SPECTROSCOPIC CHARACTERIZATION OF THE INTERNAL MOTIONS IN ACRYLIC AND CROTONIC ACID DERIVATIVES

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The recent detection of cyano-substituted alkenes in a dark molecular cloud (TMC-1) of the interstellar medium[1] raises the question whether other corresponding alkene-based carboxylic acid derivatives are also formed and could be present in this astrochemical environment. For the simplest case, acrylic acid (three carbons), both the nitrile[2] and the aldehyde[3] have been identified. However, it is interesting to note that acrolein, like many larger oxygen-rich molecules (COMs), tends to be observed in warmer regions nearby stars, unlike acrylonitrile, although small amounts have also been found in cold TMC-1. Of the alkene molecules with four carbon atoms, only crotonitrile and methacrylonitrile have been identified to date. While methacrylic acid[4] and its methyl ester methyl methacrylate[5] have been studied in our laboratory, we have now extended spectroscopic characterizations or reinvestigations to the remaining methyl ester of acrylic acid (methyl acrylate)[6] and derivatives of crotonic acid (four carbon atoms). All of these molecules undergo internal rotation of one or two methyl groups. The resulting feature of the rotational spectrum (splitting of the rotational transitions into different components corresponding to different symmetry species) can lead to a decrease in the overall signal intensity, potentially complicating identification in radio astronomical data. This and a contextualization of the V_3 values are discussed.

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