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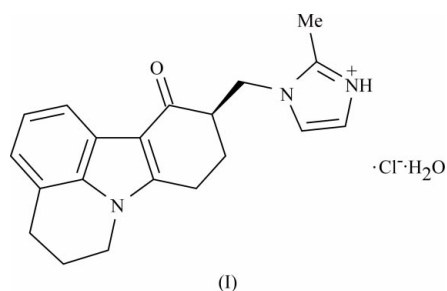
## Key indicators

Single-crystal X-ray study  
*T* = 123 K  
Mean  $\sigma(\text{C}-\text{C})$  = 0.005 Å  
Disorder in main residue  
*R* factor = 0.058  
*wR* factor = 0.105  
Data-to-parameter ratio = 13.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Cilansetron hydrochloride monohydrate,  
modification B (orthorhombic)

The absolute configuration of the orthorhombic form of the title compound, (–)-5,6,9,10-tetrahydro-10-[(2-methyl-1*H*-imidazol-1-yl)methyl]-4*H*-pyrido[3,2,1-*jk*]carbazol-11(8*H*)-one monohydrochloride monohydrate,  $\text{C}_{20}\text{H}_{22}\text{N}_3\text{O}^+\cdot\text{Cl}^-\cdot\text{H}_2\text{O}$ , was established as *R* at the asymmetric carbon adjacent to the carbonyl function. This form [*cf.* the monoclinic form; Jones *et al.* (2003). *Acta Cryst. E* **59**, o38–o40] also involves two independent formula units with different ring conformations of the six-membered N-heterocycle, and somewhat different orientations of the imidazole ring. Classical hydrogen bonding leads to a helical chain of alternating water and chloride residues, with cations hydrogen bonded laterally to the water molecules.

## Comment

In the previous paper (Jones *et al.*, 2003), we described the structure of the monoclinic form (modification A) of cilansetron hydrochloride monohydrate, (I); introductory material is presented there. We describe here the structure of the orthorhombic form (modification B).



In common with the monoclinic form, the title compound crystallizes with two independent formula units in the asymmetric unit (Fig. 1); the cations again differ in the ring conformation involving the methylene groups C4, C5 and C6, and in the orientation of the imidazole ring. A brief selection of relevant torsion angles is shown in Table 1. A least-squares fit of the cations is shown in Fig. 2. Molecular dimensions may be regarded as normal.

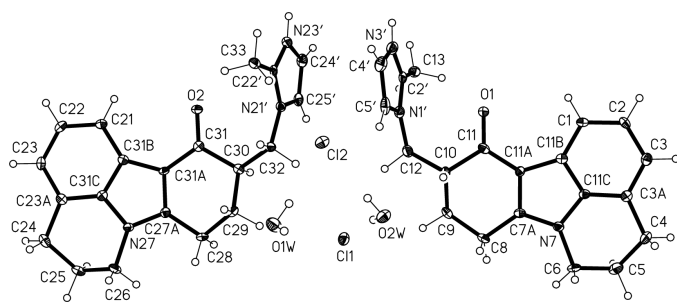
The *R* absolute configuration at the asymmetric centre C10 (C30 in the second molecule) was confirmed by the Flack (1983) parameter (see *Experimental*).

The crystal packing differs significantly from that in the monoclinic form. An analysis of the classical hydrogen bonds (Table 2) again reveals the presence of helical chains [ $\cdots\text{Cl}\cdots\text{H}-\text{O}-\text{H}\cdots$ ], but now with overall direction parallel to the *a* axis and involving both formula units in the same chain; the cations are again attached laterally to these helices, but now by contacts  $\text{N}-\text{H}\cdots\text{O}_{\text{water}}$  rather than  $\text{N}-\text{H}\cdots\text{Cl}$

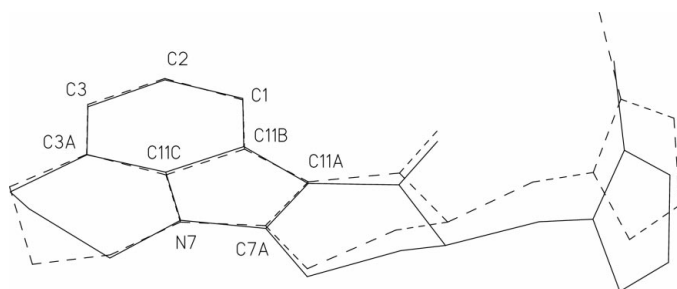
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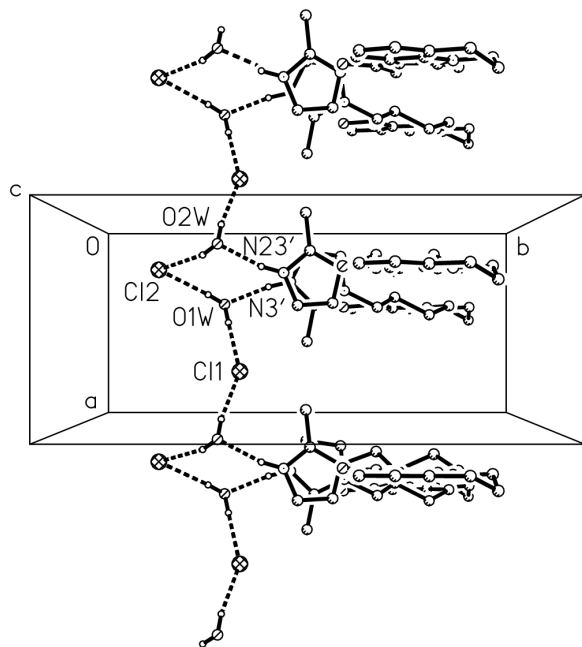
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**Figure 1**  
The asymmetric unit of the title compound in the crystal. Ellipsoids are drawn at the 30% probability level.



**Figure 2**  
Least-squares fit of both independent cations, calculated using the labelled atoms.



**Figure 3**  
The helical hydrogen-bonding chain of the title compound. Hydrogen bonds are indicated by dashed lines. H atoms not involved in hydrogen bonding have been omitted.

(Fig. 3). The chains form hydrophilic regions at  $z \approx 0.25, 0.75, \text{etc.}$

A considerable number of non-classical (weak) hydrogen bonds of the form  $C-H \cdots Cl$  and  $C-H \cdots O$  are observed (Table 2), but only one of these ( $C25'-H25' \cdots Cl2$ ) is especially short, at 2.55 Å; it joins neighbouring chains.

## Experimental

A single crystal was selected by IR microscopy from a mixture of modifications A and B crystallized from 0.1 M HCl.

### Crystal data

$C_{20}H_{22}N_3O^+ \cdot Cl^- \cdot H_2O$   
 $M_r = 373.87$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 7.396$  (2) Å  
 $b = 16.460$  (3) Å  
 $c = 30.263$  (6) Å  
 $V = 3684.2$  (14) Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 1.348$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
 Cell parameters from 5470 reflections  
 $\theta = 2-25^\circ$   
 $\mu = 0.23$  mm<sup>-1</sup>  
 $T = 123$  (2) K  
 Lath, colourless  
 $0.70 \times 0.23 \times 0.04$  mm

### Data collection

Stoe-Huber-Siemens area-detector diffractometer  
 $\varphi$  scans  
 61 630 measured reflections  
 6553 independent reflections  
 5335 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.112$   
 $\theta_{\text{max}} = 25.1^\circ$   
 $h = -8 \rightarrow 8$   
 $k = -19 \rightarrow 19$   
 $l = -36 \rightarrow 36$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.058$   
 $wR(F^2) = 0.105$   
 $S = 1.15$   
 6553 reflections  
 500 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.018P)^2 + 3.9789P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.36$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.27$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), 2820 Friedel pairs  
 Flack parameter =  $-0.03$  (9)

**Table 1**

Selected torsion angles ( $^\circ$ ).

C3A—C4—C5—C6	−50.0 (5)	C23A—C24—C25—C26	47.0 (6)
C4—C5—C6—N7	48.8 (5)	C24—C25—C26—N27	−47.5 (6)
C11A—C7A—C8—C9	15.6 (5)	C31A—C27A—C28—C29	21.4 (5)

**Table 2**

Hydrogen-bonding geometry (Å,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N3'-H3' \cdots O1W^i$	0.88 (4)	1.85 (4)	2.724 (5)	170 (5)
$N23'-H23' \cdots O2W^i$	0.88 (4)	1.87 (4)	2.741 (5)	167 (4)
$O1W-HO1 \cdots Cl2$	0.84 (3)	2.28 (3)	3.117 (3)	173 (5)
$O1W-HO2 \cdots Cl1^{ii}$	0.84 (3)	2.27 (3)	3.113 (4)	178 (5)
$O2W-HO3 \cdots Cl1$	0.85 (3)	2.24 (3)	3.076 (3)	170 (4)
$O2W-HO4 \cdots Cl2$	0.84 (3)	2.26 (3)	3.086 (3)	165 (5)
$C9-H9A \cdots Cl1$	0.99	2.88	3.797 (4)	154
$Cl2-H12B \cdots Cl1$	0.99	2.85	3.775 (4)	156
$Cl3-H13B \cdots Cl1^{iii}$	0.98	2.91	3.685 (4)	137
$C29-H29A \cdots Cl1$	0.99	2.81	3.761 (4)	161
$C32-H32B \cdots Cl1$	0.99	2.96	3.887 (4)	156
$C24'-H24' \cdots Cl1^{iii}$	0.95	2.70	3.632 (4)	167
$Cl2-H12A \cdots Cl2^{iv}$	0.99	2.88	3.528 (4)	124
$Cl3-H13C \cdots Cl2^{iv}$	0.98	2.85	3.782 (4)	159
$C5'-H5' \cdots Cl2$	0.95	2.73	3.507 (4)	139
$C33-H33C \cdots Cl2$	0.98	2.73	3.665 (4)	160
$C25'-H25' \cdots Cl2^{iv}$	0.95	2.55	3.438 (4)	155
$C5-H5A \cdots O1^v$	0.99	2.62	3.479 (5)	145
$C2-H2 \cdots O2^{vi}$	0.95	2.61	3.482 (5)	152
$C25-H25B \cdots O2^{vii}$	0.99	2.54	3.398 (6)	145
$C3-H3 \cdots O2W^v$	0.95	2.53	3.479 (5)	173
$C23-H23 \cdots O1W^{vii}$	0.95	2.67	3.586 (5)	164

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

H atoms bonded to oxygen or nitrogen were refined freely but with chemically equivalent bond lengths restrained to be equal. Methyl H atoms were identified in difference syntheses, idealized and refined as rigid groups allowed to rotate but not tip. Other H atoms were included using a riding model. Fixed C–H bond lengths: methyl = 0.98, methylene = 0.99, methine = 1.00 and  $sp^2C-H = 0.95$  Å. In the second cation, the atom C25 is disordered over two positions. The major component has an occupation factor of 0.767 (12). The minor position was refined isotropically. Appropriate similarity restraints were employed.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

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