HIGH-RESOLUTION SPECTROSCOPY OF TWO CONFORMERS OF 2-CYANOBUTANE BETWEEN 10 AND 400 GHZ

MARIUS HERMANNS, NADINE WEHRES, FRANK LEWEN, HOLGER S. P. MÜLLER, STEPHAN SCHLEMMER, *I. Physikalisches Institut, Universität zu Köln, Köln, Germany*.

We present high-resolution rotational spectroscopy of two out of three conformers of 2-cyanobutane. Spectra were taken between 10-26 GHz by means of chirped-pulse spectroscopy. Spectra between 36 and 402 GHz were recorded by means of frequency modulated (FM) absorption spectroscopy. The analysis yields precise rotational constants and higher order distortion constants, as well as a set of ^{14}N nuclear electric quadrupole coupling parameters. In addition, quantum chemical calculations were performed assisting the assignments. Calculations of vibrational frequencies yield insight into the vibrational energy structure from which partition functions and vibrational correction factors are determined. These are used to determine experimentally and computationally the energy difference between the conformers. Overall, this study provides precise spectroscopic constants for the search of 2-cyanobutane in the interstellar medium. In particular, this molecule appears as an interesting case to test our knowledge of (branched) molecule formation in space.