HIGH RESOLUTION MEASUREMENTS ON THE ROTATIONAL SPECTRA OF HYDROGEN CYANIDE ISOTOPOMERS UP TO 2 THz

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Employing the Cologne Terahertz Spectrometer in Sub-Doppler resolution between 150 GHz and 1 THz, the rotational spectra of the hydrogen cyanide isotopic species $H^{13}CN$, $HC^{15}N$, $H^{13}C^{15}N$, DCN, $D^{13}CN$, $DC^{15}N$ and $D^{13}C^{15}N$ were recorded in the vibrational ground and first excited bending states ($v_2 = 0, 1$). Thereby, R-branch transitions from $J = 2 \leftarrow 1$ to $J = 11 \leftarrow 10$ for the H-containing species and from $J = 3 \leftarrow 2$ to $J = 13 \leftarrow 12$ for the deuterated species could be covered. This very high resolution ($\sim$70 kHz) and precise ($\pm$ 3-10 kHz) saturation dip measurements allowed resolving the hyperfine structure due to the ^{14}N nucleus in $H^{13}CN$, DCN and $D^{13}CN$ for transitions as high as $J = 8 \leftarrow 7$ and $J = 10 \leftarrow 9$, respectively. Additional, high lying R-branch transitions have been recorded in Doppler resolution between 1.75 and 2.01 THz with the Cologne Sideband Spectrometer for Terahertz Applications (COSSTA). For some isotopomers also direct ℓ-type ($\Delta J = 0$) transitions in the frequency region from 65 to 270 GHz were measured in Doppler resolution.

These new experimental data, together with available infrared rovibrational data and low frequency direct ℓ-type transitions, were subjected to a global least squares analysis for each isotopomer. This yielded highly precise sets of molecular constants for the ground and first excited vibrational states of all isotopomers, including the nuclear quadrupole and magnetic dipole constants of the ^{14}N nucleus for $H^{13}CN$, DCN and $D^{13}CN$. The hyperfine structure due to the D, ^{13}C and ^{15}N nuclei could not be resolved, but led to a broadening of the observed saturation dips.