

Accurate rest frequencies for propargylamine in the ground and low-lying vibrational states

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Context. To date, several complex organic molecules have been detected in the interstellar medium, and they have been suggested as precursors of biologically important species. Propargylamine ($\text{HC}\equiv\text{C}-\text{CH}_2-\text{NH}_2$) is structurally similar to a number of other organic molecules which have already been identified by radioastronomy, making it a good candidate for astrophysical detection.

Aims. This work provides accurate rest frequencies of propargylamine, from the centimeter-wave to the submillimeter-wave region, useful to facilitate the detection of this molecule in the interstellar medium.

Methods. An extensive laboratory study of the rotational spectrum of propargylamine has been performed using a pulsed-jet Fourier Transform Microwave (FTMW) spectrometer (7–19 GHz frequency range) and a frequency modulation microwave spectrometer (75–560 GHz). Several hundred rotational transitions of propargylamine were recorded in the ground and three lowest excited vibrational states. The experiments were supported by high-level ab initio computations, mainly employed to characterize the vibrational state structure and to predict spectroscopic parameters unknown prior to this study.

Results. The measured transition frequencies yielded accurate rotational constants and the complete sets of quartic and sextic centrifugal distortion constants for propargylamine in its vibrational ground state. ^{14}N -nuclear quadrupole coupling constants were also determined. Rotational and quartic centrifugal distortion constants were also obtained for the low-lying excited states $\nu_{13} = 1$ (A'), $\nu_{20} = 1$ (A''), and $\nu_{21} = 1$ (A''). The a -type Coriolis resonance which couples the $\nu_{13} = 1$ and $\nu_{21} = 1$ levels was analyzed.

Conclusions. The determined spectroscopic constants allowed for the compilation of a dataset of highly accurate rest frequencies for astrophysical purposes in the millimeter and submillimeter regions with 1σ uncertainties that are smaller than 0.050 MHz, corresponding to 0.03 km s^{-1} at 500 GHz in radial equivalent velocity.

Słowa kluczowe

molecular data-methods, laboratory, molecular-techniques,
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