

The 4051 Å Comet Band of $^{13}\text{C}_3$

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Abstract. The tricarbon C_3 molecule has been detected in a number of translucent interstellar clouds via its $A^1\Pi_u - X^1\Sigma_g^+$ (000-000) electronic ‘comet’ band around 4051 Å. So far, it is the largest molecule unambiguously identified in the diffuse interstellar medium. In this work, rotationally resolved laboratory spectra are presented for the corresponding transition of the $^{13}\text{C}_3$ isotopologue. The spectra are recorded in direct absorption using cavity ring-down spectroscopy in combination with a supersonic plasma jet. A rotational analysis yields accurate spectroscopic parameters. In contrast to $^{12}\text{C}_3$, no significant perturbations are found for (*e*- or *f*-parity) levels up to $J' = 18$ in the $A^1\Pi$ upper electronic state.

Keywords. methods: laboratory, ISM: molecules, molecular data, $^{13}\text{C}_3$.

1. Introduction

The 4051 Å band of C_3 has attracted much interest of astronomers and spectroscopists since it was first observed in the emission spectrum of comet Tebbutt (Huggins 1881). The spectrum was unambiguously assigned to the linear pure carbon species C_3 following an isotopic ^{13}C -substitution experiment (Douglas 1951, Clusius & Douglas 1954). Later Gausset *et al.* (1965) assigned the optical spectra in the 3900 – 4140 Å range as originating from the $A^1\Pi_u - X^1\Sigma_g^+$ electronic system and a detailed rotational analysis was presented for a number of bands. In the dense interstellar medium (ISM) the presence of C_3 was proven using its mid- and far-infrared vibrational transitions (Hinkle *et al.* 1988, Cernicharo *et al.* 2000, Giesen *et al.* 2001). More recently, C_3 was identified in the diffuse interstellar medium, initially by Maier *et al.* (2001) and later in a number of other studies (Adamkovics *et al.* 2003, Galazutdinov *et al.* 2002, Schmidt *et al.* 2013) along a number of different lines of sight. These studies allowed to derive column densities and temperatures.

The spectroscopic interpretation of C_3 has been far from trivial. A number of laboratory studies have been performed over the past half century to comprehensively understand the $A - X$ electronic system. It was confirmed that the lower J levels in the upper $A^1\Pi_u$ state of $^{12}\text{C}_3$ are perturbed and some of the unassigned rotational lines observed by McCall *et al.* (2003) were found to be due to transitions into two long-lived perturbing states (Zhang *et al.* 2005, Tanabashi *et al.* 2005). Previous spectroscopic studies on C_3 have focused on the main $^{12}\text{C}_3$ isotopologue. The only laboratory study on the $^{13}\text{C}_3$ has been reported by Clusius & Douglas (1954). Their emission spectrum of the 4051 Å band has been instrumental in confirming the identification of the cometary band to triatomic carbon, C_3 . In these proceedings, we present the high-resolution spectrum of the $A^1\Pi_u - X^1\Sigma_g^+$ (000 – 000) origin band of $^{13}\text{C}_3$ isotopologue. The full details of this study will be available soon from Haddad *et al.* (2013).

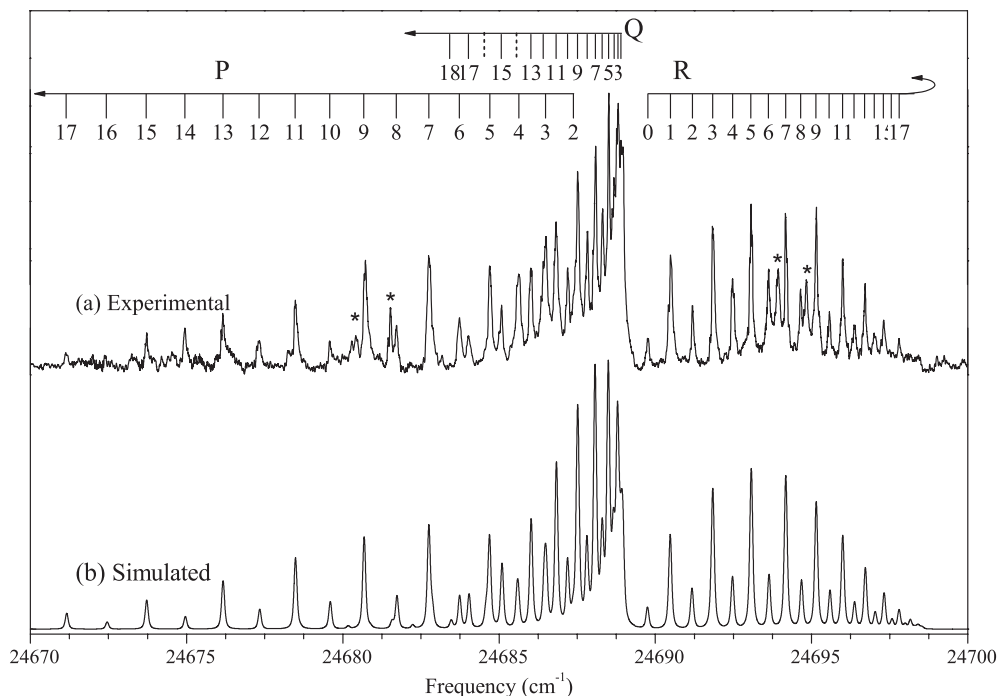


Figure 1. The rotationally resolved spectrum of the $A^1\Pi_u - X^1\Sigma_g^+$ electronic origin band of $^{13}\text{C}_3$ around 4051 \AA (upper trace). The lower trace shows a simulated spectrum for a rotational temperature of $\sim 40 \text{ K}$ and using a $^1\Pi-^1\Sigma$ Hamiltonian and convolution with a Lorentzian line width of 0.07 cm^{-1} and a Gaussian width of 1.0 cm^{-1} . The lines marked with an asterisk are due to blending transitions of small species like $^{13}\text{C}_2$ and ^{13}CH .

2. Experimental

Supersonically jet-cooled $^{13}\text{C}_3$ radicals are produced in an expanding planar plasma by discharging a high pressure (8 bar) gas pulse of 0.2% $^{13}\text{C}_2\text{H}_2$ diluted in an He:Ar $\sim 1:1$ gas mixture that expands through a $30 \text{ mm} \times 300 \text{ }\mu\text{m}$. Details of the slit nozzle system are available from (Motylewski *et al.* 1999, Zhao *et al.* 2011). The gas expansion crosses 5 mm downstream the optical axis of a high finesse cavity that is used for cavity ring-down spectroscopy. Tunable violet light around $\sim 4050 \text{ \AA}$ is generated by frequency-doubling the near infrared output of a pulsed dye laser running on (Styryl 9) dye. The wavelengths in the recorded C_3 spectra are calibrated by detection of the Ar I line at 24656.83 cm^{-1} (405.4 nm) (Kramida *et al.* 2012) in the plasma and by recording transmission fringes of two solid etalons. This yields an absolute laser frequency accuracy better than 0.04 cm^{-1} over the full scanning range.

3. Results and discussion

Figure 1 (upper trace) shows a spectrum of the $A^1\Pi_u - X^1\Sigma_g^+$ origin band of $^{13}\text{C}_3$ recorded around $\sim 4051 \text{ \AA}$. As typical for $^1\Pi-^1\Sigma$ transitions the system is dominated by its Q-branch. In total 16 transitions in the P branch, 14 transitions in the Q-branch and 18 transitions in the R-branch have been identified. The rotational assignments (J) are given in Fig. 1.

The $^{13}\text{C}_3$ band is blue shifted with respect to the $^{12}\text{C}_3$ band. Because of spin-statistics; the intensity alternation ratio for $^{13}\text{C}_3$ is 1:3 for rotational levels with even and odd J

numbers, respectively, due to nuclear spin of ^{13}C ($I = 1/2$) whereas in $^{12}\text{C}_3$ transitions starting from odd levels are missing. As a consequence, the $^{13}\text{C}_3$ spectrum is more dense than the spectrum of the tricarbon main isotopologue. The experimentally determined transition frequencies are fitted using Pgpopher (PGOPHER) and employing a standard Hamiltonian for a $A^1\Pi_u - X^1\Sigma_u^+$ transition. Here, the $X^1\Sigma_g^+$ ground state constants, B_0'' , D'' , are fixed to the values reported by Moazzenahmadi *et al.* (1993) and the $A^1\Pi_u$ state constants T_{00} , B_0' , and q' are set as variable parameters in the fit. Inclusion of a free running centrifugal distortion constant D' does not improve the rms of the fit. Therefore, the constant D' has been fixed to a value that is estimated from the D''/D' ratio as obtained for $^{12}\text{C}_3$.

The fit yields $B' = 0.38072(10) \text{ cm}^{-1}$, $q' = 2.01(28) \times 10^{-4} \text{ cm}^{-1}$ and $T_{00} = 24688.99(5) \text{ cm}^{-1}$. The band origin is $\sim 13.5 \text{ cm}^{-1}$ blue shifted with respect to the value found for $^{12}\text{C}_3$. The simulated spectrum calculated from the obtained constants is shown in the lower trace of Fig. 1. The observed minus calculated values are well within the experimental uncertainties. This indicates that for levels $J' < 18$ in the upper $A^1\Pi_u$ state, no significant perturbations occur for either e -parity or f -parity levels. The ratio of B_0''/B_0' amounts to 1.042 for $^{13}\text{C}_3$, nearly identical to the value found for $^{12}\text{C}_3$ (1.043) and this is typical for an increase of effective length upon electronic excitation. As stated before, full details are available from Haddad *et al.* (2013).

The direct astronomical relevance of this study is limited. In principle, the data provide for a first time the necessary tools to search for $^{13}\text{C}_3$ in translucent clouds, but given the relative low ^{13}C natural abundance an unambiguous identification is currently out of reach, despite the recent improvements realized for regular $^{12}\text{C}_3$ (Schmidt *et al.* 2013).

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