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# Isomerism Effects in the Collisional Excitation of Cyanoacetylene by Molecular Hydrogen

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## INTRODUCTION

The carbon rich circumstellar envelope (IRC+10216) and starless and prestellar cores of the Taurus Molecular Cloud (TMC) are among the richest astronomical sources of carbon chain molecules. TMC-1 is distinguished by its high abundance of  $C_2H_2$  and its derivatives which are the precursors of nitriles through ion-molecule reactions. Nitriles likely preceded the origin of life on Earth and they are present with a relatively large abundance in planet formation regions. One group of nitriles (the cyanopolyynes) has particular astrophysical interests. For instance, (i)  $HC_3N$  is a good gas tracer, thanks to its low rotational constant and large dipole moment, (ii) based on  $HC_3N$  and  $HC_5N$ , chemical model predictions unveiled a crucial part of the IRAS 16293-2422 history. In star forming regions, the abundance ratio of isomers are useful tool to probe the physical and chemical conditions. Therefore, determining the abundance ratios between  $HC_3N$  and its isomers ( $HC_2NC$  and  $HNC_3$ ) may reveal important information in media where they were observed (TMC-1 and L1544). Fully exploiting the spectral emission lines of these isomers and deriving their abundance using a non-LTE approach require the prior computation of their collisional rate coefficients.

## METHODS

\* From the 4D PESs, we derived inelastic cross sections for the 31 low-lying rotational levels of  $HC_3N^1$ ,  $HC_2NC$  and  $HNC_3$  using the close-coupling method<sup>2</sup> as implemented in the MOLS-CAT code<sup>3</sup>.

\* From the so-computed inelastic cross sections, we derive the corresponding rotational rate coefficients for temperatures ranging up to 80 K.

\* The radiative transfer calculations were done using the RADEX computer code<sup>4</sup>.

## RESULTS AND DISCUSSIONS

Fig. 1 highlights the importance of computing rate coefficients specific to each isomer as the difference among two sets of data can reach an order of magnitude.

Fig. 2 shows the excitation temperature ( $T_{ex}$ ) varies from  $\sim 2.73$  K (which corresponds to the cosmic background temperature,  $T_{CMB}$ ) to 10 and 50 K for the top panels and bottom panels, respectively. In fact, at low (high)  $H_2$  density, radiative (collisional) processes outweigh leading to  $T_{ex} = T_{CMB}$  ( $T_{ex} = T_k$ , i.e. LTE is reached).

Fig. 3 depicts the dependence of the brightness temperature of the isomers on the  $H_2$  density. Large differences are observed mainly in the intermediary region ( $10^4 \leq n \leq 10^6 \text{ cm}^{-3}$ ) where both radiative and collisional processes are likely in competition. These differences point out the need of computing rate coefficients of each isomer to accurately determine their abundance.

Fig. 4, shows the line intensity (which is proportional to  $T_B$ ) ratios of the isomers. At high  $H_2$  density ( $n \geq 10^6 \text{ cm}^{-3}$ ), towards LTE where radiative processes are dominant, the column density ratios are not equal to unity due to the difference between the dipole moments of the  $HC_3N$  isomers.

## RATE COEFFICIENTS

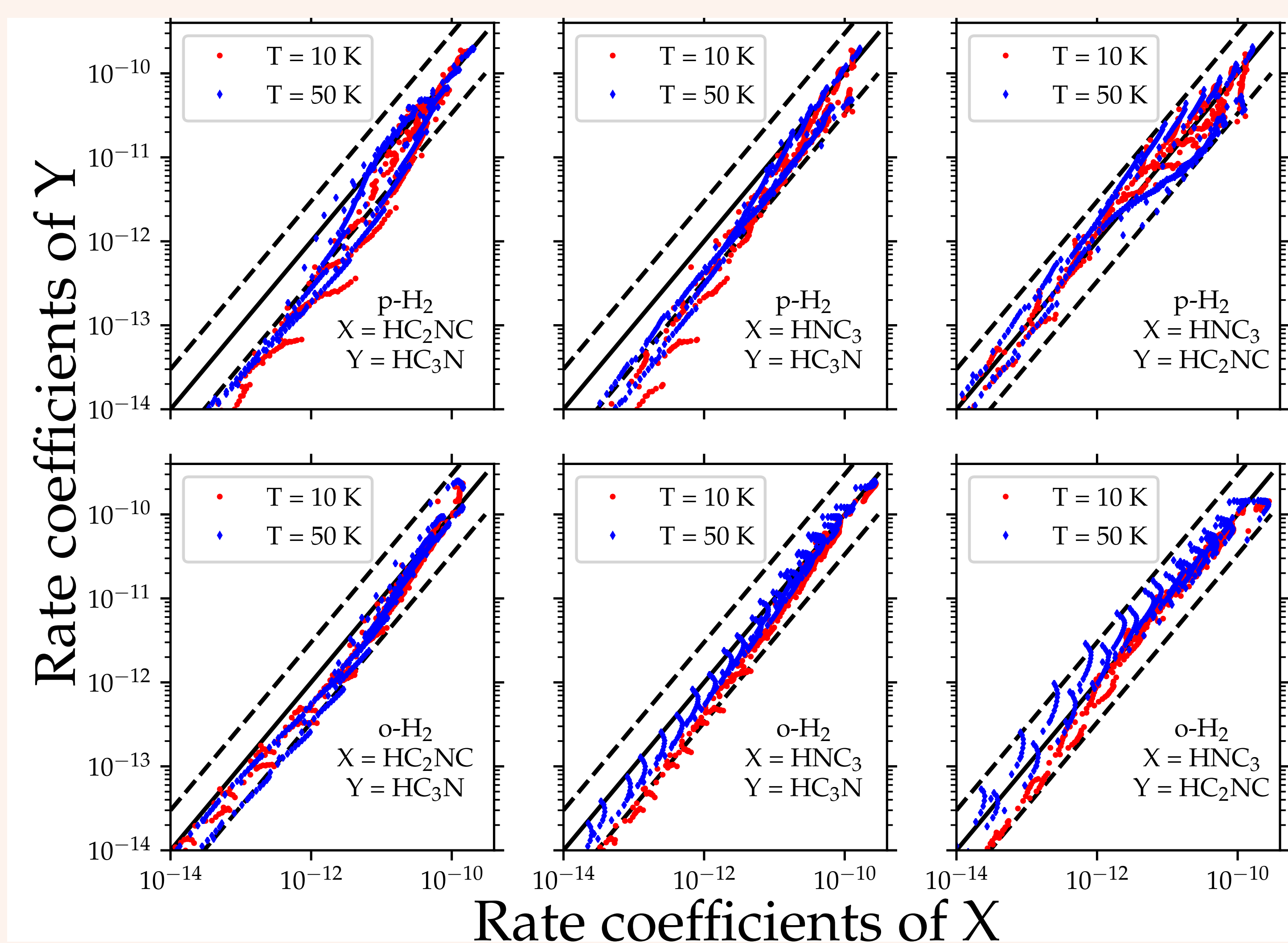


Fig. 1: Comparison of the rate coefficients of the  $HC_3N$  isomers at  $T = 10$  K and 50 K. The collisions treated in the p- $H_2$  (o- $H_2$ ) ladder are represented in the top (bottom) panels. In each panel, the solid line stands for  $y = x$  and the dashed lines wrap the rate coefficients which differ by less than a factor of three.

## EXCITATION TEMPERATURE

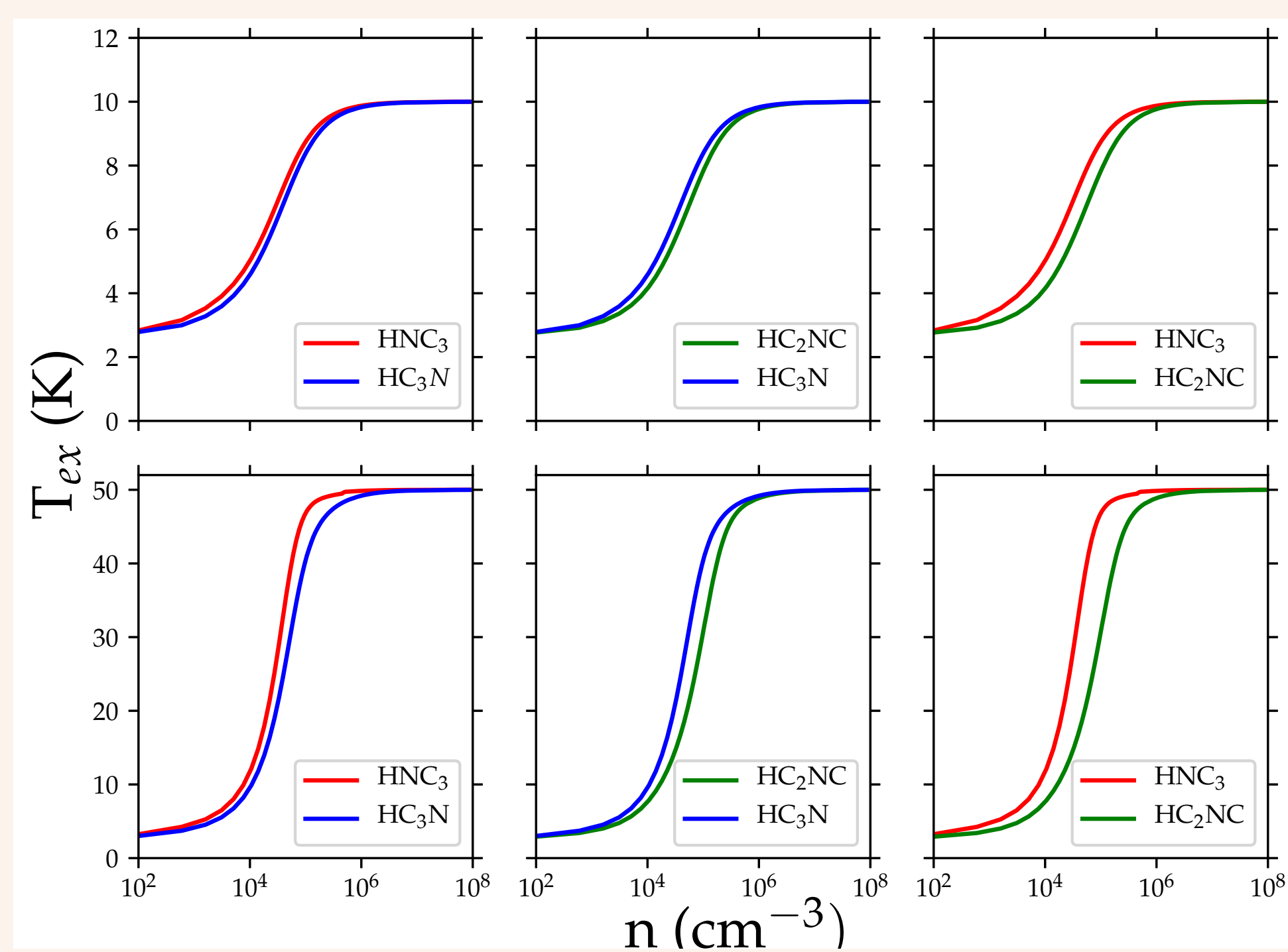


Fig. 2: Excitation temperature for the  $j_1 = 8 - 7$  line of  $HC_3N$ ,  $HC_2NC$  and  $HNC_3$  calculated for temperatures  $T_k = 10$  K (top panels) and 50 K (bottom panels) and a fixed column density of  $10^{13} \text{ cm}^{-2}$ , for all isomers.

## BRIGHTNESS TEMPERATURE

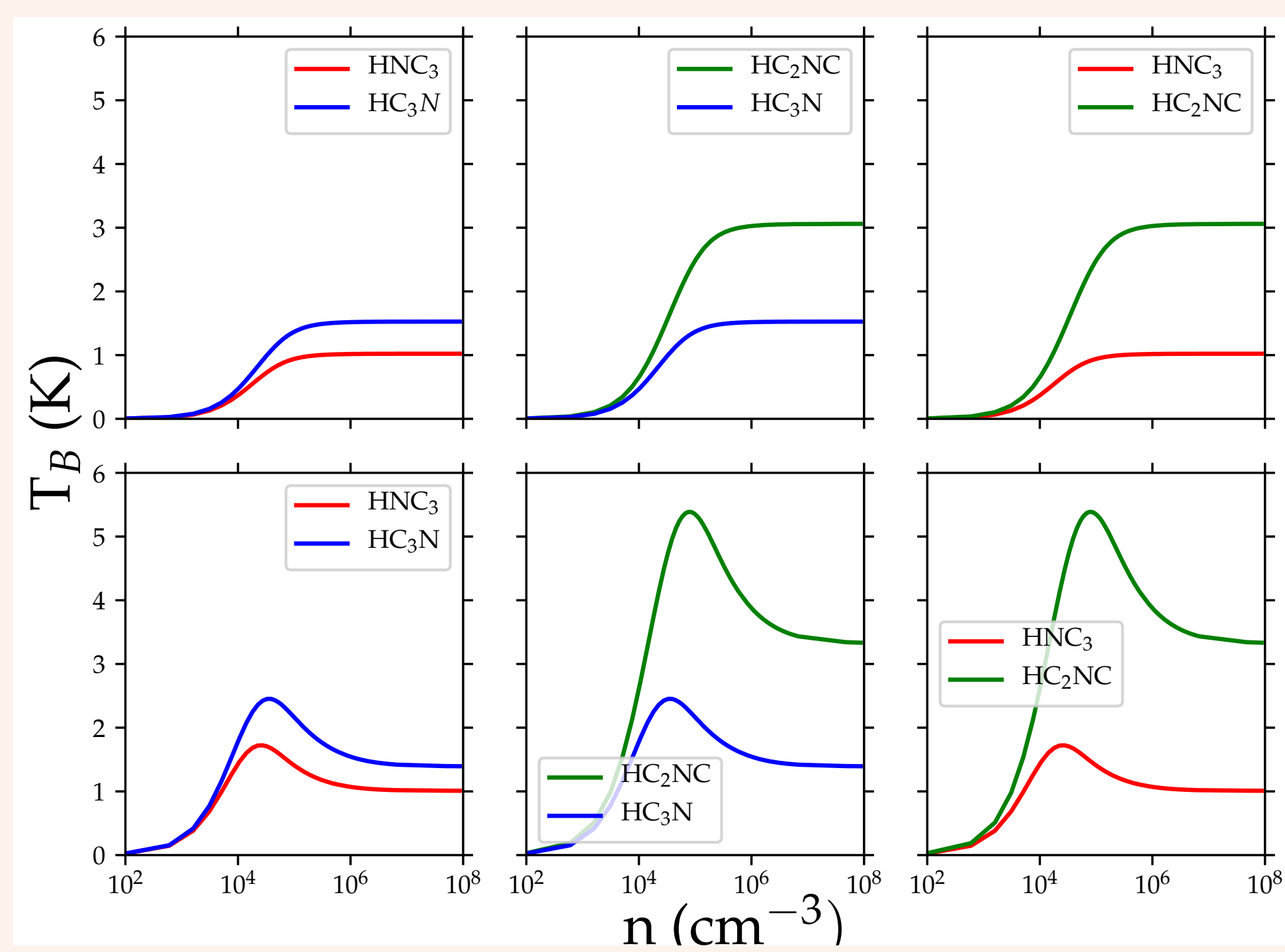


Fig. 3: Brightness temperature for the  $j_1 = 8 - 7$  line of  $HC_3N$ ,  $HC_2NC$  and  $HNC_3$  calculated for temperatures of  $T_k = 10$  K (top panels) and 50 K (bottom panels) and a fixed column density of  $10^{13} \text{ cm}^{-2}$ , for all isomers.

## LINE INTENSITY RATIO

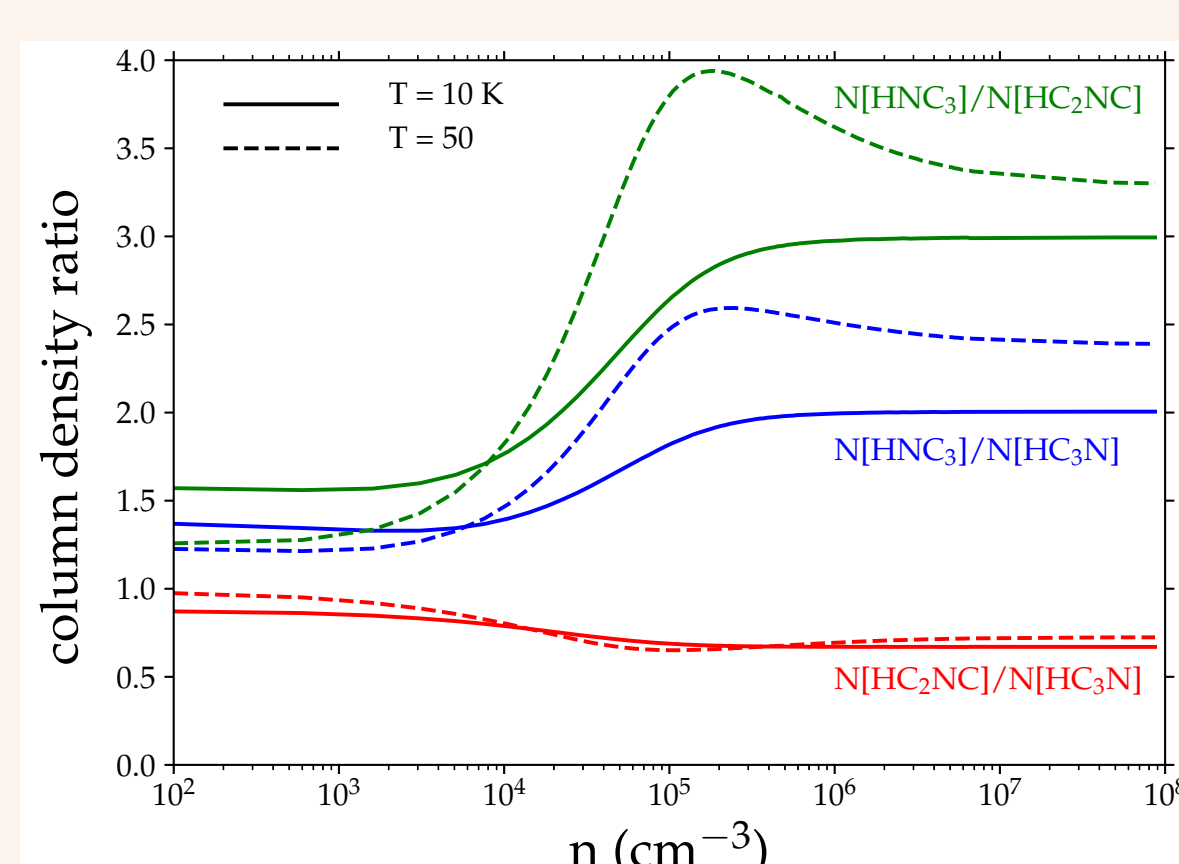


Fig. 4: Comparison of line intensities.

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