Experimental Charge Density Analysis for Doxycycline

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The results of experimental charge density analysis for the wide spectrum antibiotic doxycycline in its monohydroxide form are presented. The tautomeric form adopted by the antibiotic in the monohydrate crystal is identical to the tautomeric form observed in the antibiotic-protein interactions.
The network of intra- and intermolecular interactions of the doxycycline is analyzed and classified in terms of topological analysis, interaction energies and source function contributions. Interaction energies are also compared with the results of theoretical periodic calculations.

The conformation of the antibiotic in the crystal lattice is compared with the conformation known for the antibiotic-target protein complexes deposited in PDB. The major difference is the breaking of the intramolecular hydrogen bond network in order to form two protein-ligand contacts. The differences are also explored by means of Hirshfeld surface analysis of the doxycycline in the crystal network and doxycycline in the protein environment.

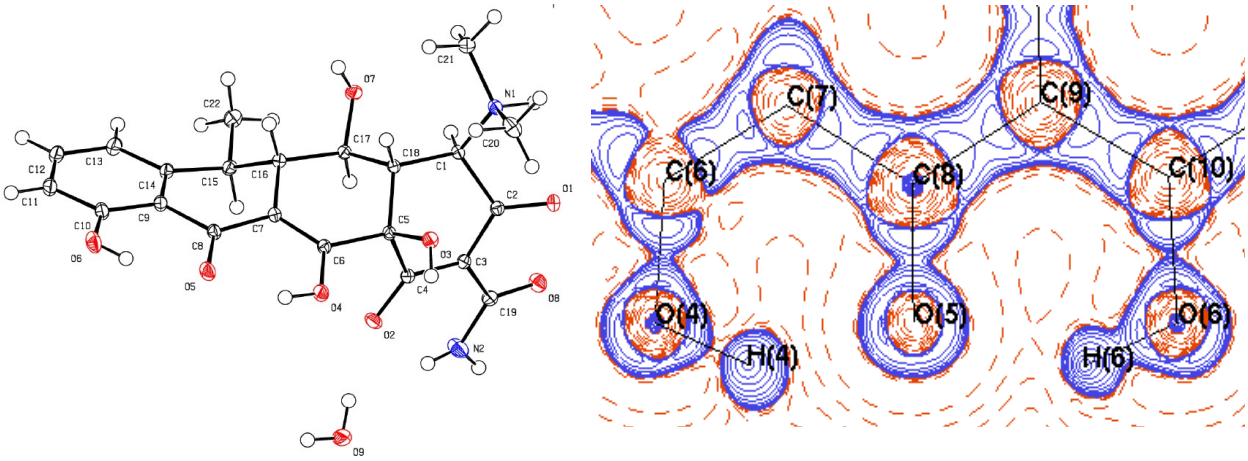

Fig. The ORTEP representation of the doxycycline and the Laplacian map for the intramolecular network of hydrogen bonds.

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