

Structure and Hirshfeld Surface analysis of a new structure of oxymetazoline chloride

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The resolution of crystalline structures is conventionally carried out by the single crystal method, however, there are materials where obtaining this single crystals is difficult or in some cases impossible, for this reason, resolving structures by powder x-ray diffraction has become an effective technique for knowing a molecule thoroughly. The oxymetazoline hydrochloride (OxyCl) is a drug that is used as a nasal decongestant. The powder pattern of OxyCl is different from the reported in PDF-4 (00-033-1792) and the pattern calculate from the single crystal data contained in CSD (REFCODE: ZIVKEU). This compound crystallizes in a monoclinic unit cell $P2_1/c$ with parameters: $a= 14.2876(13) \text{ \AA}$, $b= 9.5145(9) \text{ \AA}$, $c= 12.4476(17) \text{ \AA}$, $\beta=103.864(9)$ and $V= 1642.81(32) \text{ \AA}^3$. The structure of OxyCl (Figure 1) was determined using the EXPO14 program and refined using the Rietveld method with the GSASII. The Hirshfeld surface analysis shows that the packing is defined by intermolecular hydrogen bonds: $\text{Cl}\cdots\text{H}$: 8.7%, $\text{O}\cdots\text{H}$: 3.7%, $\text{N}\cdots\text{H}$: 2.1% and $\text{C}\cdots\text{H}$: 8.9%.

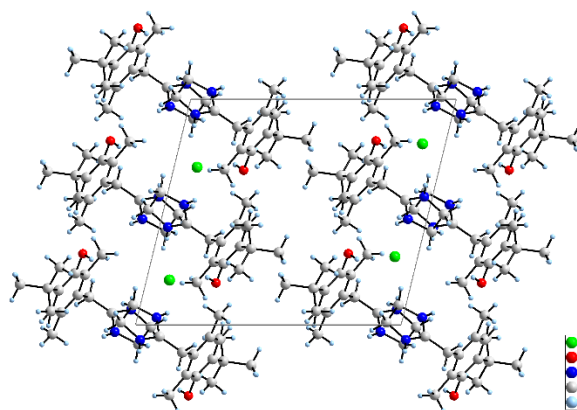


Figure 1. Structure of oxymetazoline chloride.

References

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