Crystal and Molecular Structure of the Natural Product Strictosidinic Acid: Structural, Occupational Disorders and Statistical Analysis.

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The Palicourea coriacea species, popularly known as Douradinha, is a typical plant of cerrado, whose tea is used in the kidney stones treatment, kidney and urethra inflammation, as well as effective diuretic action. The roots and leaves extract, when submitted to antimicrobial test shows growth inhibition of gram positives bacteria such as Staphylococcus aureus, Bacillus subtilis, Micrococcus luteus and under certain conditions inhibits also Escherichia coli. Strictosidinic acid, a alkaloid that has important biological properties, was isolated from the roots of Palicourea coriacea. The structures were elucidated on the basis of x-ray diffraction data. The widespread popular use and the lack of crystallographic information in literature about the isolated alkaloid are the main motivation of this work.

The strictosidinic acid was crystallized by the slow evaporation technique using methanol as solvent. Selected sample for x-ray experiment has prismatic shape. Diffraction data were collected in a KappaCCD diffractometer using Mo-Kα radiation at room temperature. The unit cell of monoclinic system is a = 7,5983(2)Å, b = 23,5833(6) Å and c=15,9734(3) Å, β= 91,039(1)°. The space group is $P2_1$ and displays two independents molecules per asymmetric unit. In the interstitium molecular there is a cavity partially completed by six water molecules showing high occupational disorder, causing structural disorder in the molecule. Due to the absent of hydrogen bond involving the water molecules each site has a high displacement and the occupancy varies from 20% to 100%. The initial model presented a residual wR2 of 35%, after the modeling of structural and occupational disorder, the final model had index adjustment wR2 of 25,7%. The software SHELXL-97 was used in this modeling. The crystal packing is mediated by intermolecular hydrogen bonds of types N-H...O.

A statistical analysis on the structural parameters of the title compound based on structures deposited in the Cambridge Structural Database, showed some relevant differences, mainly in the bond lengths, which can be assigned to structural disorder in the molecule due to the partial filled water cavities.

References

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