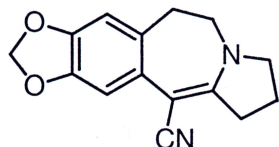


f0.m0.p0 Charge density of a putative intermediary product in the total synthesis of the cephalotaxine

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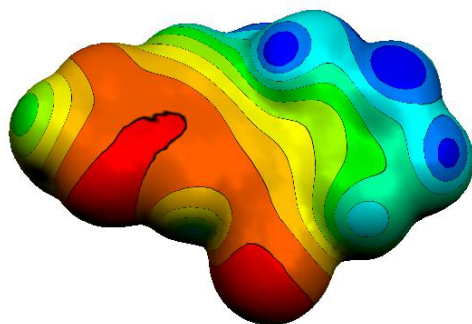
Keywords: homoharringtonine, charge density, electrostatic potential

A high resolution diffraction measurement have been performed on a putative precursor of cephalotaxine; using a Brücker CCD detector. The compound crystallizes in $P2_1/n$ space group ($V = 1174.49(2) \text{ \AA}^3$). 161121 reflections were collected leading to 10690 independent reflections up to $1,11 \text{ \AA}^{-1}$ ($R_{\text{int}} = 0,0215$). Multipole refinement (Hansen and Coppens model [1]) converges with reliability factors



($R(F) = 0,0283$ and $GOF = 1,32$). Electron deformation maps show up a strong delocalization over the four cycles. The calculation of the atomic net charges deduced from a κ refinement are in agreement with the reactivity (or the non-reactivity) of the compound. The topological properties at the bond critical points (3, -1) are reported and are also in a quite good agreement with the chemistry.

Finally the electrostatic potential has been calculated [2] and two different representations are used in order to characterize the compound: 3D isopotential surfaces, and 3D isodensity molecular surface colored by the electrostatic potential (figure).



[1] Hansen N. Coppens P., Acta Crystallogr. 1978, A34, 909

[2] Ghermani N.E., Bouhaida N., Lecomte C., Internal report UMR CNRS 7036, Université H. Poincaré, Nancy 1, UMR CNRS 8612, Université Paris XI and Université Cadi Ayyad, Morocco