COMPREHENSIVE ROTATIONAL SPECTROSCOPY OF METHYL CYANOACETATE FOR ASTRONOMICAL SEARCHES

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Out of the more than 200 individual molecular species already identified in the ISM, nearly 16% of the molecules contain a cyano functional group (see www.astro.uni-koeln.de/cdms/molecules). An interesting extension to this is studying molecules that contain an additional functional group. We present a comprehensive study on methyl cyanoacetate (MCA) whose condensed formula is $NCCH_2COOCH_3$. It is a molecule whose two functional groups (cyano, -CN, and ester, $-COOCH_3$) have already been identified individually in the ISM.

The rotational spectrum of MCA was obtained in the frequency range of 2-26 GHz using two chirped-pulse Fourier transform microwave (CP-FTMW) spectrometers, namely the COMPACT spectrometer and the 18-26 GHz spectrometer. The ^{14}N nucleus (I=1) in the cyano group, is responsible for the observation of the nuclear quadrupole hyperfine splitting (HFS) of rotational transitions. The ester functional group contains a methyl top that rotates with respect to the molecular frame and couples with the overall rotation (computed barrier height for internal rotation, V_3 is 309 cm^{-1}), giving rise to further splitting of each transition into A and E states. Both the nuclear quadrupole HFS and the methyl internal rotation splitting were resolved, and it was possible to obtain a single fit for all the rotational parameters using the XIAM program.[1]

This study of MCA in the 2-26 GHz region would provide insights into how the barrier height is affected by the presence of electron-withdrawing/donating moieties attached to the ester group. For example, in methyl carbamate,[2] V_3 is 352 cm^{-1}, while in methyl acetate,[3] V_3 is 425 cm^{-1}. Furthermore, the experimental data obtained from this study can facilitate searches for this molecule with various radio observatories, for example, the Jansky Very Large Array (JVLA) and the Radio Telescope Effelsberg.

(1) H.Hartwig and H.Dreizler, Z. Naturforsch 51a, 923-932 (1996) (2) J. Sheridan et al. J. Mol. Spectrosc. 80, 1-11 (1980) (3) B. Bakri et al. J. Mol. Spectrosc. 215, 312–316 (2002)