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Crystal structure of methyl chloroformate

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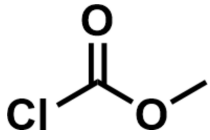
The crystal structure of methyl chloroformate, $C_2H_3ClO_2$, was determined by single-crystal X-ray diffraction data at 200 and 100 K. A suitable single crystal was grown in a capillary directly on the goniometer *via* Ostwald ripening around its melting point at 210 K. The $ClC(O)OCH_3$ molecule has a staggered conformation and is planar (without H atoms) with point group C_S. In the crystal, methyl chloroformate features weak Cl···O interactions forming chains along [100], which again extend into a network *via* intermolecular C···O dipole interactions, consistent with Hirshfeld surface analysis. Complementary quantum chemical calculations at the DFT-def2-TZVP/PBE0-D3 level of theory were performed to compare with the experimental Raman data in both the liquid and solid state.

1. Chemical context

Methyl chloroformate, $ClC(O)OCH_3$, is a liquid at room temperature with a melting point of 212 K (GESTIS, 2025). It is widely used in organic chemistry to introduce a methoxycarbonyl functionality to a suitable nucleophile (Chiarucci *et al.*, 2012). Methyl chloroformate is well characterized, including its conformational properties by vibrational spectroscopy, microwave spectra (Groner *et al.*, 1990), and gas phase electron diffraction (O'Gorman *et al.*, 1950). Herein, we report on its hitherto unknown crystal structure on the basis of diffraction data recorded at 200 and 100 K. Additional quantum chemical calculations were performed and are consistent with the experimental findings and allow for the assignment of the vibrational modes.



2. Structural commentary

Methyl chloroformate crystallizes in the orthorhombic crystal system with the centrosymmetric space group *Pnma*. It has been shown that crystals of small molecular compounds can exhibit extensive polymorphism in the solid state, thus undergoing phase transitions at temperatures somewhere below their melting temperatures (Cruz-Cabeza *et al.*, 2015). However, lowering the temperature starting from 200 K did not lead to a phase transition. The unit cell contains four formula units (Z = 4) and one independent molecule in the asymmetric unit (Fig. 1). In the crystal structure, individual molecules are arranged in an *AB* stacking pattern (Fig. 2).

In the solid state, $ClC(O)OCH_3$ adopts C_S symmetry with the molecule lying on a mirror plane and thus displaying a

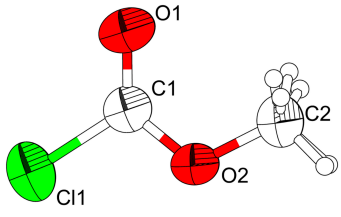


Table 1
Comparison of selected interatomic distances (Å, °) of methyl chloroformate (X-ray, this work), methyl chloroformate (electron diffraction; O'Gorman *et al.*, 1950), phosgene (Zaslow *et al.*, 1952) and dimethyl carbonate (Whitfield, 2023).

	X-ray 200 K	X-ray 100 K	Electron diffraction	Phosgene	Dimethyl carbonate 82 K
C═O	1.186 (2)	1.195 (2)	1.19 (3)	1.15 (2)	1.219 (2)
C—Cl	1.7504 (13)	1.7502 (13)	1.75 (2)	1.74 (2)*	–
(CO)—O	1.306 (2)	1.309 (2)	1.36 (4)	–	1.337 (2)*
O—CH_3	1.456 (2)	1.462 (2)	1.47 (4)	–	1.456 (2)*
Cl—C═O	122.46 (10)	122.47 (10)	–	124(1.5)*	–
Cl—C—O	108.61 (9)	108.75 (9)	112 (3)	–	–
O═C—O	128.93 (11)	128.78 (11)	126 (4)	–	125.58 (11)*

*Mean values.

torsion angle Cl1—C1—O2—C2 of exactly 180°. Due to the symmetry restrictions of point group C_S, the methyl group is in a staggered orientation with respect to the carbonyl group. Also, the O—CH_3 moiety is orientated *syn* relative to the C═O bond, with bond lengths similar to those determined by electron diffraction and comparable to those of phosgene (Zaslow *et al.*, 1952) and dimethyl carbonate (Whitfield, 2023). A comparison of the structural parameters is given in Table 1.

3. Supramolecular features

The crystal packing of methyl chloroformate is dominated by short intermolecular Cl···O contacts with a distance of $d_{Cl\cdots O}$ = 3.0442 (9) Å, forming infinite chains along [100] (Fig. 2). Within these chains, the molecules are aligned in a zigzag fashion. However, individual chains are not interconnected into layers, but instead form a framework through weak intermolecular dipole interactions between the carbonyl oxygen atom and the central carbon atom of two parallel molecules along [010].

A Hirshfeld surface analysis was performed using *CrystalExplorer* (Spackman *et al.*, 2021) to quantify and visualize the intermolecular interactions in the crystal structure of the title compound. The Hirshfeld surface was mapped with the d_{norm} function (Fig. 3), highlighting attractive interactions shorter

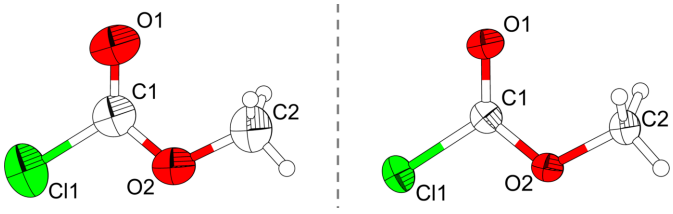


Figure 1
Molecular structure of a methyl chloroformate molecule in the solid state measured at 200 K (left) and 100 K (right). Atoms are drawn with displacement ellipsoids at the 70% probability level.

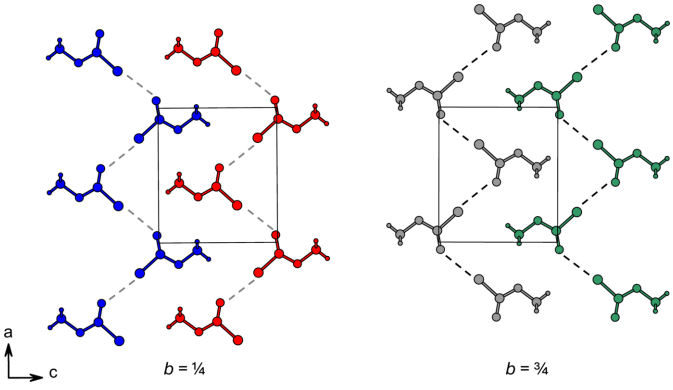


Figure 2
AB stacking in the crystal structure of methyl chloroformate viewed along [010]. Repeating layers: *A* (left) and *B* (right).

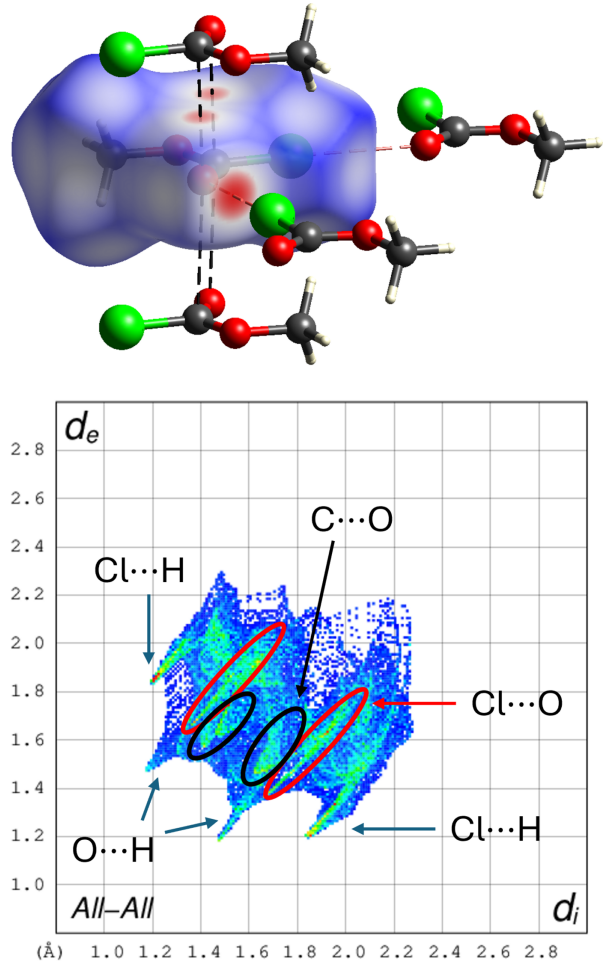


Figure 3
Hirshfeld surface (top) and fingerprint plot (bottom) mapped for methyl chloroformate on basis of 100 K data. Red areas indicate short contacts shorter than the sum of the van der Waals radii. Color code: C gray, O red, Cl green, H white.

Table 2
Vibrational band positions (cm^{-1}) and band assignments of the Raman spectra of liquid and solid methyl chloroformate based on the DFT calculation. Symmetry modes are given in parentheses..

$\nu_{calc.}$	$\nu_{obs.}$(liquid)	$\nu_{obs.}$(solid)	**Assignment**	$\nu_{calc.}$	$\nu_{obs.}$(liquid)	$\nu_{obs.}$(solid)	**Assignment**
182 (B_{2g})	–	195	out-of-plane δ(C—O—C)	1248 (A_g)	1206	1206	ν(C—O)+δ(CH_3)
191 (B_{1g})				1253 (B_{3g})			
272 (B_{3g})	281	283	in-plane δ(C—O—C)	1470 (B_{3g})	1457	1435	δ_s(CH_3)
272 (A_g)				1474 (A_g)			
409 (B_{3g})	407	411	in-plane δ(C—O—C—Cl)	1485 (A_g)		1452	δ_s(CH_3)
410 (A_g)				1486 (B_{3g})			
488 (A_g)	485	481	ν(C—Cl)	1491 (B_{1g})		1459	δ_{as}(CH_3)
490 (B_{3g})		486		1494 (B_{2g})			
719 (B_{1g})	–	–	out-of-plane ν_{as}(O—C—O) wagging	1875 (A_g)	1788	1756	ν(C═O)
723 (B_{2g})	–	–		1884 (B_{3g})		1778	
845 (A_g)	823	824	δ(C—O—C—Cl) scissoring	3087 (A_g)	2967	2964	ν_s(CH_3)
852 (B_{3g})				3088 (B_{3g})			
996 (A_g)	950	950	ν(O—CH_3)	3180 (B_{2g})	3026	3029	ν_{as}(CH_3)
1004 (B_{3g})		975		3180 (B_{1g})			
1174 (B_{1g})	1155	1148	δ(CH_3) rocking	3222 (A_g)	3053	3056	ν_{as}(CH_3)
1175 (B_{2g})				3222 (B_{3g})			
1198 (A_g)		1155	δ(CH_3) rocking				
1212 (B_{3g})		1168					

Notes: ν = stretching vibration, δ = bending vibration, *s* = symmetric, *as* = asymmetric, – = not observed.

than the sum of the van der Waals radii in red and equal or longer contacts in white and blue, respectively. Akin to the observations above, relevant contributions arise from Cl···O and C···O short contacts accounting for only 12.6% and 7.6% to the overall Hirshfeld plot. Other major contributions include Cl—H (35.0%) and O—H (27.4%) intermolecular contacts. However, those are equal to or longer than the sum of their van der Waals radii.

4. Vibrational spectroscopy

Experimental Raman spectra of liquid and solid methyl chloroformate were recorded at room temperature and at 153 K, confirming the molecular structure as determined by X-ray analysis. The experimental spectra are confirmed by quantum chemical calculations at the DFT-def2-TZVP/PBE0-D3 level of theory (Weigend & Ahlrichs, 2005; Karttunen *et al.*, 2015; Dovesi *et al.*, 2018; Zicovich *et al.*, 2004; Pascale *et al.*, 2004; Maschio *et al.*, 2013; Grimme *et al.*, 2010) on the basis of the crystal structure of methyl chloroformate. The recorded and calculated spectra are in good agreement, as shown in Fig. 4. The vibrational frequencies have been calculated within the harmonic approximation and therefore are overestimated, especially at higher wavenumbers. Nevertheless, the vibrational band at 2845 cm^{-1} is not reproduced in the calculated spectrum. A comparison of calculated and observed vibrational bands is given in Table 2.

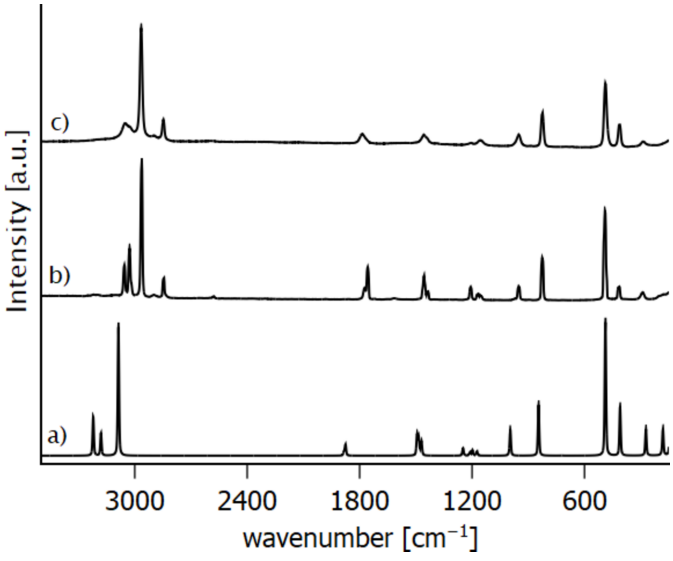


Figure 4
Calculated (*a*) and recorded Raman spectra of methyl chloroformate (*b*) at room temperature (liquid) and (*c*) at 153 K (crystalline). Calculated Raman spectra of solid $ClC(O)OCH_3$ at the DFT-TZVP/PBE0 level of theory.

5. Synthesis and crystallization

Methyl chloroformate (Fisher Scientific GmbH, 99%) was used as received. Its purity was checked with vibrational IR and Raman spectroscopy. A borosilicate glass capillary (0.3 mm, Hilgenberg) was filled with a small amount of methyl chloroformate and flame-sealed at ambient pressure. The capillary was mounted onto the goniometer of the diffractometer and shock-cooled at 100 K using an open-flow cryostat to obtain a polycrystalline sample. The sample was incrementally heated at a rate of 180 K min^{-1} until partial melting was observed at around 213 K. Subsequently, a suitable single crystal was grown through Ostwald ripening between 200 and 213 K in three cycles. Full datasets were collected at 200 and 100 K and reflections of the strongest scattering individuum integrated.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The positions of the hydrogen

Table 3
Experimental details.

	100 K	200 K
Crystal data		
Chemical formula	$C_2H_3ClO_2$	$C_2H_3ClO_2$
M_r	94.49	94.49
Crystal system, space group	Orthorhombic, *Pnma*	Orthorhombic, *Pnma*
a, *b*, *c* (Å)	8.4404 (5), 6.2019 (4), 7.4314 (4)	8.526 (2), 6.3454 (15), 7.4619 (16)
V (Å^3)	389.01 (4)	403.67 (16)
Z	4	4
Radiation type	Cu *Kα*	Cu *Kα*
μ (mm^{-1})	7.23	6.97
Crystal size (mm)	0.30 × 0.05 (radius)	0.30 × 0.15 (radius)
Data collection		
Diffractometer	Stoe Stadivari	Stoe Stadivari
Absorption correction	Multi-scan (*LANA*; Koziskova *et al.*, 2016)	Multi-scan (*LANA*; Koziskova *et al.*, 2016)
T_{min}, T_{max}	0.161, 0.337	0.231, 0.512
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8421, 432, 415	10088, 453, 432
R_{int}	0.018	0.022
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.627	0.625
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.018, 0.049, 1.08	0.022, 0.064, 1.11
No. of reflections	432	453
No. of parameters	38	39
H-atom treatment	All H-atom parameters refined	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.17	0.18, −0.16

Computer programs: *X-AREA* (Stoe, 2022), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

atoms were obtained through difference-Fourier synthesis in both datasets.

Funding information

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Crystal structure of methyl chloroformate

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Computing details

Methyl chloroformate (srx03)

Crystal data

$C_2H_3ClO_2$
M_r = 94.49
Orthorhombic, *Pnma*
a = 8.4404 (5) Å
b = 6.2019 (4) Å
c = 7.4314 (4) Å
V = 389.01 (4) Å^3
Z = 4
F(000) = 192
D_x = 1.613 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54186 Å
Cell parameters from 30155 reflections
θ = 5.3–75.7°
μ = 7.23 mm^{-1}
T = 100 K
Block, clear colourless
0.30 × 0.15 × 0.15 × 0.05 (radius) mm

Data collection

Stoe Stadivari diffractometer
Radiation source: microfocus sealed X-ray tube, XENOCS GENIX 3D CU HIGH FLUX
Graded multilayer mirror monochromator
Detector resolution: 5.81 pixels mm^{-1}
ω and *φ* scans
Absorption correction: multi-scan (*LANA*; Koziskova *et al.*, 2016)
T_{min} = 0.161, T_{max} = 0.337
8421 measured reflections
432 independent reflections
415 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 75.4°, θ_{min} = 8.0°
h = −8→10
k = −7→7
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.049
S = 1.08
432 reflections
38 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 0.0604P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 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}
Cl1	0.72372 (4)	0.750000	0.33814 (4)	0.02357 (16)
O2	0.65970 (11)	0.750000	0.66663 (10)	0.0201 (2)
O1	0.44492 (10)	0.750000	0.48536 (12)	0.0235 (2)
C1	0.58441 (15)	0.750000	0.51257 (16)	0.0179 (3)
C2	0.55644 (18)	0.750000	0.82457 (17)	0.0238 (3)
H2A	0.4907 (18)	0.622 (2)	0.8235 (14)	0.033 (3)*
H2B	0.622 (2)	0.750000	0.919 (3)	0.037 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0234 (2)	0.0267 (2)	0.0206 (2)	0.000	0.00467 (10)	0.000
O2	0.0148 (5)	0.0269 (5)	0.0186 (5)	0.000	0.0001 (4)	0.000
O1	0.0174 (5)	0.0283 (5)	0.0246 (5)	0.000	−0.0034 (4)	0.000
C1	0.0190 (6)	0.0154 (6)	0.0193 (6)	0.000	0.0008 (5)	0.000
C2	0.0213 (7)	0.0327 (8)	0.0174 (6)	0.000	0.0014 (5)	0.000

Geometric parameters (Å, º)

Cl1—C1	1.7502 (13)	C2—H2A	0.968 (14)
O2—C1	1.3094 (15)	C2—H2A^{i}	0.968 (14)
O2—C2	1.4619 (15)	C2—H2B	0.90 (2)
O1—C1	1.1945 (15)		
C1—O2—C2	114.37 (10)	O2—C2—H2A	109.6 (7)
O2—C1—Cl1	108.75 (9)	O2—C2—H2B	105.1 (12)
O1—C1—Cl1	122.47 (10)	H2A—C2—H2A^{i}	110.1 (17)
O1—C1—O2	128.78 (11)	H2A—C2—H2B	111.2 (9)
O2—C2—H2A^{i}	109.6 (7)	H2B—C2—H2A^{i}	111.2 (9)
C2—O2—C1—Cl1	180.000 (1)	C2—O2—C1—O1	0.000 (1)

Symmetry code: (i) *x*, −*y*+3/2, *z*.

Methyl chloroformate (srx02)

Crystal data

$C_2H_3ClO_2$
M_r = 94.49
Orthorhombic, *Pnma*
a = 8.526 (2) Å
b = 6.3454 (15) Å
c = 7.4619 (16) Å
V = 403.67 (16) Å³
Z = 4
F(000) = 192

D_x = 1.555 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54186 Å
Cell parameters from 21811 reflections
θ = 5.9–75.5°
μ = 6.97 mm^{-1}
T = 200 K
Block, clear colourless
0.30 × 0.15 × 0.15 × 0.15 (radius) mm

Data collection

Stoe Stadivari diffractometer
Radiation source: microfocus sealed X-ray tube, XENOCS GENIX 3D CU HIGH FLUX
Graded multilayer mirror monochromator
Detector resolution: 5.81 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*LANA*; Koziskova *et al.*, 2016)
T_{min} = 0.231, T_{max} = 0.512
10088 measured reflections
453 independent reflections
432 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 74.6°, θ_{min} = 7.9°
h = −8→10
k = −7→7
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.064
S = 1.11
453 reflections
39 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.0148P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: SHELXL-2018/3 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0081 (16)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.27937 (4)	0.750000	0.33697 (4)	0.0485 (2)
O2	0.34065 (11)	0.750000	0.66399 (10)	0.0382 (3)
O1	0.55347 (11)	0.750000	0.48601 (12)	0.0472 (3)
C1	0.41624 (15)	0.750000	0.51182 (15)	0.0333 (3)
C2	0.44070 (19)	0.750000	0.82207 (18)	0.0465 (4)
H2A	0.377 (3)	0.750000	0.917 (3)	0.068 (6)*
H2B	0.505 (2)	0.627 (2)	0.8228 (15)	0.064 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0511 (3)	0.0547 (3)	0.0396 (3)	0.000	−0.01092 (11)	0.000
O2	0.0267 (5)	0.0527 (6)	0.0352 (5)	0.000	0.0021 (3)	0.000
O1	0.0336 (5)	0.0621 (7)	0.0458 (6)	0.000	0.0086 (4)	0.000
C1	0.0334 (6)	0.0313 (6)	0.0353 (7)	0.000	0.0015 (5)	0.000
C2	0.0412 (8)	0.0649 (9)	0.0333 (7)	0.000	−0.0021 (5)	0.000

Geometric parameters (Å, º)

Cl1—C1	1.7504 (13)	C2—H2A	0.89 (2)
O2—C1	1.3057 (15)	C2—H2B^{i}	0.953 (17)
O2—C2	1.4557 (16)	C2—H2B	0.953 (17)
O1—C1	1.1856 (16)		
C1—O2—C2	114.55 (11)	O2—C2—H2B	109.9 (8)
O2—C1—Cl1	108.61 (9)	O2—C2—H2B^{i}	109.9 (8)
O1—C1—Cl1	122.46 (10)	H2A—C2—H2B	110.0 (10)
O1—C1—O2	128.93 (11)	H2A—C2—H2B^{i}	110.0 (10)
O2—C2—H2A	106.8 (14)	H2B—C2—H2B^{i}	110 (2)
C2—O2—C1—Cl1	180.000 (1)	C2—O2—C1—O1	0.000 (1)

Symmetry code: (i) x, $-y+3/2$, z.