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Abstract:Rotational spectra of four isotopically enriched, singly substituted species of acrylonitrile have been studied up to 1.2 THz. Extensive analysis of the spectra recorded for $H_2^{13}CCHCN$, $H_2CCH^{13}CN$, $H_2CCHC^{15}N$, and H_2CCDCN, revealed the presence of the same characteristic perturbations between the ground state and the $v_{11} = 1$ excited vibrational state, that have recently been identified in the parent molecule. For this reason transitions in $v_{11} = 1$ have also been assigned in each of the four isotopic species and a coupled state analysis of g.s. and $v_{11} = 1$ was performed on a total of around 3000 lines for each species. The derived precise values of $E(v_{11} = 1)$ are found to be consistent with estimates from anharmonic force field calculations. In addition, transitions for six new doubly substituted isotopic species of acrylonitrile, $H_2^{13}C^{13}CHCN$, $H_2^{13}CCH^{13}CN$, $H_2C^{13}CH^{13}CN$, $H_2^{13}CCHC^{15}N$, $H_2C^{13}CHC^{15}N$, and $H_2CCH^{13}C^{15}N$, have been assigned, and their ground state spectroscopic constants have been determined. Rotational constants for all known isotopic species of acrylonitrile have been combined with ab initio calculation of vibration-rotation constants in the first evaluation of the r_e^{SE} geometry of this molecule.

Number of references:30