

FIRST LABORATORY DETECTION OF N^{13}CO^- AND SEMIEXPERIMENTAL EQUILIBRIUM STRUCTURE OF THE NCO^- ANION

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The cyanate anion NCO^- is a species of considerable astrophysical relevance. It is widely believed to be embedded in interstellar ices present in young stellar objects but has not yet been detected in the dense gas of the interstellar medium. Here, very accurate laboratory measurements of the rotational spectrum of the N^{13}CO^- isotopologue at submillimeter wavelengths and three additional lines of the parent isotopologue up to 437.4 GHz are reported. With this new data, the rotational spectrum of both isotopologues can be predicted to better 0.25 km s^{-1} in equivalent radial velocity up to 1 THz. Moreover, a semiexperimental equilibrium structure of the anion is derived by combining the experimental ground-state rotational constants of the two isotopologues with theoretical vibrational corrections, obtained by using the coupled-cluster method with inclusion of single and double excitations and perturbative inclusion of triple excitations (CCSD(T)). The estimated accuracy of the two bond distances is on the order of $5 \times 10^{-4} \text{ \AA}$.