MILLIMETER-WAVE SPECTROSCOPY OF FLEXIBLE ORGANIC MOLECULES AND COMPARISON WITH ASTRONOMICAL SURVEYS

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The identification and quantification of molecules in space is based on spectroscopic methods (in particular rotational spectroscopy) and laboratory work is essential to provide the community with the spectral features needed to analyze the cosmological surveys. Many of the molecules which are searched for in space, are complex organic molecules which show a high degree of molecular flexibility. The high number of low energy conformations and the presence of large amplitude motions on shallow potential energy surfaces are peculiar to this kind of systems giving rise to very complex rotational spectra, which represent a challenge for spectroscopic and computational methods. Spectroscopic strategies for the rotational study of flexible organic molecules include the use of the cold and isolated conditions of a free jet expansion and heated sources for the non-volatile systems while the computational methods must deal with complex conformational surfaces and large amplitude motions which can cause tunneling splittings of the rotational transitions. As examples, we will discuss the complex conformational space of 1,2-butandiol and the problem of internal rotation in thioacetamide investigated by rotational spectroscopy in the 60-118 GHz range