Abstract

In this work the results of rotational spectroscopic investigations of selected molecular species with both astrophysical and purely spectroscopical importance are presented.

The rotational spectra of the deuterium cyanide isotopomers DCN, $D^{13}CN$, $DC^{15}N$, and $D^{13}C^{15}N$ were recorded in the vibrational ground and first excited bending state ($v_2 = 1$) up to 2 THz. R-branch transitions up to 1 THz were measured with sub-Doppler resolution. These very high resolution saturation dip measurements allowed for resolving the underlying hyperfine structure due to the nuclear spin of ^{14}N in DCN and $D^{13}CN$. Accuracies of about 3 kHz were achieved for sub-Doppler measurements of isolated lines. Additionally, high J R-branch transitions around 2 THz and direct l-type transitions ($\Delta J = 0$) between 66 and 118 GHz were recorded in Doppler-limited resolution. These new experimental data, together with available infrared rovibrational data, were subjected to a global least squares analysis for each isotopomer. This yielded precise sets of molecular constants for the ground and first excited vibrational states, including the nuclear quadrupole and magnetic spin-rotation coupling constants of the ^{14}N nucleus for DCN and $D^{13}CN$.

Two astrophysically important rotational transitions between energetically low lying levels of methylene (CH_2) have been measured with high accuracy near 2 THz for the first time. For the *in-situ* synthesis of this unstable radical and the recording of its gas-phase rotational spectrum a new absorption cell has been designed and the technique of Zeeman modulation has been introduced to the Cologne laser sideband system. A non-standard Euler expansion of the effective Hamiltonian was employed for the analysis of a global dataset, yielding precise spectroscopic parameters with improved predictive capability for astrophysical important transitions.

More than 170 rotational transitions of the two water isotopomers HDO and D_2O were measured up to high energies in the frequency range between $700 - 1000$ GHz and around 2 THz in the vibrational ground and first excited states. The global analysis of this data together with other available rotational and rovibrational transition frequencies by means of the Euler approach resulted in an improved spectroscopic parameter set on these molecules. The analysis provides highly accurate transition frequency predictions which are valuable both for atmospheric and astrophysical science.