

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Propyl 4-hydroxybenzoate

Yiwen Zhou, Guzalnur Matsadiq, Yanling Wu, Jing Xiao and Jing Cheng*

Key Laboratory of Pesticide & Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

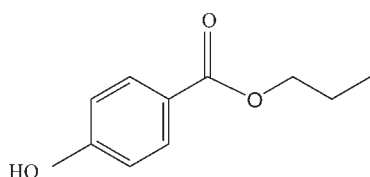
Correspondence e-mail: mdchengjing@126.com

Received 4 December 2009; accepted 4 January 2010

 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.083; wR factor = 0.189; data-to-parameter ratio = 13.8.

There are two molecules in the asymmetric unit of the title compound, $\text{C}_{10}\text{H}_{12}\text{O}_3$. In the crystal, molecules are linked by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds into chains running along [010]. Adjacent chains are joined together by weak $\pi-\pi$ interactions between benzene rings [centroid-centroid distance = 4.040 (2) Å].

Related literature

 For the structure of another *p*-hydroxybenzoate, see: Mandal & Kadirvelraj (1996).


Experimental

Crystal data

 $\text{C}_{10}\text{H}_{12}\text{O}_3$
 $M_r = 180.20$
 Monoclinic, $P2_1/c$
 $a = 12.0634$ (12) Å
 $b = 13.8419$ (14) Å
 $c = 11.7982$ (11) Å

 $\beta = 108.625$ (2)°
 $V = 1866.9$ (3) Å³
 $Z = 8$
 Mo $K\alpha$ radiation

 $\mu = 0.09$ mm⁻¹
 $T = 298$ K
 $0.30 \times 0.20 \times 0.20$ mm

Data collection

 Bruker SMART APEX CCD area-detector diffractometer
 10603 measured reflections

 3271 independent reflections
 2960 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.083$
 $wR(F^2) = 0.189$
 $S = 1.27$
 3271 reflections

 237 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.24$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O4}-\text{H4}\cdots\text{O5}^i$	0.82	1.93	2.730 (3)	167
$\text{O1}-\text{H1}\cdots\text{O2}^{ii}$	0.82	1.91	2.720 (3)	171

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

We would like to thank the National Nature Science Foundation of China (30971948) and Wuhan's program in science and technology (200760423155) for financial support for this work. We also wish to express our thanks to Meng Xianggao for his warmest help and patience.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FK2009).

References

- Bruker (2001). *SAINT-Plus* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Mandal, S. S. & Kadirvelraj, R. (1996). *Chem. Commun.* pp. 2725–2726.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supporting information

Acta Cryst. (2010). E66, o485 [https://doi.org/10.1107/S1600536810000139]

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S1. Comment

The propyl 4-hydroxybenzoate is a kind of *p*-hydroxybenzoates, which are also known as Nipagin esters. Nipagin ester is a preservative of large consumption in the world. Due to the high antibacterial activity and low toxicity of Nipagin ester, it becomes an inevitable trend that Nipagin ester replaces the traditional preservative. Here, we report the crystal structure of propyl 4-hydroxybenzoate.

There are two molecules in the asymmetric unit (Fig. 1). All bond lengths and bond angles lie in expected ranges.

As shown in Fig.2, molecules are linked by O—H···O hydrogen bonds into one-dimensional chains running along the [010] direction. Adjacent chains are further linked together by weak π – π interactions between two phenyl rings (centroid-to-centroid distance is 4.040 Å).

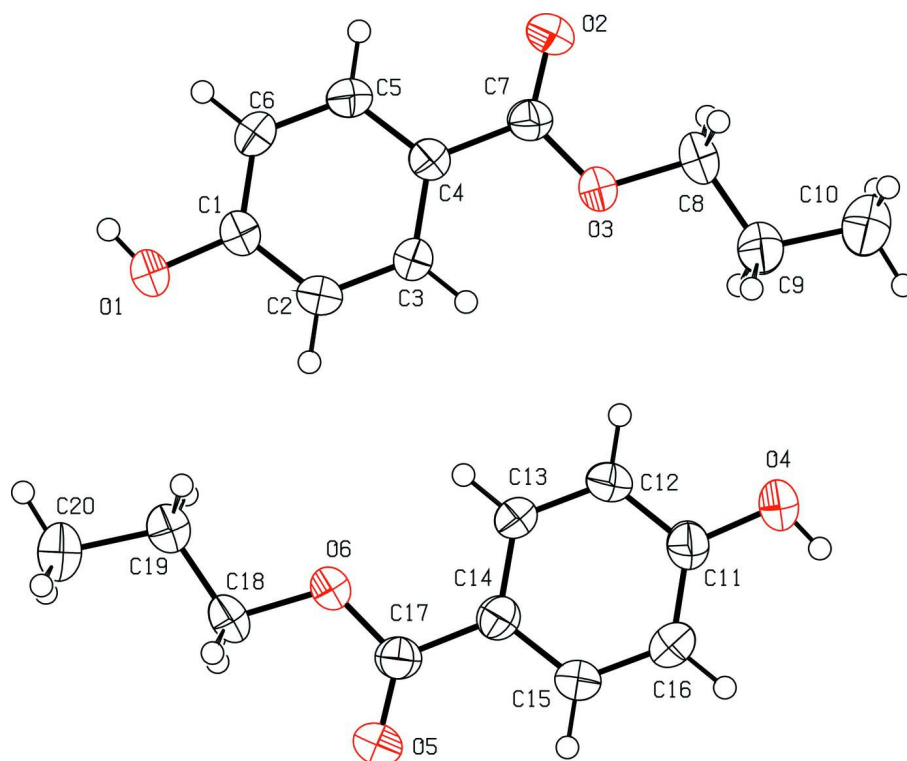
S2. Experimental

¹H-NMR (C₃D₆O, 600 MHz): δ 7.916(d, 2H, aromatic), δ 6.933(d, 2H, aromatic), δ 4.208(t, 2H, -COOCH₂-), δ 2.096(s, 1H, -OH), δ 1.752(q, 2H, -CH₂-), δ 1.004(t, 3H, -CH₃);

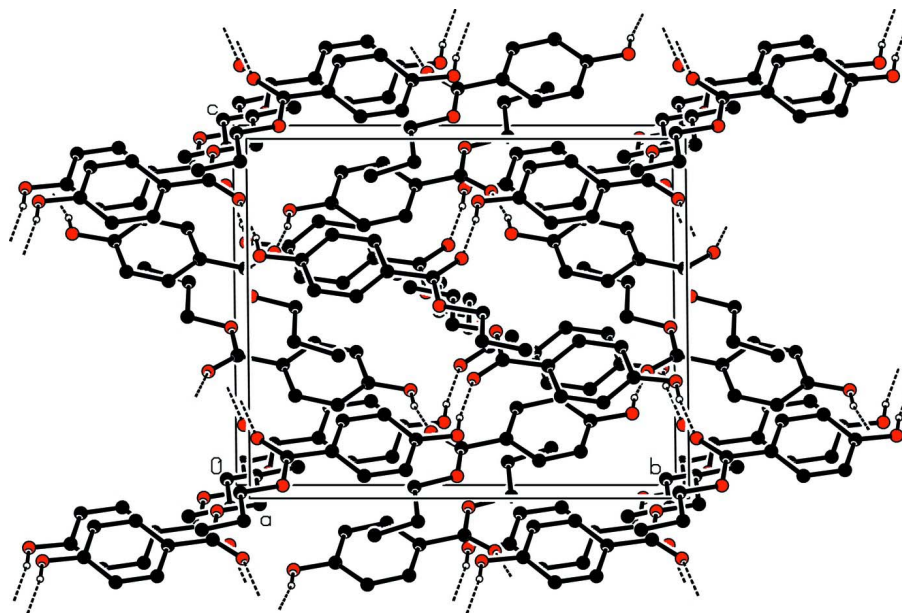
Crystals appropriate for data collection were obtained by slow evaporation of an ethanol solution at room temperature.

S3. Refinement

All the H atoms attached to carbon atoms were located from geometrical considerations with C—H = 0.93 Å (aromatic), 0.97 Å (methylene) and 0.96 Å (methyl), and $U_{eq}(H) = 1.2U_{eq}(\text{aromatic, methylene C})$ and $1.5U_{eq}(\text{methyl C})$. Hydrogen atoms H1 and H4 were found from difference maps and then placed at their ideal positions with O—H = 0.82 Å and $U_{iso}(H) = 1.5U_{eq}(O)$.

**Figure 1**

Molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

**Figure 2**

The packing of (I), with O-H...O hydrogen bonds shown as dashed lines.

Propyl 4-hydroxybenzoate

Crystal data

C₁₀H₁₂O₃ $M_r = 180.20$ Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

 $a = 12.0634$ (12) Å $b = 13.8419$ (14) Å $c = 11.7982$ (11) Å $\beta = 108.625$ (2)° $V = 1866.9$ (3) Å³ $Z = 8$ $F(000) = 768$ $D_x = 1.282$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4791 reflections

 $\theta = 2.3$ – 28.3 ° $\mu = 0.09$ mm⁻¹ $T = 298$ K

Block, colourless

 $0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker SMART APEX CCD area-detector
diffractometerRadiation source: fine focus sealed Siemens Mo
tube

Graphite monochromator

 0.3° wide ω exposures scans

10603 measured reflections

3271 independent reflections

2960 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.027$ $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.3^\circ$ $h = -14 \rightarrow 12$ $k = -16 \rightarrow 16$ $l = -11 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.083$ $wR(F^2) = 0.189$ $S = 1.27$

3271 reflections

237 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
map

Hydrogen site location: geom and difmap

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0626P)^2 + 1.2781P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.001$ $\Delta\rho_{\text{max}} = 0.24$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.9740 (2)	0.97287 (14)	0.3245 (2)	0.0657 (7)
H1	1.0093	0.9797	0.2760	0.098*
O2	0.9063 (2)	0.51536 (14)	0.3293 (2)	0.0608 (6)
O3	0.82019 (18)	0.56944 (13)	0.45749 (18)	0.0488 (5)
C1	0.9519 (3)	0.87795 (19)	0.3346 (3)	0.0447 (7)

C2	0.8980 (3)	0.8521 (2)	0.4176 (3)	0.0545 (8)
H2	0.8777	0.8996	0.4631	0.065*
C3	0.8744 (3)	0.75689 (19)	0.4330 (3)	0.0461 (7)
H3	0.8381	0.7403	0.4890	0.055*
C4	0.9044 (2)	0.68486 (19)	0.3652 (2)	0.0370 (6)
C5	0.9577 (3)	0.7118 (2)	0.2820 (3)	0.0460 (7)
H5	0.9781	0.6646	0.2362	0.055*
C6	0.9810 (3)	0.8072 (2)	0.2660 (3)	0.0467 (7)
H6	1.0162	0.8242	0.2093	0.056*
C7	0.8785 (2)	0.5822 (2)	0.3806 (3)	0.0403 (7)
C8	0.7870 (3)	0.4715 (2)	0.4759 (3)	0.0527 (8)
H8A	0.8560	0.4335	0.5156	0.063*
H8B	0.7463	0.4414	0.3997	0.063*
C9	0.7087 (4)	0.4766 (2)	0.5519 (3)	0.0672 (10)
H9A	0.7509	0.5067	0.6277	0.081*
H9B	0.6418	0.5170	0.5124	0.081*
C10	0.6668 (4)	0.3798 (3)	0.5749 (4)	0.0862 (13)
H10A	0.6203	0.3516	0.5006	0.129*
H10B	0.6202	0.3864	0.6270	0.129*
H10C	0.7327	0.3389	0.6120	0.129*
O4	0.5717 (2)	0.61479 (15)	0.7201 (2)	0.0742 (8)
H4	0.5298	0.6082	0.7622	0.111*
O5	0.5895 (2)	1.07375 (15)	0.6687 (2)	0.0594 (6)
O6	0.68661 (18)	1.01843 (13)	0.55031 (18)	0.0492 (5)
C11	0.5838 (3)	0.7104 (2)	0.7005 (3)	0.0482 (7)
C12	0.6369 (3)	0.7352 (2)	0.6165 (3)	0.0610 (9)
H12	0.6633	0.6871	0.5766	0.073*
C13	0.6507 (3)	0.8303 (2)	0.5919 (3)	0.0497 (8)
H13	0.6860	0.8462	0.5349	0.060*
C14	0.6125 (2)	0.9033 (2)	0.6512 (2)	0.0385 (6)
C15	0.5595 (3)	0.8775 (2)	0.7353 (3)	0.0441 (7)
H15	0.5335	0.9256	0.7757	0.053*
C16	0.5447 (3)	0.7818 (2)	0.7602 (3)	0.0470 (7)
H16	0.5088	0.7656	0.8166	0.056*
C17	0.6265 (2)	1.0062 (2)	0.6259 (2)	0.0403 (7)
C18	0.7092 (3)	1.11661 (19)	0.5211 (3)	0.0476 (7)
H18A	0.7597	1.1491	0.5916	0.057*
H18B	0.6365	1.1524	0.4918	0.057*
C19	0.7673 (3)	1.1111 (2)	0.4270 (3)	0.0526 (8)
H19A	0.7162	1.0776	0.3577	0.063*
H19B	0.8390	1.0741	0.4571	0.063*
C20	0.7954 (3)	1.2110 (2)	0.3895 (3)	0.0672 (10)
H20A	0.7243	1.2470	0.3571	0.101*
H20B	0.8337	1.2047	0.3300	0.101*
H20C	0.8461	1.2443	0.4579	0.101*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1019 (19)	0.0285 (11)	0.0922 (17)	-0.0029 (11)	0.0670 (15)	0.0030 (11)
O2	0.0824 (16)	0.0342 (11)	0.0856 (16)	-0.0030 (10)	0.0544 (14)	-0.0113 (11)
O3	0.0671 (14)	0.0298 (10)	0.0629 (13)	-0.0052 (9)	0.0393 (11)	-0.0006 (9)
C1	0.0551 (18)	0.0306 (14)	0.0554 (18)	-0.0010 (12)	0.0275 (15)	0.0017 (12)
C2	0.078 (2)	0.0349 (15)	0.069 (2)	0.0015 (15)	0.0485 (18)	-0.0054 (14)
C3	0.0614 (19)	0.0340 (15)	0.0558 (18)	-0.0001 (13)	0.0370 (16)	0.0031 (12)
C4	0.0394 (15)	0.0325 (14)	0.0419 (15)	-0.0006 (11)	0.0168 (12)	-0.0009 (11)
C5	0.0575 (18)	0.0392 (15)	0.0520 (17)	-0.0024 (13)	0.0325 (15)	-0.0083 (13)
C6	0.0606 (19)	0.0425 (16)	0.0486 (17)	-0.0022 (14)	0.0337 (15)	0.0032 (13)
C7	0.0398 (15)	0.0372 (15)	0.0479 (16)	0.0008 (12)	0.0198 (13)	-0.0033 (12)
C8	0.068 (2)	0.0302 (15)	0.066 (2)	-0.0044 (14)	0.0305 (17)	0.0049 (13)
C9	0.101 (3)	0.0448 (18)	0.072 (2)	-0.0123 (18)	0.051 (2)	-0.0045 (16)
C10	0.121 (4)	0.063 (2)	0.099 (3)	-0.018 (2)	0.070 (3)	0.000 (2)
O4	0.107 (2)	0.0348 (12)	0.111 (2)	-0.0041 (12)	0.0776 (17)	0.0060 (12)
O5	0.0821 (16)	0.0367 (12)	0.0756 (15)	0.0051 (10)	0.0478 (13)	-0.0039 (10)
O6	0.0660 (13)	0.0292 (10)	0.0655 (13)	-0.0020 (9)	0.0395 (11)	-0.0008 (9)
C11	0.0502 (17)	0.0375 (15)	0.0637 (19)	-0.0021 (13)	0.0279 (15)	0.0039 (14)
C12	0.079 (2)	0.0347 (16)	0.093 (3)	0.0007 (15)	0.061 (2)	-0.0071 (16)
C13	0.0618 (19)	0.0394 (16)	0.065 (2)	-0.0035 (14)	0.0435 (17)	-0.0034 (14)
C14	0.0347 (14)	0.0397 (15)	0.0427 (15)	-0.0020 (11)	0.0145 (12)	-0.0007 (12)
C15	0.0544 (18)	0.0368 (15)	0.0475 (16)	0.0010 (13)	0.0254 (14)	-0.0052 (12)
C16	0.0520 (17)	0.0494 (17)	0.0483 (17)	0.0005 (14)	0.0281 (15)	0.0023 (14)
C17	0.0412 (15)	0.0390 (15)	0.0422 (15)	0.0020 (12)	0.0154 (13)	-0.0028 (12)
C18	0.0585 (19)	0.0271 (14)	0.0614 (19)	-0.0043 (12)	0.0250 (15)	-0.0014 (13)
C19	0.063 (2)	0.0368 (16)	0.067 (2)	-0.0039 (14)	0.0330 (17)	-0.0001 (14)
C20	0.081 (3)	0.0498 (19)	0.084 (3)	-0.0122 (18)	0.045 (2)	0.0050 (18)

Geometric parameters (Å, °)

O1—C1	1.353 (3)	O4—C11	1.360 (3)
O1—H1	0.8206	O4—H4	0.8191
O2—C7	1.210 (3)	O5—C17	1.213 (3)
O3—C7	1.326 (3)	O6—C17	1.328 (3)
O3—C8	1.449 (3)	O6—C18	1.449 (3)
C1—C2	1.384 (4)	C11—C16	1.381 (4)
C1—C6	1.385 (4)	C11—C12	1.383 (4)
C2—C3	1.374 (4)	C12—C13	1.369 (4)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.397 (4)	C13—C14	1.389 (4)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.386 (4)	C14—C15	1.387 (4)
C4—C7	1.478 (4)	C14—C17	1.476 (4)
C5—C6	1.375 (4)	C15—C16	1.381 (4)
C5—H5	0.9300	C15—H15	0.9300
C6—H6	0.9300	C16—H16	0.9300

C8—C9	1.497 (4)	C18—C19	1.492 (4)
C8—H8A	0.9700	C18—H18A	0.9700
C8—H8B	0.9700	C18—H18B	0.9700
C9—C10	1.488 (5)	C19—C20	1.523 (4)
C9—H9A	0.9700	C19—H19A	0.9700
C9—H9B	0.9700	C19—H19B	0.9700
C10—H10A	0.9600	C20—H20A	0.9600
C10—H10B	0.9600	C20—H20B	0.9600
C10—H10C	0.9600	C20—H20C	0.9600
C1—O1—H1	109.5	C11—O4—H4	109.5
C7—O3—C8	117.4 (2)	C17—O6—C18	117.6 (2)
O1—C1—C2	117.5 (3)	O4—C11—C16	122.4 (3)
O1—C1—C6	122.8 (3)	O4—C11—C12	117.6 (3)
C2—C1—C6	119.7 (3)	C16—C11—C12	120.0 (3)
C3—C2—C1	120.4 (3)	C13—C12—C11	120.4 (3)
C3—C2—H2	119.8	C13—C12—H12	119.8
C1—C2—H2	119.8	C11—C12—H12	119.8
C2—C3—C4	120.4 (3)	C12—C13—C14	120.7 (3)
C2—C3—H3	119.8	C12—C13—H13	119.7
C4—C3—H3	119.8	C14—C13—H13	119.7
C5—C4—C3	118.5 (2)	C15—C14—C13	118.4 (3)
C5—C4—C7	120.6 (2)	C15—C14—C17	120.1 (2)
C3—C4—C7	120.8 (2)	C13—C14—C17	121.5 (2)
C6—C5—C4	121.2 (3)	C16—C15—C14	121.3 (3)
C6—C5—H5	119.4	C16—C15—H15	119.3
C4—C5—H5	119.4	C14—C15—H15	119.3
C5—C6—C1	119.8 (3)	C15—C16—C11	119.3 (3)
C5—C6—H6	120.1	C15—C16—H16	120.4
C1—C6—H6	120.1	C11—C16—H16	120.4
O2—C7—O3	122.2 (3)	O5—C17—O6	122.3 (3)
O2—C7—C4	124.8 (3)	O5—C17—C14	125.3 (3)
O3—C7—C4	113.0 (2)	O6—C17—C14	112.4 (2)
O3—C8—C9	107.6 (2)	O6—C18—C19	107.3 (2)
O3—C8—H8A	110.2	O6—C18—H18A	110.3
C9—C8—H8A	110.2	C19—C18—H18A	110.3
O3—C8—H8B	110.2	O6—C18—H18B	110.3
C9—C8—H8B	110.2	C19—C18—H18B	110.3
H8A—C8—H8B	108.5	H18A—C18—H18B	108.5
C10—C9—C8	112.5 (3)	C18—C19—C20	111.8 (3)
C10—C9—H9A	109.1	C18—C19—H19A	109.3
C8—C9—H9A	109.1	C20—C19—H19A	109.3
C10—C9—H9B	109.1	C18—C19—H19B	109.3
C8—C9—H9B	109.1	C20—C19—H19B	109.3
H9A—C9—H9B	107.8	H19A—C19—H19B	107.9
C9—C10—H10A	109.5	C19—C20—H20A	109.5
C9—C10—H10B	109.5	C19—C20—H20B	109.5
H10A—C10—H10B	109.5	H20A—C20—H20B	109.5

C9—C10—H10C	109.5	C19—C20—H20C	109.5
H10A—C10—H10C	109.5	H20A—C20—H20C	109.5
H10B—C10—H10C	109.5	H20B—C20—H20C	109.5

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O4—H4 \cdots O5 ⁱ	0.82	1.93	2.730 (3)	167
O1—H1 \cdots O2 ⁱⁱ	0.82	1.91	2.720 (3)	171

Symmetry codes: (i) $-x+1, y-1/2, -z+3/2$; (ii) $-x+2, y+1/2, -z+1/2$.