ROTATIONAL SPECTROSCOPY OF ISOCYANIC MOLECULES: ALLYL ISOCYANIDE AND DIISOCYANOMETHANE

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Isocyanides are less stable isomers of nitriles and some of them have already been observed in the interstellar medium (HNC, $CH_3NC$, HCCNC). But still there exists a lack of experimental spectroscopic data on simple isocyanic molecules that can represent potential astrophysical interest. In this view we have performed high resolution studies of rotational spectra of allyl isocyanide ($CH_2$=CH–$CH_2$–NC) and diisocyanomethane (CN–$CH_2$–NC). The rotational spectra of allyl isocyanide have been measured in the frequency range 6 – 18 GHz by means of FTMW spectrometer in Bilbao and in the frequency range 150 – 945 GHz by means of classic absorption spectroscopy in Lille. Two stable confomers of allyl isocyanide have been observed in both series of measurements. In addition, all $^{13}$C-monosubstituted isotopologues and $^{15}$N isotopologues were detected in natural abundance. Due to much lower kinetic stability the rotational spectrum of diisocyanomethane has been measured only in absorption using the Lille spectrometer. The spectral assignments have been supported by high-level quantum chemical calculations. For both molecules accurate sets of rotational and centrifugal distortion constants (up to the octics) have been produced. As a result, reliable predictions of transitions frequencies suitable for astrophysical detection have been obtained for both molecules. Finally, the effective and substitution structures were determined for the two conformers of allyl isocyanide, comparing the result with ab initio data.

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