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Title:Analysis of the terahertz rotational spectrum of the three mono- ¹³C ethyl cyanides (¹³C-CH<inf>3</inf>CH<inf>2</inf>CN)
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Abstract:Context. Millimeter-and submillimeter-wave spectra of regions such as the Orion molecular cloud show many rotational-torsional lines that are caused by the emission of complex organic molecules (COM). Previous laboratory investigations have been conducted for three isotopologues of ethyl cyanide up to 360 GHz, and subsequently, several hundred lines of the three isotopologues have been detected in Orion IRc2 using the IRAM 30 m radiotelescope. Aims. In this survey we present the analysis based on a Watson Hamiltonian for an asymmetric one-top rotor of the ¹³C-substituted ethyl cyanide ¹³CH<inf>3</inf>CH<inf>2</inf>CN, CH<inf>3</inf>¹³CH <inf>2</inf>CN and CH<inf>3</inf>CH<inf>2</inf>¹³CN in the frequency range 480-650 GHz and 780-990 GHz. Methods. The rotational spectra of the three species were measured with a submillimeter spectrometer (50-990 GHz) using solid-state sources. Results. A new set of spectroscopic parameters was determined from a least-squares fit procedure for each isotopologue. These parameters permit a new accurate prediction of rotational lines suitable for an astrophysical detection in the submillimeter wave range. © ESO, 2012.
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