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Modeling of N_2^+ and $^{14}N^{15}N^+$ fluorescence spectrum in comets

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1. Introduction

C/2016 R2 (PanSTARRS) was a surprising comet. Detected on September 7, 2016 by Pan-STARRS it showed an unusual composition when it became a bright comet at the end of 2017 and the beginning of 2018. It developed a coma at large (~6 au) heliocentric distance and observations showed that it had a highly unusual composition: no water molecules (or OH radical) could be detected, and the abundances of the usual radicals (CN, C_2, C_3) were unusually low, with a surprising coma composition dominated by CO, CO_2 and N_2 molecules with bright CO^+ and N_2^+ emission lines in the visible range. A high CO production rate of about 10^{29} molecules s^{-1} was measured (Biver et al. 2018; Wierzchos & Womack 2018) as well as a high CO_2 production rate (CO_2/CO=1.1 from Opitom et al. 2019), and a high ratio N_2/CO varying between 0.06 and 0.09 (Biver et al. 2018; Cochran & McKay 2018a,b; Opitom et al. 2019; Venkataramani et al. 2020).

The detection of such bright N_2^+ emission lines in this comet highlighted the necessity of a good modeling of the N_2^+ fluorescence spectrum in comets. The high-quality spectra published by Opitom et al. (2019) provided a good opportunity to test such a model. This model also permits to compute the fluorescence spectrum of the $^{14}N^{15}N^+$ species, leading to the possibility of future measurements of the $^{14}N/^{15}N$ isotopic ratio in the N_2 molecules, one of the main constituant of the solar nebula.

2. Observations

The spectra used for this work have been obtained with the UVES spectrograph mounted on the ESO 8.2 m UT2 telescope of the VLT. Three different observing nights have been used, corresponding to February 11, 13 and 14, 2018. One single exposure of 4800 s of integration time was obtained during each night and we used a 0.44" wide slit, providing a resolving power R~80,000. The slit length was 8" corresponding to about 14,500 km at the distance of the comet (geocentric distance of 2.4 au). The average heliocentric distance was 2.76 au. Opitom et al. (2019) describe in more details the data processing.

From the 2D spectra having a spatial extension of 30 rows, each of them corresponding to a different cometocentric distance, we extracted different 1D spectra for each night. These spectra were then averaged for similar cometocentric distances allowing a detailed comparison of these spectra at different cometocentric distances, the furthest one corresponding to 2x4 rows at the two extremities of the slit (i.e. at a cometocentric distance varying between 4800 and 6600 km).

3. Modeling the N_2^+ fluorescence spectrum

We developed a new fluorescence model for modeling our observational spectra. The transition involved in this spectrum is the first negative group, i.e. the $B^2\Sigma_u^+$ -> $X^{2+}\Sigma_g^+$ electronic transition with the (0,0) bandhead appearing near 3914 Å. We considered the first three vibrational levels (v = 0; 1; 2) for both $X^{2+}\Sigma_g^+$ and $B^2\Sigma_u^+$ state, each of them with all the rotational levels from N = 0 to 40.

N_2^+ having no permanent dipole moment, the pure rotational and vibrational transitions are forbidden (or have a very low probability, through quadrupolar transitions, not taken into account in our model). For that reason it takes a long time for this species to reach its fluorescence equilibrium because it needs a few tens of absorption / emission cycles between the $X^{2+}\Sigma_g^+$ and $B^2\Sigma_u^+$ states to reach this equilibrium. A comparison of the spectrum obtained on the nucleus with the one obtained at the edges of the slit revealed clear differences due to different rotational relative populations. For that reason we decided to model the N_2^+ fluorescence spectrum with a Monte-Carlo simulation. Such a computational method allows to compute a spectrum at different times from an initial relative population distribution. Our model starts with a Boltzmann relative population distribution of 80 K (representing an estimate of the kinetic temperature in the inner coma) and uses 10,000 s of evolution time.

We managed to explain satisfactorily the observed N_2^+ emission spectrum. Fig. 1 presents a close up view around the (0,0) bandhead. This work, presented in more details in Rousselot et al. (2022) also allowed to compute accurate fluorescence efficiencies.

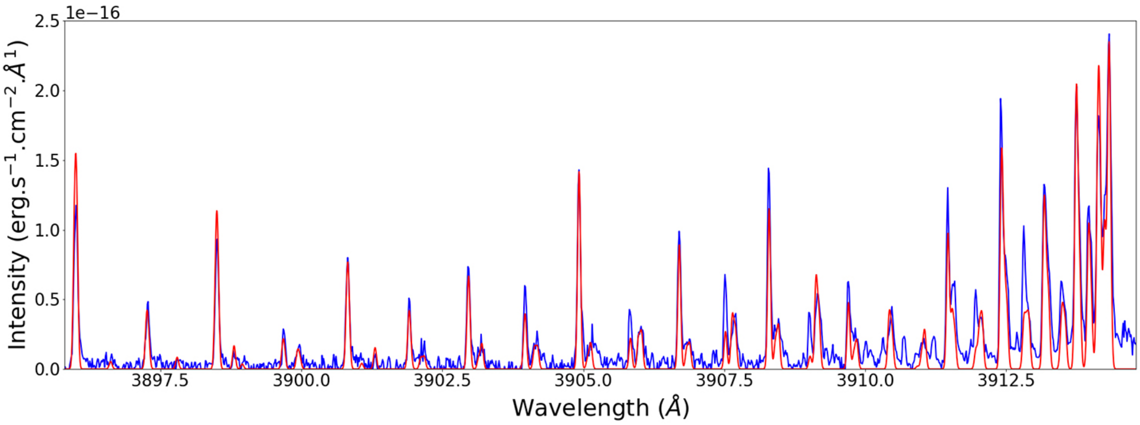

Figure 1: Comparison of the observed VLT UVES spectrum of comet C/2016 R2 (blue) obtained at the ends of the slit with our N_2^+ model (red).

4. $^{14}N^{15}N^+$ fluorescence spectrum

Our modeling of the N_2^+ fluorescence spectrum can be used to compute the $^{14}N^{15}N^+$ fluorescence spectrum, leading to the possibility of measuring the $^{14}N/^{15}N$ isotopic ratio in N_2 molecules. We will present such a spectrum as well as a search for this isotopologue in the C/2016 R2 spectra. Such comets are rare but future observations will reveal other comets similar in composition to C/2016 R2. With future observing facilities now under construction (such as the ESO ELT) $^{14}N/^{15}N$ measurements for N_2 molecules will probably become possible, leading to new constraints on this isotopic ratio.

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