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ACCEPTED MANUSCRIPT

Infrared spectroscopic study of the formation of fossil resin analogs with temperature using *trans*-communic acid as precursor

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Abstract

For million years resin exudates have undergone chemical alterations by heat, pressure, radiation, water, oxygen, microorganisms, and have suffered processes of sedimentation and diagenesis. These agents have affected the organic functional groups present in the terpenes of the resins, giving rise to what we nowadays know as fossil resins. In this work, we try to get further insight in the chemical formation of fossil resins. As the simulation of the natural process is quite complex, we have focused on the temperature induced reactivity of the *trans*-communic acid, the main component of the *Class* I resins. Using this terpene derivate as a very basic model of a resin exudate, we have monitored their thermal changes by infrared spectroscopy, differential scanning calorimetry and thermogravimetric analysis within the range of 25 to 340 ºC. The temperature-induced transformation, both in presence and absence of inert atmosphere, is discussed on the basis of the reactivity of the conjugated double-bond, the exocyclic bond and the carboxylic acid group present in the *trans*-communic acid. The results obtained in these series of experiments agree with the maturation scheme accepted in the literature for natural resins, i.e. an initial cross-linked polymerization and a subsequent maturation reaction. From combined DSC/TGA and infrared spectroscopy results, we conclude that chemical changes produced in the *trans*-communic acid in the range 130-175 ºC may mimic the initial polymerization-like process in the natural resins, whereas those produced between 180 to 340 ºC seem to correspond to the maturation pathways described in the literature for fossil resins *Class Ib*. Spectral assignment of the most relevant infrared-active modes of the *trans*-communic acid at 25 ºC is also provided with the aid of Density Functional Theory calculations.

Keywords: Infrared Spectroscopy; Communic Acid; Fossil Resins; Amber.

1. Introduction

Amber and other fossil resins are wanted not only by jewelry collectors but also by scientists, since these substances allow us to record Earth's History. Fossil resins are not ores but fossilized organic matter from ancient trees naturally formed by the cross-linked polymerization of organic compounds. Fossil resins are mostly derived from natural terpenes-based polymers and therefore have an organic origin [1,2]. They are

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