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	116B	0.117*
C17A-0.0340 (2)0.38920 (14)0.71684 (11)0H17A0.05370.44270.75000C18A0.27580 (17)0.69571 (12)0.83820 (8)0C19A0.4474 (2)0.70544 (17)0.96434 (10)0H19A0.54960.75070.99680H19B0.45530.62840.95390H19C0.35860.70670.99240O1B1.29774 (17)1.18987 (11)1.37809 (7)0O2B1.1832 (2)1.06673 (10)1.26819 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	416C	0.117*
H17A0.05370.44270.75000C18A0.27580 (17)0.69571 (12)0.83820 (8)0C19A0.4474 (2)0.70544 (17)0.96434 (10)0H19A0.54960.75070.99680H19B0.45530.62840.95390H19C0.35860.70670.99240O1B1.29774 (17)1.18987 (11)1.37809 (7)0O2B1.1832 (2)1.06673 (10)1.26819 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	C17A	0.0613 (4)
C18A0.27580 (17)0.69571 (12)0.83820 (8)0C19A0.4474 (2)0.70544 (17)0.96434 (10)0H19A0.54960.75070.99680H19B0.45530.62840.95390H19C0.35860.70670.99240O1B1.29774 (17)1.18987 (11)1.37809 (7)0O2B1.1832 (2)1.06673 (10)1.26819 (7)0O3B1.12347 (15)1.32548 (10)1.01612 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	117A	0.074*
C19A0.4474 (2)0.70544 (17)0.96434 (10)0H19A0.54960.75070.99680H19B0.45530.62840.95390H19C0.35860.70670.99240O1B1.29774 (17)1.18987 (11)1.37809 (7)0O2B1.1832 (2)1.06673 (10)1.26819 (7)0O3B1.12347 (15)1.32548 (10)1.01612 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	C18A	0.0436 (3)
H19A0.54960.75070.99680H19B0.45530.62840.95390H19C0.35860.70670.99240O1B1.29774 (17)1.18987 (11)1.37809 (7)0O2B1.1832 (2)1.06673 (10)1.26819 (7)0O3B1.12347 (15)1.32548 (10)1.01612 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	C19A	0.0729 (5)
H19B0.45530.62840.95390H19C0.35860.70670.99240O1B1.29774 (17)1.18987 (11)1.37809 (7)0O2B1.1832 (2)1.06673 (10)1.26819 (7)0O3B1.12347 (15)1.32548 (10)1.01612 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	419A	0.109*
H19C0.35860.70670.99240O1B1.29774 (17)1.18987 (11)1.37809 (7)0O2B1.1832 (2)1.06673 (10)1.26819 (7)0O3B1.12347 (15)1.32548 (10)1.01612 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	119B	0.109*
O1B1.29774 (17)1.18987 (11)1.37809 (7)0O2B1.1832 (2)1.06673 (10)1.26819 (7)0O3B1.12347 (15)1.32548 (10)1.01612 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	119C	0.109*
O2B1.1832 (2)1.06673 (10)1.26819 (7)0O3B1.12347 (15)1.32548 (10)1.01612 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	D1B	0.0731 (4)
O3B1.12347 (15)1.32548 (10)1.01612 (7)0O4B1.04928 (12)1.21083 (8)1.14210 (5)0	D2B	0.0812 (4)
O4B 1.04928 (12) 1.21083 (8) 1.14210 (5)	03B	0.0654 (3)
	04B	0.0453 (2)
O5B 0.7023 (2) 0.91721 (12) 1.11274 (8)	D5B	0.0979 (5)
C1B 1.2973 (2) 1.49121 (13) 1.18301 (9) (C1B	0.0533 (4)
H1B 1.1923 1.4422 1.1666 (11B	0.064*

C2B	1.3363 (2)	1.59176 (14)	1.15034 (11)	0.0637 (4)
H2B	1.2567	1.6106	1.1125	0.076*
C3B	1.4919 (2)	1.66485 (15)	1.17302 (11)	0.0667 (5)
H3B	1.5172	1.7326	1.1506	0.080*
C4B	1.6089 (2)	1.63690 (15)	1.22894 (11)	0.0685 (5)
H4B	1.7145	1.6854	1.2440	0.082*
C5B	1.5709 (2)	1.53742 (14)	1.26295 (10)	0.0587 (4)
H5B	1.6509	1.5200	1.3014	0.070*
C6B	1.41469 (18)	1.46261 (12)	1.24054 (8)	0.0460 (3)
C7B	1.37621 (18)	1.36008 (13)	1.28042 (9)	0.0473 (3)
H7B	1.4189	1.3692	1.3355	0.057*
C8B	1.28832 (17)	1.25531 (12)	1.24876 (8)	0.0435 (3)
C9B	1.22565 (18)	1.21970 (13)	1.16011 (8)	0.0447 (3)
H9B1	1.2822	1.2754	1.1299	0.054*
H9B2	1.2470	1.1468	1.1449	0.054*
C10B	0.96683 (17)	1.16893 (12)	1.06435 (8)	0.0426 (3)
C11B	0.84002 (18)	1.06988 (12)	1.05216 (9)	0.0476 (3)
C12B	0.7411 (2)	1.03311 (14)	0.97533 (10)	0.0594 (4)
H12B	0.6534	0.9685	0.9673	0.071*
C13B	0.7728 (2)	1.09160 (15)	0.91246 (10)	0.0632 (4)
H13B	0.7069	1.0662	0.8616	0.076*
C14B	0.9019 (2)	1.18846 (14)	0.92324 (9)	0.0577 (4)
H14B	0.9239	1.2266	0.8794	0.069*
C15B	0.99822 (19)	1.22864 (12)	0.99897 (9)	0.0484 (3)
C16B	1.1582 (3)	1.38958 (19)	0.95210 (12)	0.0898 (7)
H16D	1.2485	1.4552	0.9723	0.135*
H16E	1.0619	1.4136	0.9291	0.135*
H16F	1.1879	1.3433	0.9115	0.135*
C17B	0.8112 (2)	1.00228 (14)	1.11870 (10)	0.0616 (4)
H17B	0.8818	1.0270	1.1685	0.074*
C18B	1.2594 (2)	1.16990 (13)	1.30624 (9)	0.0508 (4)
C19B	1.1463 (4)	0.97776 (18)	1.31915 (15)	0.1193 (10)
H19D	1.0918	0.9068	1.2861	0.179*
H19E	1.0752	0.9967	1.3535	0.179*
H19F	1.2475	0.9708	1.3516	0.179*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0527 (6)	0.0632 (7)	0.0429 (6)	-0.0024 (5)	-0.0035 (5)	0.0188 (5)
O2A	0.0648 (7)	0.0522 (6)	0.0551 (6)	-0.0041 (5)	0.0021 (5)	0.0186 (5)
O3A	0.0669 (7)	0.0720 (8)	0.0502 (6)	0.0178 (6)	-0.0018 (5)	0.0172 (6)
O4A	0.0418 (5)	0.0463 (5)	0.0446 (5)	0.0123 (4)	0.0035 (4)	0.0019 (4)
O5A	0.1161 (12)	0.0530 (8)	0.0974 (10)	0.0087 (7)	0.0142 (9)	0.0254 (7)
C1A	0.0791 (11)	0.0507 (9)	0.0529 (9)	0.0140 (8)	0.0204 (8)	0.0130 (7)
C2A	0.1036 (15)	0.0701 (12)	0.0463 (9)	0.0214 (11)	0.0194 (9)	0.0151 (8)
C3A	0.1022 (15)	0.0667 (12)	0.0617 (11)	0.0232 (11)	0.0262 (10)	0.0313 (9)
C4A	0.0986 (14)	0.0498 (10)	0.0734 (12)	0.0122 (9)	0.0245 (11)	0.0219 (9)

supporting information

C5A	0.0776 (12)	0.0507 (9)	0.0545 (10)	0.0029 (8)	0.0117 (8)	0.0118 (7)
C6A	0.0506 (8)	0.0481 (8)	0.0485 (8)	0.0096 (7)	0.0106 (7)	0.0149 (7)
C7A	0.0479 (8)	0.0472 (8)	0.0441 (8)	0.0081 (6)	0.0054 (6)	0.0104 (6)
C8A	0.0442 (7)	0.0427 (7)	0.0391 (7)	0.0130 (6)	0.0067 (6)	0.0074 (6)
C9A	0.0438 (7)	0.0449 (8)	0.0411 (7)	0.0132 (6)	0.0061 (6)	0.0054 (6)
C10A	0.0431 (8)	0.0487 (8)	0.0427 (8)	0.0122 (6)	0.0059 (6)	-0.0020 (6)
C11A	0.0519 (9)	0.0473 (8)	0.0529 (9)	0.0099 (7)	0.0128 (7)	-0.0013 (7)
C12A	0.0603 (10)	0.0566 (10)	0.0731 (12)	0.0009 (8)	0.0139 (9)	-0.0068 (9)
C13A	0.0512 (10)	0.0788 (13)	0.0739 (13)	0.0029 (9)	0.0000 (9)	-0.0163 (10)
C14A	0.0551 (10)	0.0851 (13)	0.0510 (10)	0.0198 (9)	-0.0040 (8)	-0.0066 (9)
C15A	0.0522 (9)	0.0604 (10)	0.0436 (8)	0.0167 (7)	0.0061 (7)	0.0009 (7)
C16A	0.0868 (14)	0.0971 (15)	0.0559 (11)	0.0384 (12)	0.0037 (9)	0.0244 (10)
C17A	0.0712 (11)	0.0468 (9)	0.0646 (10)	0.0111 (8)	0.0141 (8)	0.0083 (8)
C18A	0.0457 (8)	0.0426 (8)	0.0414 (7)	0.0092 (6)	0.0074 (6)	0.0064 (6)
C19A	0.0722 (11)	0.0837 (13)	0.0488 (10)	0.0002 (10)	-0.0074 (8)	0.0276 (9)
O1B	0.1041 (10)	0.0693 (8)	0.0423 (7)	0.0151 (7)	0.0101 (6)	0.0163 (6)
O2B	0.1318 (12)	0.0456 (7)	0.0557 (7)	0.0084 (7)	0.0048 (7)	0.0166 (6)
O3B	0.0734 (8)	0.0593 (7)	0.0506 (6)	-0.0068 (6)	0.0032 (5)	0.0218 (5)
O4B	0.0458 (5)	0.0503 (6)	0.0354 (5)	0.0058 (4)	0.0065 (4)	0.0019 (4)
O5B	0.1163 (12)	0.0733 (9)	0.0750 (9)	-0.0361 (9)	0.0218 (8)	0.0103 (7)
C1B	0.0493 (8)	0.0524 (9)	0.0559 (9)	0.0090 (7)	0.0073 (7)	0.0111 (7)
C2B	0.0691 (11)	0.0580 (10)	0.0648 (11)	0.0171 (9)	0.0088 (8)	0.0191 (8)
C3B	0.0824 (13)	0.0489 (9)	0.0659 (11)	0.0053 (9)	0.0204 (10)	0.0124 (8)
C4B	0.0652 (11)	0.0587 (10)	0.0677 (11)	-0.0079 (8)	0.0091 (9)	0.0045 (9)
C5B	0.0558 (9)	0.0584 (10)	0.0522 (9)	0.0038 (8)	0.0000 (7)	0.0042 (7)
C6B	0.0498 (8)	0.0465 (8)	0.0391 (7)	0.0085 (6)	0.0078 (6)	0.0030 (6)
C7B	0.0476 (8)	0.0534 (9)	0.0385 (7)	0.0113 (7)	0.0031 (6)	0.0067 (6)
C8B	0.0459 (8)	0.0479 (8)	0.0391 (7)	0.0161 (6)	0.0069 (6)	0.0094 (6)
C9B	0.0483 (8)	0.0472 (8)	0.0402 (7)	0.0143 (6)	0.0090 (6)	0.0073 (6)
C10B	0.0460 (8)	0.0438 (8)	0.0370 (7)	0.0107 (6)	0.0069 (6)	0.0023 (6)
C11B	0.0524 (8)	0.0428 (8)	0.0442 (8)	0.0069 (6)	0.0101 (6)	0.0000 (6)
C12B	0.0619 (10)	0.0513 (9)	0.0534 (9)	0.0012 (8)	0.0027 (8)	-0.0037 (7)
C13B	0.0735 (11)	0.0591 (10)	0.0464 (9)	0.0120 (9)	-0.0062 (8)	-0.0026 (8)
C14B	0.0725 (11)	0.0590 (10)	0.0410 (8)	0.0179 (8)	0.0052 (7)	0.0110 (7)
C15B	0.0550 (9)	0.0439 (8)	0.0443 (8)	0.0094 (7)	0.0074 (7)	0.0091 (6)
C16B	0.0915 (15)	0.0893 (15)	0.0724 (13)	-0.0126 (12)	0.0048 (11)	0.0455 (11)
C17B	0.0712 (11)	0.0522 (9)	0.0531 (9)	-0.0027 (8)	0.0161 (8)	0.0046 (7)
C18B	0.0608 (9)	0.0489 (9)	0.0441 (9)	0.0178 (7)	0.0068 (7)	0.0106 (7)
C19B	0.199 (3)	0.0553 (12)	0.0878 (16)	0.0041 (15)	0.0135 (17)	0.0348 (11)

Geometric parameters (Å, °)

01A—C18A	1.3360 (17)	O1B—C18B	1.1971 (18)	
01A—C19A	1.4400 (18)	O2B—C18B	1.327 (2)	
O2A-C18A	1.2019 (17)	O2B—C19B	1.449 (2)	
O3A—C15A	1.358 (2)	O3B—C15B	1.3620 (18)	
O3A—C16A	1.417 (2)	O3B—C16B	1.419 (2)	
O4A—C10A	1.3808 (17)	O4B—C10B	1.3785 (16)	

O4A—C9A	1.4488 (17)	O4B—C9B	1.4481 (17)
O5A—C17A	1.202 (2)	O5B—C17B	1.1993 (19)
C1A—C6A	1.382 (2)	C1B—C2B	1.376 (2)
C1A—C2A	1.382 (2)	C1B—C6B	1.393 (2)
C1A—H1A	0.9300	C1B—H1B	0.9300
C2A—C3A	1.372 (3)	C2B—C3B	1.378 (3)
C2A—H2A	0.9300	C2B—H2B	0.9300
C3A—C4A	1.364 (3)	C3B—C4B	1.371 (3)
СЗА—НЗА	0.9300	СЗВ—НЗВ	0.9300
C4A—C5A	1.381 (2)	C4B—C5B	1.376 (2)
C4A—H4A	0.9300	C4B—H4B	0.9300
C5A—C6A	1.392 (2)	C5B—C6B	1.391 (2)
C5A—H5A	0.9300	C5B—H5B	0.9300
С6А—С7А	1.470 (2)	C6B—C7B	1.463 (2)
C7A—C8A	1.339 (2)	C7B—C8B	1.334 (2)
С7А—Н7А	0.9300	C7B—H7B	0.9300
C8A—C18A	1.4844 (19)	C8B—C18B	1.488 (2)
C8A—C9A	1.4902 (19)	C8B—C9B	1.5002 (19)
С9А—Н9А1	0.9700	C9B—H9B1	0.9700
С9А—Н9А2	0.9700	C9B—H9B2	0.9700
C10A—C11A	1.385 (2)	C10B—C11B	1.389 (2)
C10A—C15A	1.403 (2)	C10B—C15B	1.403 (2)
C11A—C12A	1.403 (2)	C11B—C12B	1.400 (2)
C11A—C17A	1.470 (2)	C11B—C17B	1.469 (2)
C12A—C13A	1.362 (3)	C12B—C13B	1.359 (2)
C12A—H12A	0.9300	C12B—H12B	0.9300
C13A—C14A	1.384 (3)	C13B—C14B	1.383 (2)
С13А—Н13А	0.9300	C13B—H13B	0.9300
C14A—C15A	1.382 (2)	C14B—C15B	1.382 (2)
C14A—H14A	0.9300	C14B—H14B	0.9300
C16A—H16A	0.9600	C16B—H16D	0.9600
C16A—H16B	0.9600	C16B—H16E	0.9600
C16A—H16C	0.9600	C16B—H16F	0.9600
C17A—H17A	0.9300	C17B—H17B	0.9300
C19A—H19A	0.9600	C19B—H19D	0.9600
C19A—H19B	0.9600	C19B—H19E	0.9600
C19A—H19C	0.9600	C19B—H19F	0.9600
C18A—O1A—C19A	115.45 (12)	C18B—O2B—C19B	115.86 (15)
C15A—O3A—C16A	118.01 (14)	C15B—O3B—C16B	118.03 (13)
C10A—O4A—C9A	112.60 (10)	C10B—O4B—C9B	116.89 (10)
C6A—C1A—C2A	120.38 (16)	C2B—C1B—C6B	120.19 (15)
C6A—C1A—H1A	119.8	C2B—C1B—H1B	119.9
C2A—C1A—H1A	119.8	C6B—C1B—H1B	119.9
C3A—C2A—C1A	120.54 (17)	C1B—C2B—C3B	120.84 (17)
СЗА—С2А—Н2А	119.7	C1B—C2B—H2B	119.6
C1A—C2A—H2A	119.7	C3B—C2B—H2B	119.6
C4A—C3A—C2A	119.68 (17)	C4B—C3B—C2B	119.44 (17)

С4А—С3А—Н3А	120.2	C4B—C3B—H3B	120.3
С2А—С3А—НЗА	120.2	C2B—C3B—H3B	120.3
C3A—C4A—C5A	120.48 (17)	C3B—C4B—C5B	120.37 (17)
C3A—C4A—H4A	119.8	C3B—C4B—H4B	119.8
C5A—C4A—H4A	119.8	C5B—C4B—H4B	119.8
C4A—C5A—C6A	120.41 (17)	C4B—C5B—C6B	120.89 (16)
С4А—С5А—Н5А	119.8	C4B—C5B—H5B	119.6
С6А—С5А—Н5А	119.8	C6B—C5B—H5B	119.6
C1A—C6A—C5A	118.48 (14)	C5B—C6B—C1B	118.27 (14)
C1A—C6A—C7A	122.41 (14)	C5B—C6B—C7B	119.47 (14)
C5A—C6A—C7A	119.08 (14)	C1B—C6B—C7B	122.19 (13)
C8A—C7A—C6A	128.24 (14)	C8B—C7B—C6B	128.96 (13)
C8A—C7A—H7A	115.9	C8B—C7B—H7B	115.5
C6A—C7A—H7A	115.9	C6B—C7B—H7B	115.5
C7A—C8A—C18A	120.49 (13)	C7B—C8B—C18B	116.47 (13)
C7A—C8A—C9A	124.49 (13)	C7B—C8B—C9B	123.79 (13)
C18A - C8A - C9A	114 79 (12)	C18B - C8B - C9B	119 68 (13)
O4A - C9A - C8A	110.18 (11)	O4B - C9B - C8B	108.60 (11)
O4A - C9A - H9A1	109.6	O4B—C9B—H9B1	110.0
C8A—C9A—H9A1	109.6	C8B—C9B—H9B1	110.0
04A—C9A—H9A2	109.6	O4B—C9B—H9B2	110.0
C8A—C9A—H9A2	109.6	C8B—C9B—H9B2	110.0
H9A1—C9A—H9A2	108.1	H9B1—C9B—H9B2	108.4
O4A— $C10A$ — $C11A$	119.70 (13)	O4B— $C10B$ — $C11B$	118.40 (12)
04A—C10A—C15A	120.06 (13)	O4B—C10B—C15B	121.71 (13)
C11A—C10A—C15A	120.19 (14)	C11B—C10B—C15B	119.66 (13)
C10A—C11A—C12A	119.64 (16)	C10B—C11B—C12B	119.55 (14)
C10A—C11A—C17A	120.45 (14)	C10B—C11B—C17B	120.62 (13)
C12A—C11A—C17A	119.90 (15)	C12B—C11B—C17B	119.82 (14)
C13A—C12A—C11A	119.87 (17)	C13B—C12B—C11B	120.21 (15)
C13A—C12A—H12A	120.1	C13B—C12B—H12B	119.9
C11A—C12A—H12A	120.1	C11B—C12B—H12B	119.9
C12A—C13A—C14A	120.74 (17)	C12B—C13B—C14B	120.83 (15)
C12A—C13A—H13A	119.6	C12B—C13B—H13B	119.6
C14A—C13A—H13A	119.6	C14B—C13B—H13B	119.6
C15A—C14A—C13A	120.63 (17)	C15B—C14B—C13B	120.14 (15)
C15A—C14A—H14A	119.7	C15B—C14B—H14B	119.9
C13A—C14A—H14A	119.7	C13B—C14B—H14B	119.9
O3A—C15A—C14A	125.62 (15)	O3B—C15B—C14B	124.42 (14)
O3A—C15A—C10A	115.46 (13)	O3B-C15B-C10B	116.01 (13)
C14A—C15A—C10A	118.91 (16)	C14B—C15B—C10B	119.55 (14)
O3A—C16A—H16A	109.5	O3B—C16B—H16D	109.5
O3A—C16A—H16B	109.5	O3B—C16B—H16E	109.5
H16A—C16A—H16B	109.5	H16D—C16B—H16E	109.5
O3A—C16A—H16C	109.5	O3B—C16B—H16F	109.5
H16A—C16A—H16C	109.5	H16D—C16B—H16F	109.5
H16B—C16A—H16C	109.5	H16E—C16B—H16F	109.5
O5A—C17A—C11A	124.33 (17)	O5B—C17B—C11B	124.08 (16)

O5A—C17A—H17A	117.8	O5B—C17B—H17B	118.0
C11A—C17A—H17A	117.8	C11B—C17B—H17B	118.0
O2A - C18A - O1A	122 83 (13)	O1B-C18B-O2B	123 09 (15)
$O_{2A} = C_{18A} = C_{8A}$	122.03(13) 123.07(13)	$\begin{array}{cccc} 01B & 010B & 02B \\ 01B & 018B & 08B \\ \end{array}$	125.07(15) 125.27(15)
O_{2A} C_{18A} C_{8A}	123.97(13)	$\begin{array}{c} \text{OID} \\ OID$	123.27(13)
OIA—CI8A—C8A	113.20 (12)	02B	111.64 (13)
OIA—CI9A—HI9A	109.5	O2B—C19B—H19D	109.5
O1A—C19A—H19B	109.5	O2B—C19B—H19E	109.5
H19A—C19A—H19B	109.5	H19D—C19B—H19E	109.5
O1A—C19A—H19C	109.5	O2B-C19B-H19F	109.5
H19A—C19A—H19C	109.5	H19D—C19B—H19F	109.5
H19B—C19A—H19C	109 5	H19F—C19B—H19F	109 5
			10,10
	0.5(2)	CAD CID COD COD	0.0.(2)
COA - CTA - CZA - CSA	-0.3(3)	COB - CIB - C2B - C3B	0.9(3)
CIA—C2A—C3A—C4A	0.4 (3)	CIB—C2B—C3B—C4B	-0.1 (3)
C2A—C3A—C4A—C5A	0.5 (3)	C2B—C3B—C4B—C5B	-0.8(3)
C3A—C4A—C5A—C6A	-1.4 (3)	C3B—C4B—C5B—C6B	1.0 (3)
C2A—C1A—C6A—C5A	-0.4 (3)	C4B—C5B—C6B—C1B	-0.3 (2)
C2A—C1A—C6A—C7A	-178.36 (16)	C4B—C5B—C6B—C7B	-177.33 (15)
C4A—C5A—C6A—C1A	1.3 (3)	C2B—C1B—C6B—C5B	-0.7(2)
C4A—C5A—C6A—C7A	179.34 (16)	C2B—C1B—C6B—C7B	176.33 (15)
C1A—C6A—C7A—C8A	-402(2)	C5B-C6B-C7B-C8B	$-141\ 00\ (17)$
C_{5A} C_{6A} C_{7A} C_{8A}	141.79(17)	C1B - C6B - C7B - C8B	42 0 (2)
C_{6A} C_{7A} C_{8A} C_{18A}	171.79(17)	C6P $C7P$ $C8P$ $C18P$	-175 41 (14)
C(A = C7A = C8A = C8A	170.94(14)	$C(D = C/B = C\delta B = C\delta B$	-1/3.41(14)
C6A - C/A - C8A - C9A	-6.8(2)	C0B - C/B - C8B - C9B	7.3 (2)
C10A—O4A—C9A—C8A	168.47 (11)	C10B—O4B—C9B—C8B	-1/4.31 (11)
C7A—C8A—C9A—O4A	104.79 (16)	C7B—C8B—C9B—O4B	-105.02 (16)
C18A—C8A—C9A—O4A	-80.66 (14)	C18B—C8B—C9B—O4B	77.76 (16)
C9A—O4A—C10A—C11A	-106.93 (14)	C9B-O4B-C10B-C11B	119.51 (14)
C9A—O4A—C10A—C15A	75.55 (16)	C9B—O4B—C10B—C15B	-66.03 (18)
O4A—C10A—C11A—C12A	-176.58(13)	O4B-C10B-C11B-C12B	172.24 (14)
C15A—C10A—C11A—C12A	0.9 (2)	C15B—C10B—C11B—C12B	-2.3(2)
O4A—C10A—C11A—C17A	4.4 (2)	O4B—C10B—C11B—C17B	-9.1(2)
$C_{15} - C_{10} - C_{11} - C_{17}$	-178.09(14)	C15B-C10B-C11B-C17B	17636(14)
C_{10A} C_{11A} C_{12A} C_{13A}	-0.7(3)	CIOR CIIR CI2R CI3R	24(2)
C17A $C11A$ $C12A$ $C12A$	0.7(3)	C17D $C11D$ $C12D$ $C13D$	2.4(2)
C1/A— $C12A$ — $C12A$ — $C13A$	1/8.30 (17)	CI/B—CIIB—CI2B—CI3B	-1/6.30(10)
CIIA—CI2A—CI3A—CI4A	-0.1(3)	CIIB—CI2B—CI3B—CI4B	-0.5 (3)
C12A—C13A—C14A—C15A	0.8 (3)	C12B—C13B—C14B—C15B	-1.6(3)
C16A—O3A—C15A—C14A	10.6 (2)	C16B—O3B—C15B—C14B	-0.2(3)
C16A—O3A—C15A—C10A	-170.80 (15)	C16B—O3B—C15B—C10B	-179.14 (17)
C13A—C14A—C15A—O3A	177.99 (16)	C13B—C14B—C15B—O3B	-177.30 (16)
C13A—C14A—C15A—C10A	-0.6(2)	C13B—C14B—C15B—C10B	1.6 (2)
O4A—C10A—C15A—O3A	-1.5(2)	O4B—C10B—C15B—O3B	4.9 (2)
C11A—C10A—C15A—O3A	-179.01(13)	C11B—C10B—C15B—O3B	179.35 (13)
04A— $C10A$ — $C15A$ — $C14A$	177 22 (14)	04B-C10B-C15B-C14B	-17406(14)
C11A - C10A - C15A - C14A	-0.3(2)	C11B C10B C15B C14B	(1, 1, 0, 0, 0, 1, 1, 1, 0, 0, 0, 1, 1, 1, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
$C_{10A} = C_{10A} = C_{1$	-170.60(17)	C10P C11P C17P OSP	(-5, (2))
C12A = C11A = C17A = O5A	1/0.09(1/)	$C_{10} = C_{11} = C_{17} = C$	1/0.01(18)
CI2A—CIIA—CI/A—OSA	10.5 (3)	CI2B—CIIB—CI/B—OSB	-2.7(3)
C19A—O1A—C18A—O2A	-2.1 (2)	C19B—O2B—C18B—O1B	0.6 (3)

C19A—O1A—C18A—C8A	177.28 (14)	C19B—O2B—C18B—C8B	-178.78 (19)
C7A—C8A—C18A—O2A	177.55 (15)	C7B—C8B—C18B—O1B	5.9 (2)
C9A—C8A—C18A—O2A	2.8 (2)	C9B—C8B—C18B—O1B	-176.72 (15)
C7A—C8A—C18A—O1A	-1.85 (19)	C7B—C8B—C18B—O2B	-174.76 (15)
C9A—C8A—C18A—O1A	-176.63 (12)	C9B—C8B—C18B—O2B	2.7 (2)

Hydrogen-bond geometry (Å, °)

	D—H	H···A	D····A	D—H…A
C17A—H17A····O2A	0.93	2.48	3.354 (2)	156
C17 <i>A</i> —H17 <i>A</i> ···O4 <i>A</i>	0.93	2.50	2.8164 (19)	100
C17 <i>B</i> —H17 <i>B</i> ···O4 <i>B</i>	0.93	2.47	2.8004 (19)	101
С9А—Н9А2…ОЗА	0.97	2.49	3.0167 (18)	114
C9 <i>B</i> —H9 <i>B</i> 1···O3 <i>B</i>	0.97	2.36	2.9416 (17)	118
C7 <i>B</i> —H7 <i>B</i> ···O1 <i>B</i>	0.93	2.41	2.7847 (18)	104
C7 <i>A</i> —H7 <i>A</i> ···O1 <i>A</i>	0.93	2.29	2.6914 (17)	106
$C9A$ — $H9A1$ ···O $4B^{i}$	0.97	2.55	3.2215 (16)	126
C19 <i>B</i> —H19 <i>D</i> ····O5 <i>A</i> ⁱⁱ	0.96	2.43	3.275 (3)	147

Symmetry codes: (i) -x+1, -y+2, -z+2; (ii) -x+1, -y+1, -z+2.