

8-Methyl-5-oxo-5,6-dihydrodipyrido[1,2-a:3',2'-e]-
pyrimidin-11-ium chloride trihydrate 120 KR. Alan Howie,^{a*} Marcelle de
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Key indicators

Single-crystal X-ray study
T = 120 K
Mean $\sigma(\text{C}-\text{C})$ = 0.003 Å
Disorder in solvent or counterion
R factor = 0.032
wR factor = 0.090
Data-to-parameter ratio = 15.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the structure of the title salt, $\text{C}_{12}\text{H}_{10}\text{N}_3\text{O}^+\cdot\text{Cl}^-\cdot 3\text{H}_2\text{O}$, the only species which do not coincide with the mirror plane in the space group $P6_3/m$ are one complete water molecule, one H atom of another water molecule and two H atoms of the methyl group of the cation. Consequently, apart from the two H atoms of the methyl group, the cation is completely planar. The hydrogen bonding between the water molecules and, through Cl^- anions, to the cations, although extensive, can be modelled satisfactorily only by treating one H atom in each of the two types of water molecules as disordered.

Comment

The title compound, (I), is an example of a more elaborate, potentially biologically active, pyridine-containing compound of the type provided by 2-chloronicotinoyl chloride, (II), as precursor, undergoing cyclization with a dinucleophilic reagent, in this case 2-amino-4-methylpyridine, (III). The asymmetric unit in the structure of (I) is shown in Fig. 1. Bond lengths and bond angles within the cation of (I) are summarized in Table 1. Particularly notable are the $\text{C}4a-\text{C}5$ and $\text{C}10a-\text{N}2$ distances of 1.468 (2) and 1.429 (2) Å, respectively, and the bond angles $\text{N}6-\text{C}5-\text{C}4a$ [114.00 (14)°] and $\text{C}6a-\text{N}6-\text{C}5$ [126.04 (14)°]. The somewhat extreme variation in bond lengths and more especially bond angles suggests that the cation is not altogether an aromatic species. This is certainly true of the lactam ring defined by $\text{C}4a/\text{C}5/\text{N}6/\text{C}6a/\text{N}2/\text{C}10a$. In the refinement of the structure of (I) described here, the only atoms which are not coincident with a mirror plane of the space group $P6_3/m$ are two H atoms of the methyl group, one H atom of the water molecule involving O2 and the entire water molecule involving O3. As a consequence the cation, with the exception of the methyl H atoms, is completely flat and the entire structure can be described in terms of well defined layers parallel to (001) at $z = \frac{1}{4}$ and $\frac{3}{4}$ such as that shown in Fig. 2. Adjacent layers are related to one another by the operation of crystallographic centres of symmetry. The layers are also connected to one another by hydrogen bonding as described later. A further consequence of the mirror symmetry is that both water molecules must be present in two distinct orientations which must be present in equal numbers resulting, therefore, in disorder. For the water molecule involving O2, H1W is ordered but H2W is distributed over two mirror-plane-related sites both of occupancy 0.5. The atom H3W is common to both orientations of the water molecule involving O3 and is accompanied by H4W in one orientation and H5W in the other. Thus, while the H3W site is fully occupied, H4W and H5W both have occupancies of 0.5. The disorder of the H atoms has serious implications for the disposition of the hydrogen bonds in which they are

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