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Área: Engenharias

Projeto: CARACTERIZAÇÃO ESPECTROSCÓPICA DE LÍQUEN PARMOTREMA TINCTORUM

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Bolsistas:

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Participantes:

Resumo:

FT-Raman spectroscopy has been used for the analytical characterization of the Parmotrema tinctorum Del. Ex Nyl. lichen. Lecanoric acid, the major lichen chemical present in the total mass, has been extracted from the lichen, purified and characterized by Raman spectroscopy supported by means of theoretical DFT calculations. The calculations indicate that the aromatic ring A of the lecanoric acid structure is kept in the molecular plane by a strong hydrogen bond between the ortho-hydroxyl group of ring A and the ester group; this hydrogen bond is shorter in the C1 isomer form, which is the main feature responsible for the Gibbs free energy difference (-2.96 kcal/mol) favouring the C1 isomer. In spite of the similarity of possible conformers and although many of the predicted Raman bands are found to be common for both forms, there is one Raman transition very characteristic of structure C2, centred at 1815 cm^{-1} , assigned to the stretching of the C=O group of the ester moiety. For the isomer C1 this transition was predicted at 1729 cm^{-1} , with a lower frequency ascribed to the stronger hydrogen bond present in the latter conformation. In the experimental spectrum two strong bands are found at 1654 and 1638 cm^{-1} (shoulder) attributed to the C=O stretching mode. The analysis of the normal modes for the corresponding transitions calculated at 1742 and 1729 cm^{-1} allowed the assignment to be made to (C=O) stretching mode from the carboxylic acid and ester moiety, respectively. Most of the other Raman bands were also assigned by comparison with the theoretical model. The Raman spectrum obtained directly from the P. tinctorum lichen shows a remarkable similarity with the isolated lecanoric acid spectrum, as well as the presence of bands at 1529 and 1156 cm^{-1} which are characteristic of a carotenoid species. The results confirm the potential of Raman spectroscopy for taxonomic characterization of lichen species.