On not yet solved problems concerning some molecular systems investigated by rotational spectroscopy along my research life

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Not yet solved aspects of the rotational spectra of some molecular systems will be discussed. They concern: 1) Unsatisfactory analyses of the spectra; 2) Non-observation of expected rotational transitions; 3) Non observation of the spectra of expected chemical species.

Rotational spectrum and molecular structure of succinic anhydride aided by computational calculations

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The cm-wave and mm-wave spectra of succinic anhydride have been studied in a pulsed supersonic jet using Fourier-transform microwave spectroscopy and in a free-jet using mm-wave absorption spectroscopy. All rotational constants, quartic centrifugal distortion constants are determined. Studies on ^{13}C and ^{18}O singly substituted isotopologues were used to assign the substitution geometry for succinic anhydride. The transitions observed in the FTMW spectrum show fine structure. The fine structure can be fitted by including spin rotation constants for the equivalent hydrogen nuclei but the resultant constants are not consistent with those predicted by computational methods. An alternative explanation involving a non planar geometry, consistent with the results of computational methods is favoured.

Pursuing the rotational spectra of large molecular systems

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In a quest for studying large molecular systems two new configurations using laser-ablation coupled with narrowband molecular beam and broadband chirped pulse Fourier-transform microwave techniques (LA-MB-FTMW and LA-CP-FTMW) have been configurated and tested in our group. The current experimental set ups have been optimized to record the rotational spectra at low frequency ranges in the 2-8 GHz region. A detailed description of the experimental systems as well as improvements in the data acquisition routines will be presented. The present state-of-the-art of microwave spectroscopy is paving the way towards the study of larger, more complex, biological systems which have been previously considered as being out of reach of high-resolution spectroscopic studies.

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Exploring the generation of new species using laser ablation Fourier transform microwave spectroscopy techniques: the study of N-carbamoyl glycine

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At the University of Valladolid, substantial advances in laser ablation procedure had made possible to transfer many thermally fragile molecules into the gas phase and to probe their rotational signatures in the isolated conditions of a supersonic expansion by Fourier transform microwave techniques.[1,2] Very recently, we have successfully applied these techniques to the generation and spectroscopic characterization of glycinamide[3] and hydantoin,[4] possible precursors of glycine. During the investigation of related acyclic hydantoic acid (N-carbamoyl glycine), for which three different conformers have been unveiled, we surprisingly observed the formation of cyclic hydantoin, glycine, urea, methyl isocyanate, and other known astrophysical species. Among the numerous unassigned lines in the spectra, cyclic glycine N-carboxyanhydride has been detected for the first time. Present results open new ways towards the generation and spectroscopic characterization of new chemical species using a laser ablation source coupled with high-resolution Fourier transform microwave techniques.

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