Chloroquine Derivatives. Conformation and Intermolecular Interactions

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Crystal structure of hydroxychloroquine (OHClQ) sulfate has been determined: a=10.5437(3)Å, b=8.8532(2)Å, c=22.0923(8)Å, α=90°, β=101.426(1)°, γ=90°, $P2_1/c$, Z=4, in order to compare its conformation and intermolecular interactions to those in the crystalline chloroquine (ClQ) phosphate [1] and quinine salicylate (QSal) monohydrate [2].

Molecular conformations of OHClQ and ClQ are comparable in both salts; the differences between corresponding torsion angles are not greater than 10°. Each of the nitrogen atoms is a proton donor in the intermolecular hydrogen bonds with the oxygen atoms of sulfate or phosphate anions. While the parameters of the N1-H1···O and N3-H3···O bonds are similar, the distance N···O within the bond N2-H2···O is much shorter in the case of OHClQ. The -OH group of OHClQ forms an additional H-bond with the oxygen atom of SO_4^{2-}.

The comparison of the hydrogen bonds formed by OHClQ and ClQ with those of quininium anion in QSal shows that these antimalarial molecules may interact with their putative receptor in a similar way.

[1] Karle J.M., Karle I.L., *Acta Cryst.,* 1988, **C44**, 1605. [2] Oleksyn B.J., Serda P., *Acta Cryst.,* 1993, **B49**, 530.

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