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7-Methoxyindan-1-one

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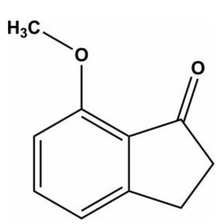
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.116; data-to-parameter ratio = 15.1.

In the title compound, $C_{10}H_{10}O_2$, the 1-indanone unit is essentially planar (r.m.s. deviation = 0.028 Å). In the crystal, molecules are linked *via* C—H⋯O hydrogen bonds, forming layers lying parallel to the *ab* plane. This two-dimensional structure is stabilized by a weak C—H⋯π interaction. A second weak C—H⋯π interaction links the layers, forming a three-dimensional structure.

Related literature

For the preparation of the title compound, see: Li *et al.* (2011). For applications of indanone derivatives, see: Borge *et al.* (2010); Cai *et al.* (2005); Cui *et al.* (2009); Fu & Wang (2008); Li *et al.* (2009); Sousa *et al.* (2011); Tang *et al.* (2011). For related structures, see: Ali *et al.* (2010*a*,*b*,*c*,*d*); Chen *et al.* (2011*a*,*b*). For C—H⋯O hydrogen bonds, see: Li *et al.* (2011*a*,*b*); Wang & Chen (2011); Xi *et al.* (2010).



Experimental

Crystal data

$C_{10}H_{10}O_2$
M_r = 162.18
Orthorhombic, *Pbca*
a = 8.5386 (7) Å
b = 10.4949 (9) Å
c = 18.8536 (16) Å
V = 1689.5 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 297 K
0.64 × 0.55 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.683, T_{max} = 1.000
8807 measured reflections
1663 independent reflections
1278 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.116
S = 1.02
1663 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

*Cg*1 is the centroid of the C1/C5–C9 ring.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C3—H3B⋯O2^{i}	0.97	2.60	3.5183 (18)	159
C7—H7A⋯O1^{ii}	0.93	2.57	3.4802 (18)	167
C10—H10B⋯O1^{iii}	0.96	2.59	3.486 (2)	156
C4—H4A⋯$Cg1^{iv}$	0.97	2.80	3.6430 (16)	146
C10—H10A⋯$Cg1^{v}$	0.96	2.82	3.6260 (16)	143

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2507).

References

Ali, M. A., Ismail, R., Choon, T. S., Rosli, M. M. & Fun, H.-K. (2010*a*). *Acta Cryst.* E**66**, o2878.
Ali, M. A., Ismail, R., Tan, S. C., Quah, C. K. & Fun, H.-K. (2010*b*). *Acta Cryst.* E**66**, o2875.
Ali, M. A., Ismail, R., Tan, S. C., Yeap, C. S. & Fun, H.-K. (2010*c*). *Acta Cryst.* E**66**, o2753.
Ali, M. A., Ismail, R., Tan, S. C., Yeap, C. S. & Fun, H.-K. (2010*d*). *Acta Cryst.* E**66**, o2864.
Borge, J., Cadierno, V., Díez, J., García-Garrido, S. E. & Gimeno, J. (2010). *Dyes Pigm.* **87**, 209–217.
Bruker (2001). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cai, X., Wu, K. & Dolbier, W. R. Jr (2005). *J. Fluor. Chem.* **126**, 479–482.
Chen, K.-Y., Fang, T.-C. & Chang, M.-J. (2011*a*). *Acta Cryst.* E**67**, o992.
Chen, K.-Y., Wen, Y.-S., Fang, T.-C., Chang, Y.-J. & Chang, M.-J. (2011*b*). *Acta Cryst.* E**67**, o927.
Cui, Y., Ren, H., Yu, J., Wang, Z. & Qian, G. (2009). *Dyes Pigm.* **81**, 53–57.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Fu, T. L. & Wang, I. J. (2008). *Dyes Pigm.* **76**, 590–595.
Li, C. J., Feng, Y. Q., Liu, X. J. & Zhang, T. Y. (2011*a*). *Chin. Chem. Lett.* **22**, 539–542.
Li, X., Kim, S.-H. & Son, Y.-A. (2009). *Dyes Pigm.* **82**, 293–298.
Li, Z., Lin, Y., Xia, J.-L., Zhang, H., Fan, F., Zeng, Q., Feng, D., Yin, J. & Liu, S. H. (2011). *Dyes Pigm.* **90**, 245–252.
Li, H. Q., Zhang, Z. B. & Li, L. (2011*b*). *Chin. Chem. Lett.* **22**, 280–283.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sousa, C. M., Berthet, J., Delbaere, S. & Coelho, P. J. (2011). *Dyes Pigm.* **92**, 537–541.
Tang, K.-C., Chang, M.-J., Lin, T.-Y., Pan, H.-A., Fang, T.-C., Chen, K.-Y., Hung, W.-Y., Hsu, Y.-H. & Chou, P.-T. (2011). *J. Am. Chem. Soc.* **133**, 17738–17745.
Wang, E. J. & Chen, G. Y. (2011). *Chin. Chem. Lett.* **22**, 847–850.
Xi, H. T., Yi, T. T. & Sun, X. Q. (2010). *Chin. Chem. Lett.* **21**, 633–636.

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7-Methoxyindan-1-one

Yuan Jay Chang and Kew-Yu Chen

S1. Comment

Indanone and its derivatives are some of the most widely used organic compounds (Tang *et al.*, 2011). They are used as dyes and pigments (Cui *et al.*, 2009; Li *et al.*, 2009), intermediates in organic synthesis (Fu & Wang, 2008; Borge *et al.*, 2010) and exhibit a wide variety of biological activities (Sousa *et al.*, 2011). In addition, 1-indanones were important precursors in the regiospecific synthesis of 2-fluoro-1-naphthols (Cai *et al.*, 2005).

The molecular structure of the title compound is shown in Figure 1. The 1-indaneone moiety is essentially planar (r.m.s. deviation = 0.028 Å), which is consistent with previous studies (Chen *et al.*, 2011*a*,*b*; Ali *et al.*, 2010*a*,*b*,*c*,*d*). There are three different kinds of C—H···O (Li *et al.*, 2011*a*,*b*; Wang *et al.*, 2011; Xi *et al.*, 2010) hydrogen bonds (Table 1) in the crystal structure (Figure 2). In addition, C—H···π hydrogen bonds further stabilize the crystal structure (2.80 Å for the C4—H4A···*Cg*1 distance and 146° for the C4—H4A—$Cg1^{i}$ angle; 2.82 Å for the C10—H10A···*Cg*1 distance and 143° for the C10—H10A—$Cg1^{ii}$ angle; *Cg*1 is the centroid of the C1/C5—C9 ring; symmetry codes: (i): *-x*, 1 - *y*,- *z* (ii): *-x*, 1/2 + *y*, 1/2 - *z*).

S2. Experimental

The title compound was synthesized by the methylation of 7-hydroxyindan-1-one with methyl iodide (Li *et al.*, 2011). Colorless parallelepiped-shaped crystals suitable for the crystallographic study reported here were isolated over a period of six weeks by slow evaporation from a chloroform solution.

S3. Refinement

The C bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

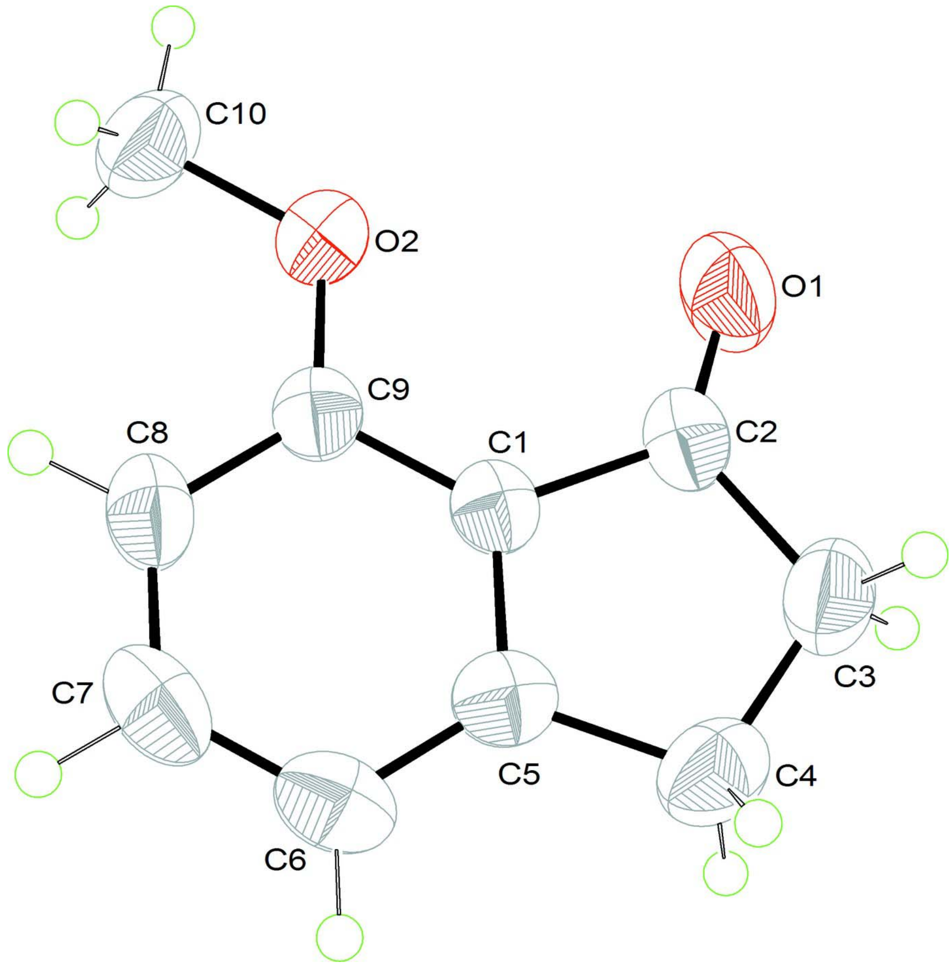

Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

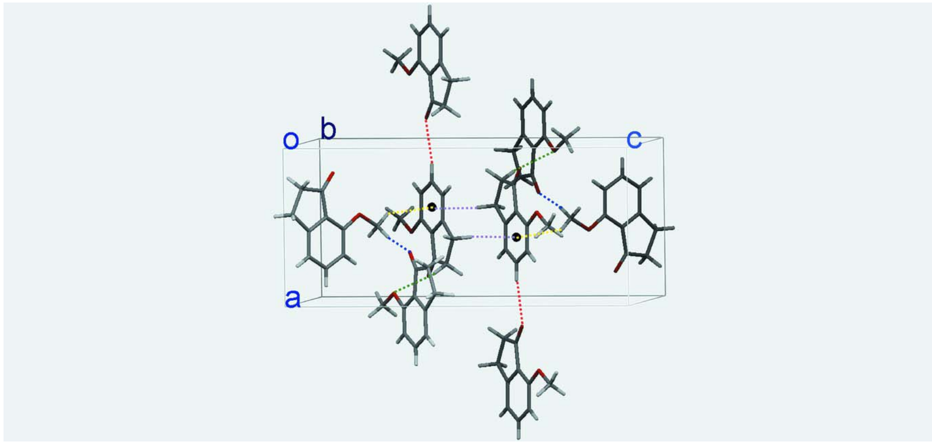

Figure 2

A section of the crystal packing of the title compound, viewed along the *b* axis. Blue, green and red dashed lines denote the intermolecular C10—H10B···O1, C3—H3B···O2 and C7—H7A···O1 hydrogen bonds, respectively. Yellow and purple dashed lines denote the intermolecular C10—H10A···*π* and C4—H4A···*π* hydrogen bonds, respectively. *Cg*1 (black circles) is the centroid of the C1/C5—C9 ring. For symmetry operators, see Table 1.

7-Methoxyindan-1-one

Crystal data

$C_{10}H_{10}O_2$
M_r = 162.18
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 8.5386 (7) Å
b = 10.4949 (9) Å
c = 18.8536 (16) Å
V = 1689.5 (2) Å^3
Z = 8
F(000) = 688
D_x = 1.275 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3629 reflections
θ = 2.9–26.0°
μ = 0.09 mm^{-1}
T = 297 K
Parallelepiped, colorless
0.64 × 0.55 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.683, T_{max} = 1.000
8807 measured reflections
1663 independent reflections
1278 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.0°, θ_{min} = 2.2°
h = −10→10
k = −12→12
l = −16→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.116
S = 1.02
1663 reflections
110 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
$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.2236P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}

Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0068 (15)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.34168 (11)	0.54158 (11)	0.13950 (7)	0.0741 (4)
O2	0.07222 (10)	0.67528 (9)	0.20144 (5)	0.0545 (3)
C1	0.06609 (14)	0.50056 (11)	0.12296 (6)	0.0412 (3)
C2	0.23519 (16)	0.47945 (13)	0.11460 (7)	0.0480 (3)
C3	0.25583 (19)	0.36302 (14)	0.06788 (8)	0.0637 (4)
H3A	0.3207	0.3835	0.0272	0.076*
H3B	0.3057	0.2948	0.0943	0.076*
C4	0.09387 (18)	0.32271 (14)	0.04396 (8)	0.0606 (4)
H4A	0.0829	0.3318	−0.0070	0.073*
H4B	0.0734	0.2348	0.0568	0.073*
C5	−0.01569 (17)	0.41149 (12)	0.08242 (7)	0.0475 (3)
C6	−0.17764 (18)	0.41110 (14)	0.08112 (8)	0.0610 (4)
H6A	−0.2322	0.3522	0.0538	0.073*
C7	−0.25596 (18)	0.49998 (16)	0.12127 (8)	0.0643 (5)
H7A	−0.3649	0.5006	0.1207	0.077*
C8	−0.17749 (16)	0.58882 (14)	0.16256 (7)	0.0560 (4)
H8A	−0.2340	0.6470	0.1896	0.067*
C9	−0.01507 (15)	0.59128 (12)	0.16371 (6)	0.0431 (3)
C10	−0.0085 (2)	0.76805 (14)	0.24349 (8)	0.0662 (4)
H10A	0.0664	0.8210	0.2674	0.099*
H10B	−0.0729	0.7255	0.2779	0.099*
H10C	−0.0730	0.8198	0.2134	0.099*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0400 (6)	0.0783 (8)	0.1039 (9)	0.0010 (5)	0.0001 (6)	−0.0157 (6)
O2	0.0529 (6)	0.0558 (6)	0.0548 (6)	0.0059 (4)	−0.0009 (4)	−0.0125 (4)
C1	0.0415 (7)	0.0426 (6)	0.0395 (6)	0.0022 (5)	0.0007 (5)	0.0071 (5)
C2	0.0418 (7)	0.0503 (7)	0.0520 (7)	0.0065 (6)	0.0016 (6)	0.0054 (6)
C3	0.0651 (9)	0.0637 (9)	0.0624 (8)	0.0227 (8)	0.0009 (7)	−0.0052 (7)
C4	0.0793 (11)	0.0469 (8)	0.0555 (8)	0.0084 (7)	−0.0041 (7)	−0.0038 (6)

C5	0.0565 (8)	0.0429 (7)	0.0432 (7)	−0.0009 (6)	−0.0041 (6)	0.0052 (5)
C6	0.0548 (9)	0.0610 (9)	0.0674 (9)	−0.0121 (7)	−0.0116 (7)	0.0017 (7)
C7	0.0380 (7)	0.0802 (11)	0.0747 (10)	−0.0061 (7)	−0.0015 (7)	0.0120 (8)
C8	0.0435 (8)	0.0664 (9)	0.0583 (8)	0.0090 (6)	0.0094 (6)	0.0041 (7)
C9	0.0440 (7)	0.0458 (7)	0.0393 (6)	0.0026 (5)	0.0020 (5)	0.0043 (5)
C10	0.0800 (10)	0.0591 (8)	0.0594 (9)	0.0161 (8)	0.0020 (8)	−0.0128 (7)

Geometric parameters (Å, º)

O1—C2	1.2134 (17)	C4—H4B	0.9700
O2—C9	1.3560 (15)	C5—C6	1.383 (2)
O2—C10	1.4321 (16)	C6—C7	1.375 (2)
C1—C5	1.3948 (17)	C6—H6A	0.9300
C1—C9	1.4061 (17)	C7—C8	1.387 (2)
C1—C2	1.4692 (18)	C7—H7A	0.9300
C2—C3	1.517 (2)	C8—C9	1.387 (2)
C3—C4	1.515 (2)	C8—H8A	0.9300
C3—H3A	0.9700	C10—H10A	0.9600
C3—H3B	0.9700	C10—H10B	0.9600
C4—C5	1.5063 (19)	C10—H10C	0.9600
C4—H4A	0.9700		
C9—O2—C10	117.90 (11)	C6—C5—C4	127.63 (13)
C5—C1—C9	120.43 (12)	C1—C5—C4	111.55 (12)
C5—C1—C2	109.40 (11)	C7—C6—C5	118.33 (13)
C9—C1—C2	130.17 (12)	C7—C6—H6A	120.8
O1—C2—C1	127.87 (13)	C5—C6—H6A	120.8
O1—C2—C3	124.79 (13)	C6—C7—C8	122.01 (14)
C1—C2—C3	107.34 (12)	C6—C7—H7A	119.0
C4—C3—C2	106.97 (12)	C8—C7—H7A	119.0
C4—C3—H3A	110.3	C7—C8—C9	120.27 (13)
C2—C3—H3A	110.3	C7—C8—H8A	119.9
C4—C3—H3B	110.3	C9—C8—H8A	119.9
C2—C3—H3B	110.3	O2—C9—C8	124.74 (12)
H3A—C3—H3B	108.6	O2—C9—C1	117.13 (11)
C5—C4—C3	104.53 (11)	C8—C9—C1	118.14 (12)
C5—C4—H4A	110.8	O2—C10—H10A	109.5
C3—C4—H4A	110.8	O2—C10—H10B	109.5
C5—C4—H4B	110.8	H10A—C10—H10B	109.5
C3—C4—H4B	110.8	O2—C10—H10C	109.5
H4A—C4—H4B	108.9	H10A—C10—H10C	109.5
C6—C5—C1	120.81 (13)	H10B—C10—H10C	109.5
C5—C1—C2—O1	176.75 (14)	C1—C5—C6—C7	−0.6 (2)
C9—C1—C2—O1	−3.7 (2)	C4—C5—C6—C7	179.00 (13)
C5—C1—C2—C3	−3.15 (14)	C5—C6—C7—C8	−0.1 (2)
C9—C1—C2—C3	176.41 (12)	C6—C7—C8—C9	0.8 (2)
O1—C2—C3—C4	−175.29 (13)	C10—O2—C9—C8	0.29 (18)

C1—C2—C3—C4	4.62 (15)	C10—O2—C9—C1	−179.75 (11)
C2—C3—C4—C5	−4.24 (15)	C7—C8—C9—O2	179.03 (12)
C9—C1—C5—C6	0.42 (18)	C7—C8—C9—C1	−0.93 (19)
C2—C1—C5—C6	−179.97 (12)	C5—C1—C9—O2	−179.63 (10)
C9—C1—C5—C4	−179.21 (11)	C2—C1—C9—O2	0.84 (18)
C2—C1—C5—C4	0.41 (14)	C5—C1—C9—C8	0.33 (17)
C3—C4—C5—C6	−177.12 (14)	C2—C1—C9—C8	−179.19 (12)
C3—C4—C5—C1	2.47 (15)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C1/C5–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*B*···O2^{i}	0.97	2.60	3.5183 (18)	159
C7—H7*A*···O1^{ii}	0.93	2.57	3.4802 (18)	167
C10—H10*B*···O1^{iii}	0.96	2.59	3.486 (2)	156
C4—H4*A*···*Cg*1^{iv}	0.97	2.80	3.6430 (16)	146
C10—H10*A*···*Cg*1^{v}	0.96	2.82	3.6260 (16)	143

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