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(±)-4,6-Dimethoxy-3-(trichloromethyl)-isobenzofuran-1(3*H*)-one

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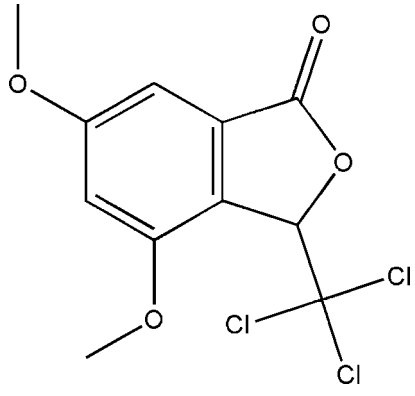
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.087; data-to-parameter ratio = 18.4.

The structure of the title compound, $C_{11}H_9Cl_3O_4$, shows two crystallographically independent but geometrically essentially identical molecules per asymmetric unit. The methoxy groups lie in the plane of the aromatic system, the relevant C—O—C—C and C—O—C—C torsion angles being −173.7 (2) and 3.1 (3)°, and 174.7 (1) and 3.2 (3)° for the two molecules. Molecules are packed in sheets parallel to the (100) plane, with various intermolecular C—H···O and C—H···Cl contacts.

Related literature

For related literature, see: Calo *et al.* (2004); Lin *et al.* (2005); Ogawa *et al.* (1996); Shan *et al.* (1997); Takenaka *et al.* (2004); Xiong & Li (2007).



Experimental

Crystal data

$C_{11}H_9Cl_3O_4$
M_r = 311.53
Monoclinic, $P2_1/c$
a = 12.478 (3) Å
b = 17.100 (4) Å
c = 12.084 (3) Å
β = 99.129 (4)°
V = 2545.8 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 153 (2) K
0.51 × 0.40 × 0.28 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.710, T_{max} = 0.824
21365 measured reflections
6059 independent reflections
5282 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.087
S = 1.04
6059 reflections
329 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C109—H109···O23^{i}	0.93	2.57	3.328 (2)	139
C202—H202···O23^{ii}	0.98	2.38	3.331 (2)	163
C206—H206···Cl32^{iii}	0.93	2.74	3.5949 (17)	154

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2237).

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supplementary materials

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(±)-4,6-Dimethoxy-3-(trichloromethyl)isobenzofuran-1(3*H*)-one

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Comment

Isobenzofuran-1-ones (phtalides) are an important class of natural products and are part of the structure of several alkaloids like bicuculline (Ogawa *et al.*, 1996). Furthermore, phtalides are intermediates towards the synthesis of several alkaloids and isocoumarins and exhibit a wide range of biological activities. Thus, 3-n-butylphtalide a constituent of celery seed oil, exhibits anticonvulsant, asthmatic, and antitumor properties (Xiong & Li, 2007); phenolphthalein a well known pH indicator, and its derivatives like 4-Fluoro-3,3-bis-(4-hydroxy-phenyl)-3*H*-isobenzofuran-1-one are low micromolar inhibitor of the enzyme Thymidylate Synthase, an important target for anticancer chemotherapy (Calo *et al.*, 2004). Diaporthelactone (3-dihydro-4-methoxy-7-methyl-3-oxo-5-isobenzo furan-carboxyaldehyde) and 7-methoxy-4,6-dimethyl-3*H*-isobenzofuran-1-one isolated from the culture of Diaporthe *sp*., show cytotoxic activity against KB and Raji cell lines (Lin *et al.*, 2005). Three isocoumarins and a benzofuran derivative Pyrenulafuran were isolated from the cultured lichen mycobionts of Pyrenula *sp*. (Takenaka *et al.*, 2004). Naphthalenone and phthalide metabolites from Lachnum papyraceum possesses weak antimicrobial and phytotoxic activities and weak cytotoxicity (Shan *et al.*, 1997)·The title compound was prepared as an intermediate towards isocoumarins and dihydroisocoumarins.

Refinement

Hydrogen atoms were located in difference syntheses, refined at idealized positions riding on the C (C–H = 0.95–0.99 Å) atoms with isotropic displacement parameters U_{iso}(H) = 1.2U(C_{eq}) and 1.5(methyl-C). Methyl H atoms were refined on the basis of rigid groups allowed to rotate but not tip.

Figures

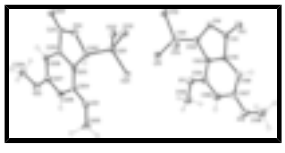


Fig. 1. Molecular structure of the title compound with atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

(±)-4,6-Dimethoxy-3-(trichloromethyl)isobenzofuran-1(3*H*)-one

Crystal data

$C_{11}H_9Cl_3O_4$	F_{000} = 1264
M_r = 311.53	D_x = 1.626 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 962 reflections
a = 12.478 (3) Å	θ = 2.6–28.3º

b = 17.100 (4) Å	μ = 0.72 mm^{-1}
c = 12.084 (3) Å	T = 153 (2) K
β = 99.129 (4)º	Prism, colourless
V = 2545.8 (11) Å^3	0.51 × 0.40 × 0.28 mm
Z = 8	

Data collection

Bruker SMART APEX diffractometer	6059 independent reflections
Radiation source: sealed tube	5282 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 153(2) K	θ_{max} = 27.9º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	h = −16→16
T_{min} = 0.710, T_{max} = 0.824	k = −22→22
21365 measured reflections	l = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.032	H-atom parameters constrained
$wR(F^2)$ = 0.087	$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.9873P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
6059 reflections	$\Delta\rho_{max}$ = 0.56 e Å^{-3}
329 parameters	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}

Cl11	0.06980 (4)	0.38817 (3)	0.63046 (4)	0.03840 (12)
Cl12	0.03253 (3)	0.22443 (3)	0.59138 (4)	0.03250 (10)
Cl13	0.08641 (3)	0.28182 (3)	0.81751 (3)	0.02977 (10)
O11	−0.11211 (11)	0.49245 (7)	0.67516 (11)	0.0356 (3)
O12	−0.19628 (11)	0.49814 (7)	1.04506 (10)	0.0344 (3)
O13	−0.19275 (10)	0.19641 (7)	0.88626 (11)	0.0331 (3)
O14	−0.14403 (9)	0.24163 (7)	0.72704 (10)	0.0259 (2)
C101	0.01528 (13)	0.30328 (9)	0.68230 (13)	0.0244 (3)
C102	−0.10748 (12)	0.31451 (9)	0.68615 (14)	0.0234 (3)
H102	−0.1470	0.3261	0.6112	0.028*
C103	−0.13292 (12)	0.37435 (9)	0.76942 (13)	0.0228 (3)
C104	−0.13137 (13)	0.45617 (10)	0.76967 (14)	0.0268 (3)
C105	−0.10805 (19)	0.57622 (11)	0.67624 (18)	0.0418 (5)
H10A	−0.1759	0.5966	0.6914	0.063*
H10B	−0.0949	0.5948	0.6046	0.063*
H10C	−0.0505	0.5934	0.7335	0.063*
C106	−0.15238 (14)	0.49424 (10)	0.86530 (15)	0.0295 (3)
H106	−0.1486	0.5485	0.8686	0.035*
C107	−0.17912 (13)	0.45283 (10)	0.95691 (14)	0.0267 (3)
C108	−0.21277 (17)	0.45821 (11)	1.14487 (16)	0.0382 (4)
H10D	−0.2807	0.4307	1.1315	0.057*
H10E	−0.2139	0.4955	1.2041	0.057*
H10F	−0.1548	0.4216	1.1660	0.057*
C109	−0.18921 (12)	0.37180 (9)	0.95425 (14)	0.0245 (3)
H109	−0.2112	0.3438	1.0127	0.029*
C110	−0.16447 (12)	0.33563 (9)	0.85902 (13)	0.0225 (3)
C111	−0.16957 (12)	0.25131 (10)	0.83304 (14)	0.0250 (3)
Cl21	0.35097 (3)	0.36154 (2)	0.86744 (4)	0.02780 (10)
Cl22	0.33480 (3)	0.27080 (2)	0.66440 (3)	0.02883 (10)
Cl32	0.38734 (3)	0.19644 (2)	0.88102 (3)	0.02798 (10)
O21	0.54062 (10)	0.46814 (6)	0.85553 (10)	0.0267 (2)
O22	0.65546 (10)	0.51642 (7)	0.50708 (10)	0.0290 (3)
O23	0.61187 (9)	0.20023 (6)	0.57770 (10)	0.0264 (2)
O24	0.56252 (9)	0.22630 (6)	0.74437 (9)	0.0220 (2)
C201	0.40543 (12)	0.28189 (8)	0.80263 (13)	0.0204 (3)
C202	0.52850 (12)	0.29374 (8)	0.80197 (13)	0.0191 (3)
H202	0.5679	0.2962	0.8788	0.023*
C203	0.55838 (11)	0.36196 (8)	0.73458 (12)	0.0193 (3)
C204	0.56441 (12)	0.44246 (9)	0.75619 (13)	0.0214 (3)
C205	0.54455 (15)	0.55076 (9)	0.87515 (15)	0.0315 (4)
H20A	0.6179	0.5688	0.8793	0.047*
H20B	0.5192	0.5619	0.9444	0.047*
H20C	0.4991	0.5769	0.8148	0.047*
C206	0.59708 (13)	0.49068 (9)	0.67534 (14)	0.0239 (3)
H206	0.5995	0.5445	0.6870	0.029*
C207	0.62647 (12)	0.46061 (9)	0.57683 (13)	0.0228 (3)
C208	0.69563 (15)	0.48998 (11)	0.40926 (15)	0.0330 (4)
H20D	0.7616	0.4612	0.4311	0.049*
H20E	0.7096	0.5342	0.3647	0.049*

H20F	0.6426	0.4568	0.3662	0.049*
C209	0.62686 (12)	0.38057 (9)	0.55670 (13)	0.0215 (3)
H209	0.6489	0.3595	0.4930	0.026*
C210	0.59189 (11)	0.33413 (8)	0.63869 (13)	0.0193 (3)
C211	0.59060 (12)	0.24800 (9)	0.64337 (13)	0.0204 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl11	0.0378 (2)	0.0371 (2)	0.0445 (3)	−0.00823 (18)	0.01931 (19)	0.00498 (19)
Cl12	0.0330 (2)	0.0393 (2)	0.0265 (2)	0.00077 (16)	0.00859 (16)	−0.01034 (16)
Cl13	0.02363 (19)	0.0419 (2)	0.0231 (2)	0.00053 (15)	0.00183 (14)	−0.00355 (16)
O11	0.0542 (8)	0.0261 (6)	0.0284 (7)	0.0020 (5)	0.0130 (6)	0.0065 (5)
O12	0.0499 (8)	0.0279 (6)	0.0275 (7)	0.0059 (5)	0.0129 (6)	−0.0031 (5)
O13	0.0386 (7)	0.0263 (6)	0.0372 (7)	−0.0086 (5)	0.0147 (5)	0.0000 (5)
O14	0.0256 (5)	0.0259 (5)	0.0271 (6)	−0.0062 (4)	0.0074 (5)	−0.0041 (4)
C101	0.0250 (7)	0.0285 (8)	0.0209 (8)	−0.0038 (6)	0.0073 (6)	−0.0031 (6)
C102	0.0227 (7)	0.0254 (7)	0.0225 (8)	−0.0024 (6)	0.0044 (6)	−0.0003 (6)
C103	0.0222 (7)	0.0261 (7)	0.0202 (8)	0.0001 (6)	0.0036 (6)	−0.0002 (6)
C104	0.0295 (8)	0.0273 (8)	0.0241 (8)	0.0025 (6)	0.0057 (6)	0.0048 (6)
C105	0.0616 (13)	0.0259 (9)	0.0403 (11)	0.0018 (8)	0.0154 (9)	0.0099 (8)
C106	0.0358 (9)	0.0227 (7)	0.0304 (9)	0.0042 (6)	0.0059 (7)	0.0016 (6)
C107	0.0269 (8)	0.0293 (8)	0.0243 (8)	0.0053 (6)	0.0051 (6)	−0.0022 (6)
C108	0.0518 (11)	0.0368 (10)	0.0288 (10)	0.0047 (8)	0.0151 (8)	−0.0041 (7)
C109	0.0235 (7)	0.0270 (8)	0.0238 (8)	0.0017 (6)	0.0064 (6)	0.0015 (6)
C110	0.0183 (7)	0.0237 (7)	0.0257 (8)	−0.0003 (5)	0.0035 (6)	0.0007 (6)
C111	0.0196 (7)	0.0282 (8)	0.0276 (9)	−0.0032 (6)	0.0050 (6)	−0.0036 (6)
Cl21	0.02578 (19)	0.02353 (18)	0.0364 (2)	−0.00070 (14)	0.01188 (16)	−0.00840 (15)
Cl22	0.02551 (19)	0.0379 (2)	0.0222 (2)	−0.00386 (15)	0.00106 (14)	−0.00351 (15)
Cl32	0.0349 (2)	0.02229 (18)	0.0293 (2)	−0.00411 (14)	0.01264 (16)	0.00259 (14)
O21	0.0390 (6)	0.0184 (5)	0.0254 (6)	−0.0044 (4)	0.0134 (5)	−0.0061 (4)
O22	0.0376 (6)	0.0239 (6)	0.0287 (6)	−0.0019 (5)	0.0149 (5)	0.0043 (5)
O23	0.0310 (6)	0.0227 (5)	0.0273 (6)	0.0014 (4)	0.0101 (5)	−0.0050 (4)
O24	0.0279 (5)	0.0176 (5)	0.0221 (6)	0.0025 (4)	0.0091 (4)	−0.0006 (4)
C201	0.0241 (7)	0.0182 (6)	0.0197 (7)	−0.0011 (5)	0.0060 (6)	−0.0009 (5)
C202	0.0209 (7)	0.0179 (6)	0.0192 (7)	0.0008 (5)	0.0054 (5)	−0.0027 (5)
C203	0.0194 (7)	0.0202 (7)	0.0187 (7)	−0.0012 (5)	0.0045 (5)	−0.0006 (5)
C204	0.0224 (7)	0.0212 (7)	0.0214 (8)	−0.0008 (5)	0.0064 (6)	−0.0038 (6)
C205	0.0451 (10)	0.0192 (7)	0.0326 (9)	−0.0033 (7)	0.0131 (7)	−0.0088 (6)
C206	0.0282 (8)	0.0179 (7)	0.0271 (8)	−0.0028 (6)	0.0085 (6)	−0.0018 (6)
C207	0.0223 (7)	0.0237 (7)	0.0231 (8)	−0.0025 (6)	0.0061 (6)	0.0030 (6)
C208	0.0392 (9)	0.0335 (9)	0.0302 (9)	−0.0006 (7)	0.0177 (7)	0.0063 (7)
C209	0.0214 (7)	0.0240 (7)	0.0199 (8)	−0.0009 (6)	0.0056 (6)	−0.0023 (6)
C210	0.0175 (6)	0.0194 (7)	0.0211 (7)	−0.0011 (5)	0.0034 (5)	−0.0025 (5)
C211	0.0186 (7)	0.0219 (7)	0.0212 (8)	0.0007 (5)	0.0049 (5)	−0.0003 (6)

Geometric parameters (Å, °)

Cl11—C101	1.7599 (17)	Cl21—C201	1.7603 (15)

Cl12—C101	1.7738 (16)	Cl22—C201	1.7709 (16)
Cl13—C101	1.7697 (17)	Cl32—C201	1.7753 (15)
O11—C104	1.354 (2)	O21—C204	1.3546 (19)
O11—C105	1.433 (2)	O21—C205	1.4321 (18)
O12—C107	1.361 (2)	O22—C207	1.3597 (18)
O12—C108	1.429 (2)	O22—C208	1.429 (2)
O13—C111	1.199 (2)	O23—C211	1.1976 (19)
O14—C111	1.378 (2)	O24—C211	1.3733 (19)
O14—C102	1.4411 (19)	O24—C202	1.4451 (17)
C101—C102	1.552 (2)	C201—C202	1.550 (2)
C102—C103	1.504 (2)	C202—C203	1.503 (2)
C102—H102	0.9800	C202—H202	0.9800
C103—C110	1.379 (2)	C203—C210	1.377 (2)
C103—C104	1.399 (2)	C203—C204	1.401 (2)
C104—C106	1.387 (2)	C204—C206	1.388 (2)
C105—H10A	0.9600	C205—H20A	0.9600
C105—H10B	0.9600	C205—H20B	0.9600
C105—H10C	0.9600	C205—H20C	0.9600
C106—C107	1.398 (2)	C206—C207	1.398 (2)
C106—H106	0.9300	C206—H206	0.9300
C107—C109	1.391 (2)	C207—C209	1.390 (2)
C108—H10D	0.9600	C208—H20D	0.9600
C108—H10E	0.9600	C208—H20E	0.9600
C108—H10F	0.9600	C208—H20F	0.9600
C109—C110	1.384 (2)	C209—C210	1.393 (2)
C109—H109	0.9300	C209—H209	0.9300
C110—C111	1.475 (2)	C210—C211	1.474 (2)
C104—O11—C105	117.45 (14)	C204—O21—C205	117.38 (13)
C107—O12—C108	116.74 (14)	C207—O22—C208	116.97 (13)
C111—O14—C102	110.31 (12)	C211—O24—C202	110.38 (11)
C102—C101—Cl11	110.35 (11)	C202—C201—Cl21	110.72 (10)
C102—C101—Cl13	110.53 (11)	C202—C201—Cl22	110.75 (11)
Cl11—C101—Cl13	109.51 (9)	Cl21—C201—Cl22	109.46 (8)
C102—C101—Cl12	109.27 (11)	C202—C201—Cl32	108.68 (10)
Cl11—C101—Cl12	108.35 (9)	Cl21—C201—Cl32	107.98 (8)
Cl13—C101—Cl12	108.78 (9)	Cl22—C201—Cl32	109.19 (8)
O14—C102—C103	104.32 (12)	O24—C202—C203	103.97 (11)
O14—C102—C101	105.71 (12)	O24—C202—C201	105.38 (11)
C103—C102—C101	114.73 (13)	C203—C202—C201	115.80 (12)
O14—C102—H102	110.6	O24—C202—H202	110.4
C103—C102—H102	110.6	C203—C202—H202	110.4
C101—C102—H102	110.6	C201—C202—H202	110.4
C110—C103—C104	118.95 (15)	C210—C203—C204	118.80 (14)
C110—C103—C102	108.39 (14)	C210—C203—C202	108.79 (12)
C104—C103—C102	132.65 (15)	C204—C203—C202	132.24 (14)
O11—C104—C106	124.74 (15)	O21—C204—C206	124.14 (14)
O11—C104—C103	117.42 (15)	O21—C204—C203	118.09 (13)
C106—C104—C103	117.82 (15)	C206—C204—C203	117.74 (14)
O11—C105—H10A	109.5	O21—C205—H20A	109.5

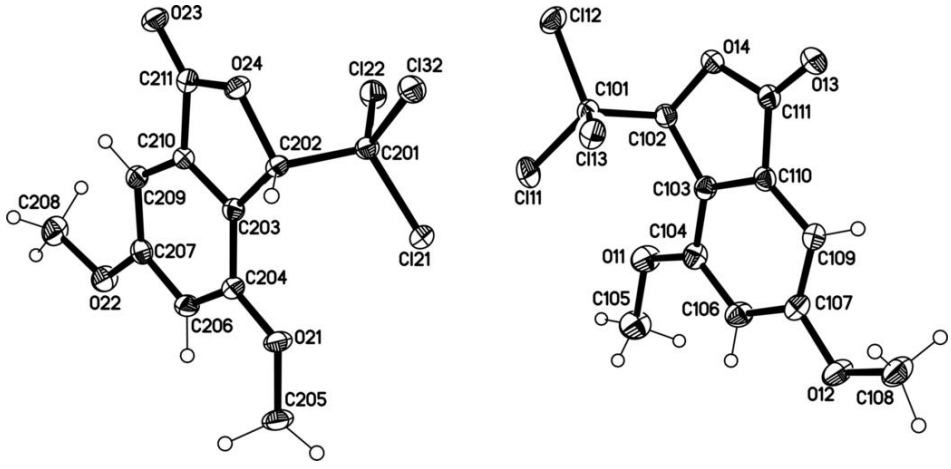
O11—C105—H10B	109.5	O21—C205—H20B	109.5
H10A—C105—H10B	109.5	H20A—C205—H20B	109.5
O11—C105—H10C	109.5	O21—C205—H20C	109.5
H10A—C105—H10C	109.5	H20A—C205—H20C	109.5
H10B—C105—H10C	109.5	H20B—C205—H20C	109.5
C104—C106—C107	121.48 (16)	C204—C206—C207	121.79 (14)
C104—C106—H106	119.3	C204—C206—H206	119.1
C107—C106—H106	119.3	C207—C206—H206	119.1
O12—C107—C109	124.06 (15)	O22—C207—C209	125.02 (14)
O12—C107—C106	114.72 (15)	O22—C207—C206	113.65 (13)
C109—C107—C106	121.21 (15)	C209—C207—C206	121.32 (14)
O12—C108—H10D	109.5	O22—C208—H20D	109.5
O12—C108—H10E	109.5	O22—C208—H20E	109.5
H10D—C108—H10E	109.5	H20D—C208—H20E	109.5
O12—C108—H10F	109.5	O22—C208—H20F	109.5
H10D—C108—H10F	109.5	H20D—C208—H20F	109.5
H10E—C108—H10F	109.5	H20E—C208—H20F	109.5
C110—C109—C107	115.66 (15)	C207—C209—C210	115.25 (14)
C110—C109—H109	122.2	C207—C209—H209	122.4
C107—C109—H109	122.2	C210—C209—H209	122.4
C103—C110—C109	124.58 (15)	C203—C210—C209	124.93 (14)
C103—C110—C111	108.08 (14)	C203—C210—C211	107.84 (13)
C109—C110—C111	127.32 (15)	C209—C210—C211	127.12 (13)
O13—C111—O14	121.03 (15)	O23—C211—O24	121.28 (14)
O13—C111—C110	131.09 (16)	O23—C211—C210	130.63 (14)
O14—C111—C110	107.87 (13)	O24—C211—C210	108.06 (12)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C109—H109···O23^{i}	0.93	2.57	3.328 (2)	139
C202—H202···O23^{ii}	0.98	2.38	3.331 (2)	163
C206—H206···Cl32^{iii}	0.93	2.74	3.5949 (17)	154

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

Fig. 1


O23
C211
O24
Cl22
Cl32
C210
C202
C201
C209
C208
C203
C207
Cl21
C204
O22
C206
O21
C205
Cl12
O14
O13
C101
C111
C102
Cl13
Cl11
C103
C110
C104
O11
C109
C105
C106
C107
O12
C108