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3-Hydroxy-3-methylisochroman-1-one–2-(carboxymethyl)benzoic acid (1/1)

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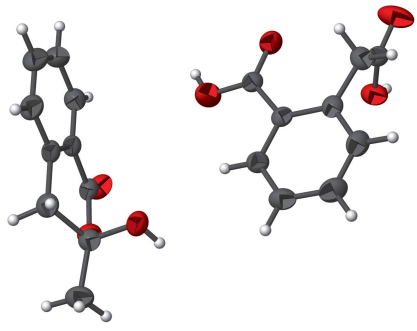
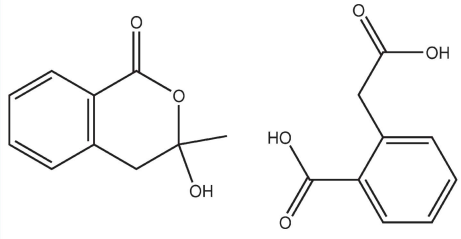
Structural data: full structural data are available from iucrdata.iucr.org

The title co-crystalline compound, $C_{10}H_{10}O_3 \cdot C_9H_8O_4$, has been synthesized and characterized in a single-crystal X-ray diffraction study. In the 3-hydroxy-3-methylisochroman-1-one molecule, the six-membered heterocyclic ring lies between an envelope and a screw-boat conformation. In the 2-carboxymethylbenzoic acid, molecule, the 2-carboxymethyl substituent is almost planar (r.m.s deviation = 0.048 Å) and makes a dihedral angle of 79.59 (7)° with the planar benzene ring. In this molecule, intramolecular C—H···O contacts generate five- and six-membered rings, forming a tricyclic ring system. In the crystal, classical O—H···O and C—H···O hydrogen bonds combine with C—H···π(ring) and unusual C═O···π(ring) contacts to generate a three-dimensional network.

3D view



Chemical scheme



Structure description

Isochromanone derivatives are generally known as regulators of plant growth (Bianchi *et al.*, 2004). Depending on their chemical structure and concentration, they can act either as inhibitors or stimulators in these processes. Some substituted isochromanones isolated from myxobacteria strains have been introduced as anti-fungal agents (Buntin *et al.*, 2008). In view of their importance and as a continuation of our work on the crystal structure analysis of isochromanone derivatives (Abou *et al.*, 2009, 2011, 2012), we report herein the synthesis and crystal structure of the title compound (Fig. 1), a (1/1) co-crystal of 3-hydoxy-3-methyl-isochroman-1-one (*A*), and 2-carboxymethyl-benzoic acid (*B*).

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

*Cg*2 is the centroid of the C3*A*/C4*A*/C10*A*–C13*A* benzene ring (molecule *A*) and *Cg*4 is the centroid of the C3*B*/C4*B*/C10*B*–C13*B* benzene ring (molecule *B*).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10*B*—H10*B*···O18*B*	0.93	2.33	2.6745 (16)	102
C2*B*—H21*B*···O17*B*	0.97	2.39	2.7870 (16)	104
C7*A*—H73*A*···O9*A*^{i}	0.96	2.60	3.4469 (17)	148
O8*A*—H8*A*···O9*A*^{ii}	0.82	2.02	2.8311 (12)	172
O15*B*—H15*B*···O17*B*^{iii}	0.82	1.88	2.6950 (13)	171
O18*B*—H18*B*···O16*B*^{iv}	0.82	1.80	2.6115 (15)	168
C2*B*—H22*B*···*Cg*2^{iii}	0.97	2.92	3.8725 (15)	169
C5*A*—H51*A*···*Cg*2^{v}	0.97	2.74	3.6346 (15)	153
C11*A*—H11*A*···*Cg*4^{vi}	0.93	2.78	3.6075 (17)	149
C14*B*—O17*B*···*Cg*4^{vii}	1.26 (1)	3.44 (1)	3.5714 (13)	86 (1)

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

In molecule *A*, the six-membered heterocyclic ring system O1*A*/C2*A*–C6*A* displays a conformation between that of an envelope and a screw-boat as judged from the puckering parameters [Q_T = 0.4319 (14) Å, θ = 120.60 (18)° and φ = 109.5 (2)°] with atom O8*A* in an axial position. In this molecule, the bond lengths and angles of the isochroman-1-one ring are within normal ranges and comparable to those found in related structures (Brockway *et al.*, 2011; Bredenkamp *et al.*, 1989).

In molecule *B*, *S*(5) and *S*(6) ring motifs arise from intramolecular C10*B*—H10*B*···O18*B* and C2*B*—H2B···O17*B* hydrogen bonds (Table 1), and generate a pseudo tricyclic ring system (Fig. 1). The planar benzoic acid (r.m.s deviation = 0.028 Å) group is almost perpendicular to the least-squares plane of the 2-carboxymethyl substituent (r.m.s deviation = 0.004), making a dihedral angle of 79.14 (7)°. The bond lengths and angles of this molecule are also generally in good agreement with those observed in related structures (Tai *et al.*, 2014; Bolte, 2009).

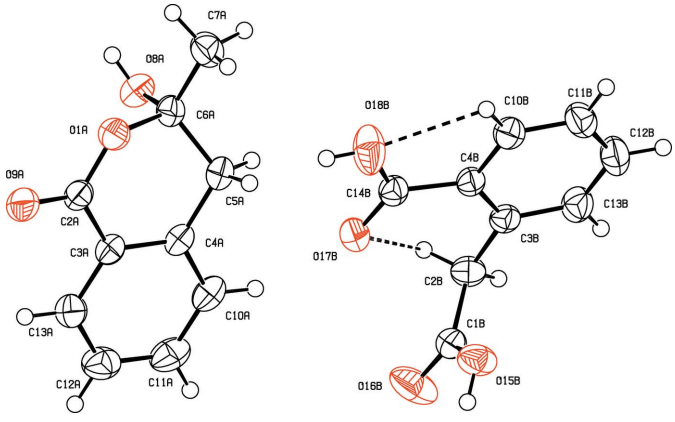


Figure 1
The asymmetric unit of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius. The dashed lines indicate intramolecular hydrogen bonds.

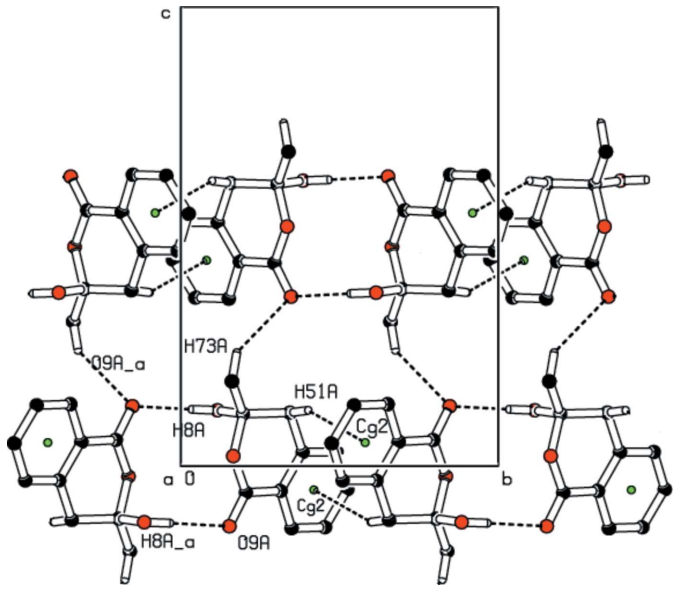


Figure 2
Sheets of type *A* molecules viewed along the the *a*-axis direction. The green dots are the centroids of the C3*A*/C4*A*/C10*A*–C13*A* benzene rings. In these packing diagrams, the dashed lines represent hydrogen bonds and H atoms not involved in hydrogen-bonding interactions have been omitted for clarity.

In the co-crystal structure, O8*A*—H8*A*···O9*A* hydrogen bonds (Table 1) link molecules of type *A* into centrosymmetric $R_2^2(12)$ dimers lying nearly parallel to the *bc* plane. These are connected by C7*A*—H73*A*···O9*A* hydrogen bonds along the *c*-axis direction and by inversion-related C5*A*—

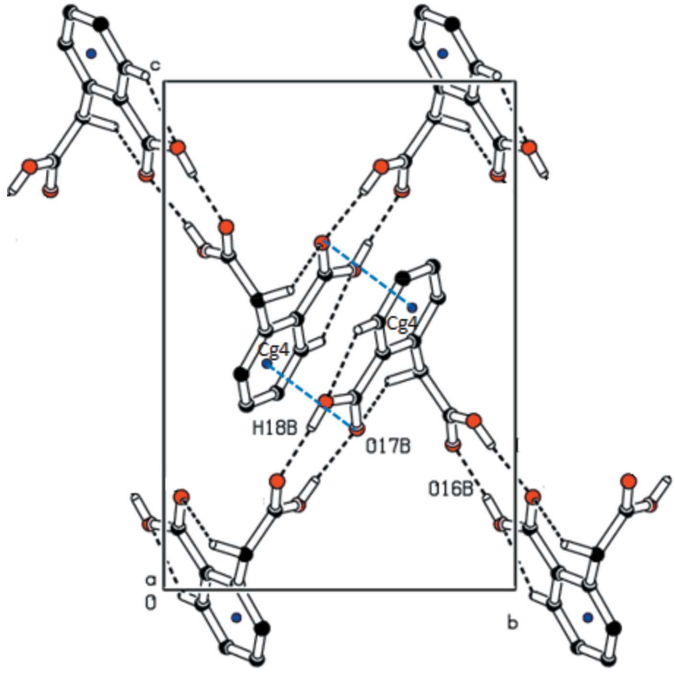


Figure 3
Part of the crystal packing of the *B* molecules in the co-crystal viewed along the the *a* axis direction. The blue dots are the centroids of the C3*B*/C4*B*/C10*B*–C13*B* benzene rings

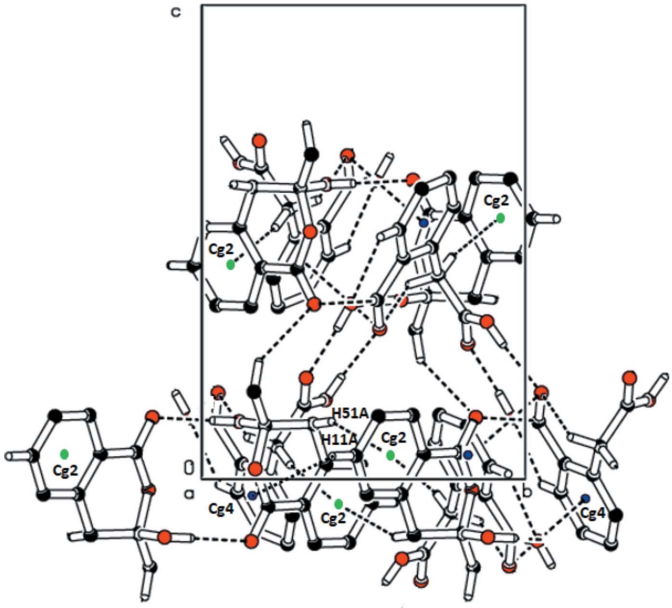


Figure 4
Overall crystal packing of the title compound, showing the supramolecular aggregation resulting from the three-dimensional hydrogen-bonded network.

H51*A*···π(ring) contacts to the benzene ring of another *A* molecule (Fig. 2). *B* molecules form unusual inversion-related C14*B*═O17*B*···*Cg*4 contacts and classical centrosymmetric head-to-head carboxylic acid–carboxyl hydrogen-bonding interactions (O15*B*—H15*B*···O17*B* and O18*B*—H18*B*···O16*B*) each generating $R_2^2(8)$ ring motifs. These contacts link the *B* molecules into an extensive *X*-shaped array along the *c*-axis direction, Fig. 3. The two sets of co-crystallized molecules are further interconnected by weak C11*A*—H11*A*···*Cg*4 and C2*B*—H22*B*···*Cg*2 hydrogen bonds (Table 1) to give a three-dimensional network (Fig. 4) (*Cg*2 and *Cg*4 are the centroids of the C3*A*/C4*A*/C10*A*–C13*A* and C3*B*/C4*B*/C10*B*–C13*B* benzene rings, respectively).

Synthesis and crystallization

300 ml of dried diethyl ether, 0.125 mol of acetic anhydride and 4 ml of dried pyridine were placed in a 500 ml flask fitted with water condenser. The mixture was stirred and 0.12 mol of homophthalic anhydride was added in small portions of 0.03 mol over 30 min. After this addition, the mixture was stirred at room temperature for 3 h. The precipitate was filtered, washed with petroleum ether to remove the pyridine and recrystallized from chloroform–pentane (1/1; *v*/*v*) solution. Colourless crystals of the title compound were obtained in a good yield (98%; m.p. 435–436 K).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Two outlier reflections ($\bar{3}08$, $\bar{3}17$) were omitted from the final refinement.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_{10}O_3{\cdot}C_9H_8O_4$
M_r	358.33
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, *b*, *c* (Å)	12.1143 (4), 9.8134 (1), 14.2602 (2)
β (°)	95.116 (1)
V (Å^3)	1688.53 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.50 × 0.30 × 0.30
Data collection	
Diffractometer	Nonius KappaCCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16894, 4368, 3717
R_{int}	0.025
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.683
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.044, 0.116, 1.05
No. of reflections	4368
No. of parameters	238
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.34

Computer programs: *COLLECT* (Hooft, 1998), *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997), *SIR2014* (Burla *et al.*, 2015), *PLATON* (Spek, 2009), *SHELXL2014* (Sheldrick, 2015), *publCIF* (Westrip, 2010) and *WinGX* (Farrugia, 2012).

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x181653 [https://doi.org/10.1107/S241431461801653X]

3-Hydroxy-3-methylisochroman-1-one–2-(carboxymethyl)benzoic acid (1/1)

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Crystal data

$C_{10}H_{10}O_3·C_9H_8O_4$
M_r = 358.33
Monoclinic, $P2_1/c$
a = 12.1143 (4) Å
b = 9.8134 (1) Å
c = 14.2602 (2) Å
β = 95.116 (1)°
V = 1688.53 (6) Å^3
Z = 4
F(000) = 752
D_x = 1.410 Mg m^{-3}
Melting point = 435–436 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 16894 reflections
θ = 3.0–29.1°
μ = 0.11 mm^{-1}
T = 298 K
Prism, colourless
0.50 × 0.30 × 0.30 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
φ & ω scans
16894 measured reflections
4368 independent reflections
3717 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 29.1°, θ_{min} = 3.0°
h = −16→16
k = −12→12
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.116
S = 1.05
4368 reflections
238 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
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.4813P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1A	−0.54160 (7)	−0.16519 (9)	−0.02214 (6)	0.0373 (2)
O9A	−0.50696 (9)	−0.15285 (9)	0.13071 (6)	0.0454 (2)
O8A	−0.40645 (7)	−0.11526 (9)	−0.12192 (7)	0.0408 (2)
H8A	−0.4248	−0.0348	−0.1239	0.061*
O15B	0.00113 (8)	0.38147 (10)	0.16774 (7)	0.0471 (2)
H15B	0.0107	0.4299	0.2146	0.071*
O17B	−0.01082 (9)	0.04983 (10)	0.18244 (6)	0.0468 (2)
C3A	−0.40072 (9)	−0.31387 (11)	0.05345 (8)	0.0325 (2)
O18B	−0.17355 (9)	−0.03915 (12)	0.13005 (8)	0.0614 (3)
H18B	−0.1638	−0.0801	0.1803	0.092*
C4B	−0.09752 (9)	0.12336 (11)	0.03329 (8)	0.0306 (2)
C2B	0.09587 (10)	0.23078 (13)	0.06993 (9)	0.0373 (3)
H21B	0.1250	0.1420	0.0890	0.045*
H22B	0.1485	0.2727	0.0314	0.045*
C5A	−0.46413 (11)	−0.34373 (12)	−0.11663 (9)	0.0377 (3)
H51A	−0.5297	−0.4010	−0.1216	0.045*
H52A	−0.4249	−0.3592	−0.1721	0.045*
C14B	−0.09202 (10)	0.04148 (12)	0.12152 (8)	0.0329 (2)
C6A	−0.49905 (10)	−0.19569 (12)	−0.11399 (8)	0.0338 (2)
C1B	0.08979 (10)	0.31608 (12)	0.15668 (8)	0.0354 (2)
C10B	−0.19361 (10)	0.10970 (12)	−0.02765 (9)	0.0366 (3)
H10B	−0.2504	0.0531	−0.0113	0.044*
O16B	0.17422 (9)	0.32251 (14)	0.21356 (8)	0.0657 (4)
C4A	−0.39103 (9)	−0.38359 (11)	−0.03078 (8)	0.0331 (2)
C13B	−0.02670 (12)	0.27947 (14)	−0.07543 (9)	0.0424 (3)
H13B	0.0289	0.3374	−0.0924	0.051*
C11A	−0.25009 (12)	−0.52470 (14)	0.04999 (12)	0.0498 (3)
H11A	−0.1996	−0.5960	0.0488	0.060*
C12B	−0.12191 (13)	0.26454 (15)	−0.13581 (9)	0.0473 (3)
H12B	−0.1295	0.3121	−0.1924	0.057*
C11B	−0.20523 (11)	0.17956 (14)	−0.11222 (9)	0.0431 (3)
H11B	−0.2691	0.1691	−0.1529	0.052*
C3B	−0.01182 (10)	0.21028 (11)	0.00992 (8)	0.0324 (2)
C13A	−0.33505 (11)	−0.34890 (13)	0.13500 (9)	0.0406 (3)
H13A	−0.3420	−0.3018	0.1908	0.049*
C2A	−0.48439 (10)	−0.20496 (11)	0.05745 (8)	0.0331 (2)
C10A	−0.31536 (11)	−0.49014 (13)	−0.03101 (10)	0.0433 (3)
H10A	−0.3086	−0.5387	−0.0862	0.052*
C7A	−0.59486 (12)	−0.16094 (16)	−0.18498 (10)	0.0483 (3)
H71A	−0.6147	−0.0670	−0.1781	0.072*
H72A	−0.6572	−0.2176	−0.1745	0.072*
H73A	−0.5736	−0.1761	−0.2474	0.072*
C12A	−0.25926 (12)	−0.45421 (15)	0.13264 (11)	0.0481 (3)
H12A	−0.2146	−0.4774	0.1867	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0383 (4)	0.0387 (5)	0.0353 (4)	0.0089 (3)	0.0059 (3)	−0.0026 (3)
O9A	0.0633 (6)	0.0381 (5)	0.0361 (5)	0.0094 (4)	0.0125 (4)	−0.0028 (4)
O8A	0.0427 (5)	0.0321 (4)	0.0487 (5)	0.0000 (3)	0.0093 (4)	0.0005 (4)
O15B	0.0446 (5)	0.0467 (5)	0.0482 (5)	0.0124 (4)	−0.0047 (4)	−0.0156 (4)
O17B	0.0585 (6)	0.0419 (5)	0.0378 (5)	−0.0058 (4)	−0.0084 (4)	0.0062 (4)
C3A	0.0325 (5)	0.0267 (5)	0.0382 (6)	−0.0018 (4)	0.0040 (4)	−0.0014 (4)
O18B	0.0465 (6)	0.0747 (8)	0.0623 (7)	−0.0108 (5)	0.0012 (5)	0.0329 (6)
C4B	0.0345 (5)	0.0276 (5)	0.0299 (5)	0.0056 (4)	0.0048 (4)	−0.0013 (4)
C2B	0.0355 (6)	0.0381 (6)	0.0386 (6)	0.0000 (5)	0.0056 (5)	−0.0062 (5)
C5A	0.0446 (7)	0.0314 (6)	0.0371 (6)	0.0010 (5)	0.0027 (5)	−0.0072 (4)
C14B	0.0344 (6)	0.0313 (5)	0.0331 (5)	0.0034 (4)	0.0045 (4)	0.0004 (4)
C6A	0.0368 (6)	0.0331 (6)	0.0317 (5)	0.0019 (4)	0.0037 (4)	−0.0037 (4)
C1B	0.0378 (6)	0.0327 (6)	0.0353 (6)	0.0026 (5)	0.0007 (5)	−0.0007 (4)
C10B	0.0355 (6)	0.0358 (6)	0.0385 (6)	0.0031 (5)	0.0029 (5)	−0.0003 (5)
O16B	0.0518 (6)	0.0896 (9)	0.0521 (6)	0.0245 (6)	−0.0164 (5)	−0.0269 (6)
C4A	0.0336 (5)	0.0253 (5)	0.0408 (6)	−0.0015 (4)	0.0062 (5)	−0.0026 (4)
C13B	0.0488 (7)	0.0403 (6)	0.0392 (6)	−0.0017 (5)	0.0103 (5)	0.0053 (5)
C11A	0.0415 (7)	0.0377 (7)	0.0701 (9)	0.0095 (5)	0.0044 (6)	0.0046 (6)
C12B	0.0569 (8)	0.0506 (8)	0.0345 (6)	0.0068 (6)	0.0041 (6)	0.0104 (5)
C11B	0.0436 (7)	0.0483 (7)	0.0363 (6)	0.0074 (5)	−0.0032 (5)	0.0013 (5)
C3B	0.0367 (6)	0.0289 (5)	0.0322 (5)	0.0029 (4)	0.0066 (4)	−0.0040 (4)
C13A	0.0413 (6)	0.0386 (6)	0.0413 (6)	−0.0026 (5)	−0.0009 (5)	−0.0012 (5)
C2A	0.0380 (6)	0.0271 (5)	0.0348 (6)	−0.0011 (4)	0.0065 (4)	−0.0013 (4)
C10A	0.0448 (7)	0.0315 (6)	0.0546 (8)	0.0052 (5)	0.0090 (6)	−0.0051 (5)
C7A	0.0503 (8)	0.0512 (8)	0.0412 (7)	0.0084 (6)	−0.0071 (6)	−0.0048 (6)
C12A	0.0401 (7)	0.0462 (7)	0.0561 (8)	0.0026 (6)	−0.0054 (6)	0.0076 (6)

Geometric parameters (Å, º)

O1A—C2A	1.3343 (14)	C5A—H52A	0.9700
O1A—C6A	1.4803 (14)	C6A—C7A	1.5095 (17)
O9A—C2A	1.2160 (14)	C1B—O16B	1.2491 (16)
O8A—C6A	1.3845 (15)	C10B—C11B	1.3834 (18)
O8A—H8A	0.8200	C10B—H10B	0.9300
O15B—C1B	1.2729 (15)	C4A—C10A	1.3907 (16)
O15B—H15B	0.8200	C13B—C12B	1.384 (2)
O17B—C14B	1.2556 (14)	C13B—C3B	1.3914 (17)
C3A—C13A	1.3922 (17)	C13B—H13B	0.9300
C3A—C4A	1.3964 (16)	C11A—C12A	1.379 (2)
C3A—C2A	1.4776 (16)	C11A—C10A	1.383 (2)
O18B—C14B	1.2798 (15)	C11A—H11A	0.9300
O18B—H18B	0.8200	C12B—C11B	1.374 (2)
C4B—C10B	1.3956 (16)	C12B—H12B	0.9300
C4B—C3B	1.4064 (16)	C11B—H11B	0.9300
C4B—C14B	1.4894 (15)	C13A—C12A	1.3848 (19)

C2B—C1B	1.5009 (16)	C13A—H13A	0.9300
C2B—C3B	1.5085 (17)	C10A—H10A	0.9300
C2B—H21B	0.9700	C7A—H71A	0.9600
C2B—H22B	0.9700	C7A—H72A	0.9600
C5A—C4A	1.4975 (17)	C7A—H73A	0.9600
C5A—C6A	1.5145 (16)	C12A—H12A	0.9300
C5A—H51A	0.9700		

C2A—O1A—C6A	119.87 (9)	C10A—C4A—C3A	118.45 (12)
C6A—O8A—H8A	109.5	C10A—C4A—C5A	122.43 (11)
C1B—O15B—H15B	109.5	C3A—C4A—C5A	119.10 (10)
C13A—C3A—C4A	120.79 (11)	C12B—C13B—C3B	121.88 (12)
C13A—C3A—C2A	119.29 (11)	C12B—C13B—H13B	119.1
C4A—C3A—C2A	119.88 (10)	C3B—C13B—H13B	119.1
C14B—O18B—H18B	109.5	C12A—C11A—C10A	120.47 (12)
C10B—C4B—C3B	120.20 (10)	C12A—C11A—H11A	119.8
C10B—C4B—C14B	116.50 (10)	C10A—C11A—H11A	119.8
C3B—C4B—C14B	123.30 (10)	C11B—C12B—C13B	120.11 (12)
C1B—C2B—C3B	116.00 (10)	C11B—C12B—H12B	119.9
C1B—C2B—H21B	108.3	C13B—C12B—H12B	119.9
C3B—C2B—H21B	108.3	C12B—C11B—C10B	119.62 (12)
C1B—C2B—H22B	108.3	C12B—C11B—H11B	120.2
C3B—C2B—H22B	108.3	C10B—C11B—H11B	120.2
H21B—C2B—H22B	107.4	C13B—C3B—C4B	117.54 (11)
C4A—C5A—C6A	112.11 (9)	C13B—C3B—C2B	117.98 (11)
C4A—C5A—H51A	109.2	C4B—C3B—C2B	124.46 (10)
C6A—C5A—H51A	109.2	C12A—C13A—C3A	119.65 (12)
C4A—C5A—H52A	109.2	C12A—C13A—H13A	120.2
C6A—C5A—H52A	109.2	C3A—C13A—H13A	120.2
H51A—C5A—H52A	107.9	O9A—C2A—O1A	117.92 (11)
O17B—C14B—O18B	122.56 (11)	O9A—C2A—C3A	123.02 (11)
O17B—C14B—C4B	121.50 (11)	O1A—C2A—C3A	119.00 (10)
O18B—C14B—C4B	115.92 (10)	C11A—C10A—C4A	120.69 (13)
O8A—C6A—O1A	107.79 (9)	C11A—C10A—H10A	119.7
O8A—C6A—C7A	113.37 (11)	C4A—C10A—H10A	119.7
O1A—C6A—C7A	103.89 (10)	C6A—C7A—H71A	109.5
O8A—C6A—C5A	108.34 (10)	C6A—C7A—H72A	109.5
O1A—C6A—C5A	109.63 (10)	H71A—C7A—H72A	109.5
C7A—C6A—C5A	113.57 (10)	C6A—C7A—H73A	109.5
O16B—C1B—O15B	123.04 (11)	H71A—C7A—H73A	109.5
O16B—C1B—C2B	117.76 (11)	H72A—C7A—H73A	109.5
O15B—C1B—C2B	119.16 (11)	C11A—C12A—C13A	119.94 (13)
C11B—C10B—C4B	120.64 (12)	C11A—C12A—H12A	120.0
C11B—C10B—H10B	119.7	C13A—C12A—H12A	120.0
C4B—C10B—H10B	119.7		

C10B—C4B—C14B—O17B	−177.63 (11)	C4B—C10B—C11B—C12B	−0.8 (2)
C3B—C4B—C14B—O17B	2.75 (17)	C12B—C13B—C3B—C4B	0.09 (18)

C10B—C4B—C14B—O18B	3.79 (16)	C12B—C13B—C3B—C2B	178.65 (12)
C3B—C4B—C14B—O18B	−175.83 (11)	C10B—C4B—C3B—C13B	−0.59 (16)
C2A—O1A—C6A—O8A	−70.24 (13)	C14B—C4B—C3B—C13B	179.02 (11)
C2A—O1A—C6A—C7A	169.20 (10)	C10B—C4B—C3B—C2B	−179.05 (11)
C2A—O1A—C6A—C5A	47.50 (14)	C14B—C4B—C3B—C2B	0.56 (17)
C4A—C5A—C6A—O8A	68.15 (13)	C1B—C2B—C3B—C13B	106.92 (13)
C4A—C5A—C6A—O1A	−49.23 (13)	C1B—C2B—C3B—C4B	−74.62 (15)
C4A—C5A—C6A—C7A	−164.94 (11)	C4A—C3A—C13A—C12A	−0.07 (19)
C3B—C2B—C1B—O16B	172.01 (13)	C2A—C3A—C13A—C12A	177.65 (12)
C3B—C2B—C1B—O15B	−10.13 (17)	C6A—O1A—C2A—O9A	163.52 (11)
C3B—C4B—C10B—C11B	0.98 (17)	C6A—O1A—C2A—C3A	−19.25 (15)
C14B—C4B—C10B—C11B	−178.66 (11)	C13A—C3A—C2A—O9A	−7.62 (18)
C13A—C3A—C4A—C10A	0.92 (17)	C4A—C3A—C2A—O9A	170.12 (11)
C2A—C3A—C4A—C10A	−176.79 (11)	C13A—C3A—C2A—O1A	175.30 (11)
C13A—C3A—C4A—C5A	179.32 (11)	C4A—C3A—C2A—O1A	−6.97 (16)
C2A—C3A—C4A—C5A	1.62 (16)	C12A—C11A—C10A—C4A	0.2 (2)
C6A—C5A—C4A—C10A	−154.37 (11)	C3A—C4A—C10A—C11A	−1.00 (19)
C6A—C5A—C4A—C3A	27.29 (15)	C5A—C4A—C10A—C11A	−179.35 (12)
C3B—C13B—C12B—C11B	0.0 (2)	C10A—C11A—C12A—C13A	0.6 (2)
C13B—C12B—C11B—C10B	0.3 (2)	C3A—C13A—C12A—C11A	−0.7 (2)

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the C3*A*/C4*A*/C10*A*–C13*A* benzene ring (molecule *A*) and *Cg*4 is the centroid of the C3*B*/C4*B*/C10*B*–C13*B* benzene ring (molecule *B*).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10*B*—H10*B*···O18*B*	0.93	2.33	2.6745 (16)	102
C2*B*—H21*B*···O17*B*	0.97	2.39	2.7870 (16)	104
C7*A*—H73*A*···O9*A*^{i}	0.96	2.60	3.4469 (17)	148
O8*A*—H8*A*···O9*A*^{ii}	0.82	2.02	2.8311 (12)	172
O15*B*—H15*B*···O17*B*^{iii}	0.82	1.88	2.6950 (13)	171
O18*B*—H18*B*···O16*B*^{iv}	0.82	1.80	2.6115 (15)	168
C2*B*—H22*B*···*Cg*2^{iii}	0.97	2.92	3.8725 (15)	169
C5*A*—H51*A*···*Cg*2^{v}	0.97	2.74	3.6346 (15)	153
C11*A*—H11*A*···*Cg*4^{vi}	0.93	2.78	3.6075 (17)	149
C14*B*—O17*B*···*Cg*4^{vii}	1.26 (1)	3.44 (1)	3.5714 (13)	86 (1)

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