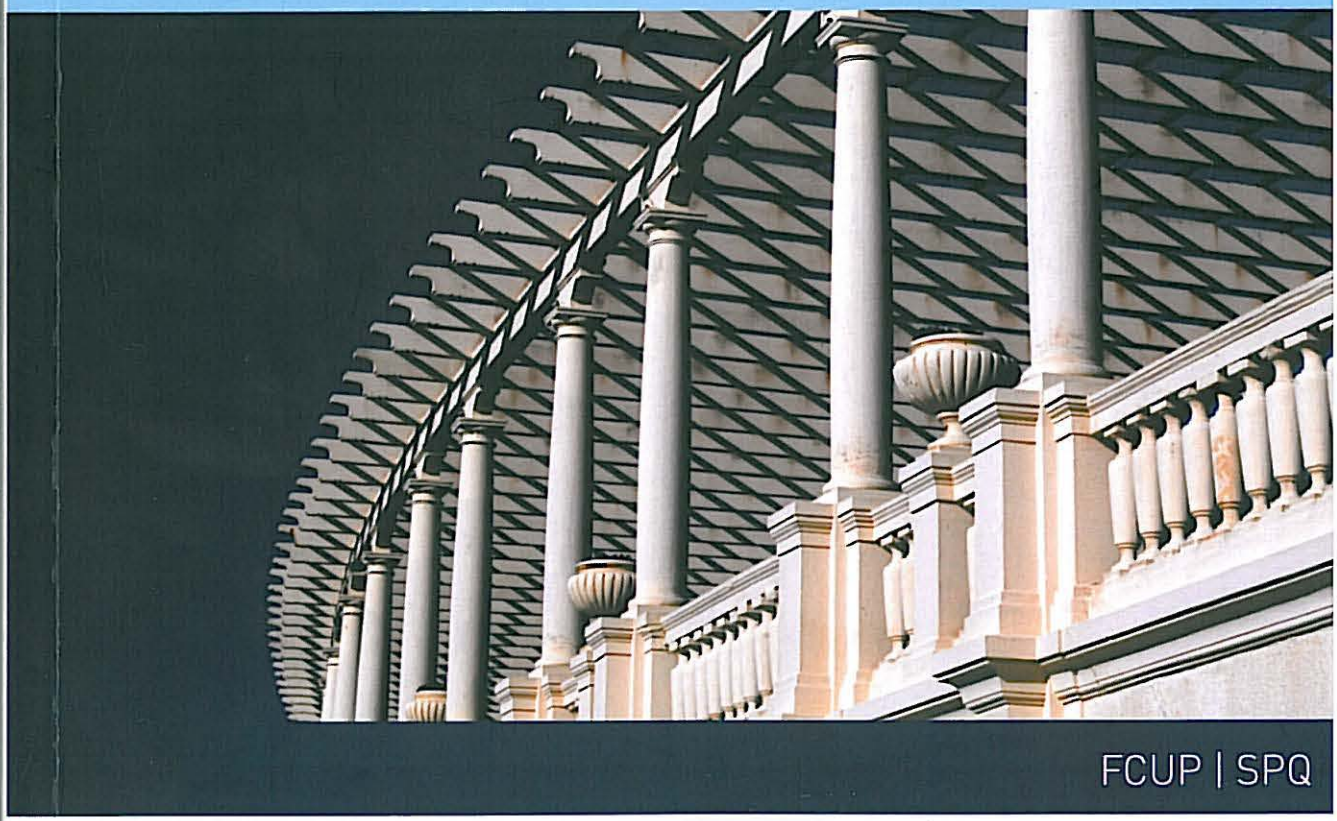
11º Encontro Nacional de Química-Física

BOOK OF ABSTRACTS



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Jorge M. Gonçalves

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SECTION D

CHEMICAL THERMODYNAMICS

SOLUBILITY OF HESPERETIN IN MIXED SOLVENTS

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The study of the solubility of flavonoids is essential to support the design of several separation processes in the food and pharmaceutical industries. Hesperetin is a flavanone with great importance for its promising biological and pharmacological properties.

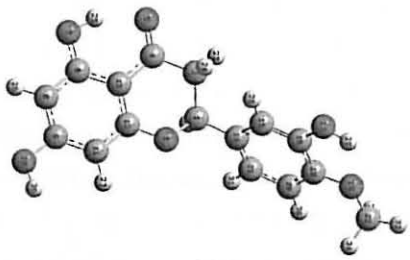

Figure 1. Hesperetin: illustration of the molecule.

Our previous studies included the measurement of the solubility of this biomolecule in several pure organic solvents [1]. In this work, new solubility data is presented for hesperetin in the binary mixed solvents water + ethanol, water + methanol, and water + acetone, at 298.15 K. The isothermal shake-flask method was applied, followed by quantitative analysis by gravimetry. The three solubility phase diagrams obtained, present quite distinct and interesting features. For these studies in aqueous mixtures, it is important to take into consideration the existence of two different crystal structures of hesperetin, already described in the literature, one corresponding to the anhydrous form [2] and another to the monohydrate form [3]. Therefore, a set of solid samples obtained from the solubility studies were analysed by Powder X-ray diffraction, Infrared Spectroscopy and Thermogravimetric Analysis. The selected solid samples, obtained from mixed solvents solutions, with higher compositions in water, showed the presence of the monohydrate form of hesperetin, while the others were anhydrous. Evidence from complex molecular interactions involving hesperetin, including intramolecular and intermolecular hydrogen bonding, was shown by the solid phase analysis.

[1] O. Ferreira, S.P. Pinho, *Ind. Eng. Chem. Res.*, **51**, 6586-6590 (2012).

[2] S. Fujii, Y. Yamagata, G.Z. Jin, K. Tomita, *Chem. Pharm. Bull.*, **42**, 1143-1145 (1994).

[3] W. Shin, S. Kim, K.S. Chun, *Acta Cryst. C*, **43**, 1946-1949 (1987).