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► **To cite this version:**

Cheikh T Bop, E. Quintas-Sánchez, R. Dawes, François Lique, A Faure. Isomerism Effects in the Collisional Excitation of Cyanoacetylene by Molecular Hydrogen. European Astronomical Society Annual Meeting, Jun 2020, Leiden, Netherlands. . hal-04072202

HAL Id: hal-04072202

<https://hal.science/hal-04072202>

Submitted on 17 Apr 2023

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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 method² as implemented in the MOLS-CAT code³.

★ 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 code⁴.

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 ~ 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

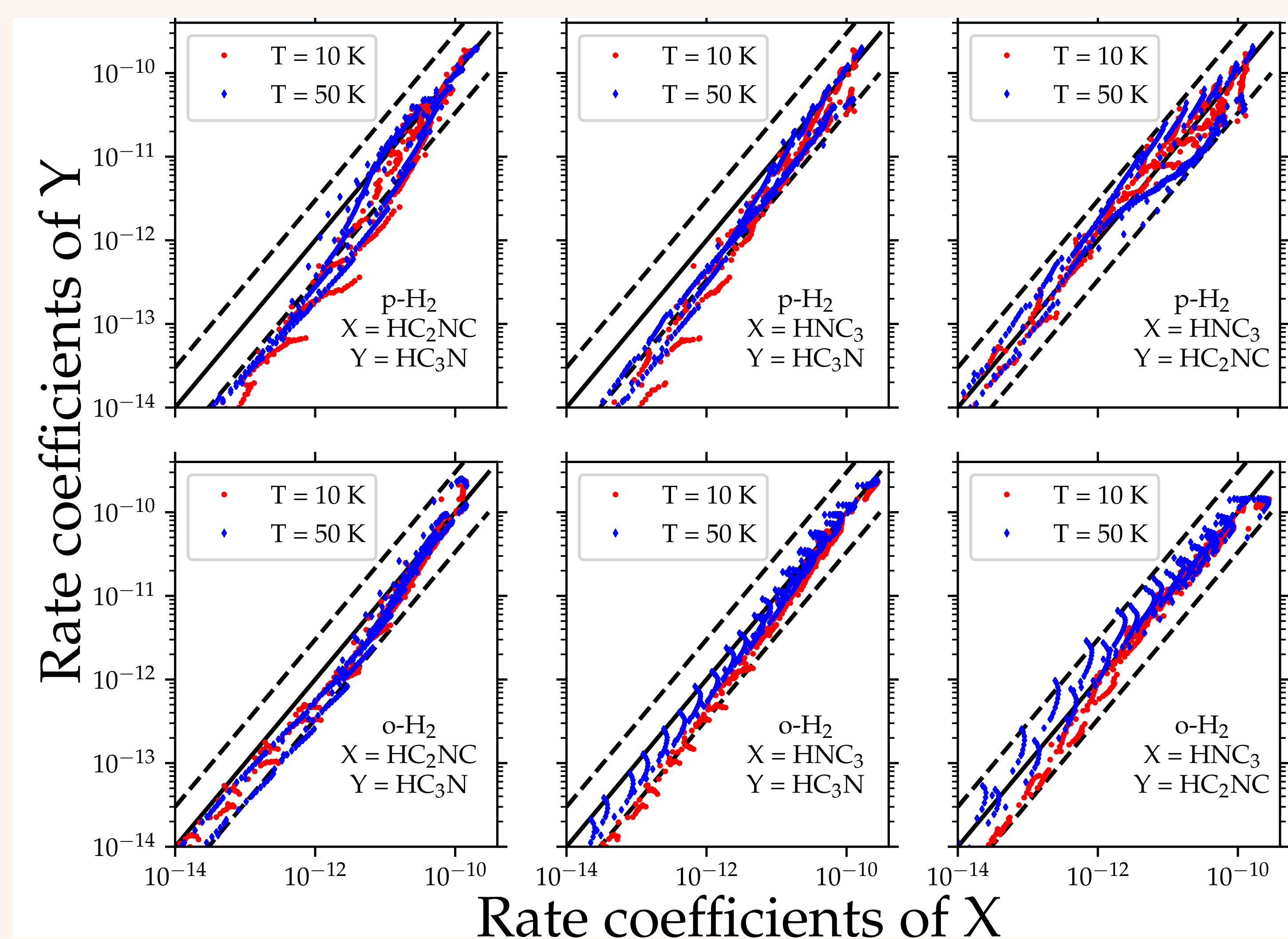


Fig. 1: Comparison of the rate coefficients of the HC_3N isomers at $T = 10$ K and 50 K. The collisions treated in the p- H_2 (o- H_2) ladder are represented in the top (bottom) panels. In each panel, the solid line stands for $y = x$ and the dashed lines wrap the rate coefficients which differ by less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

EXCITATION TEMPERATURE

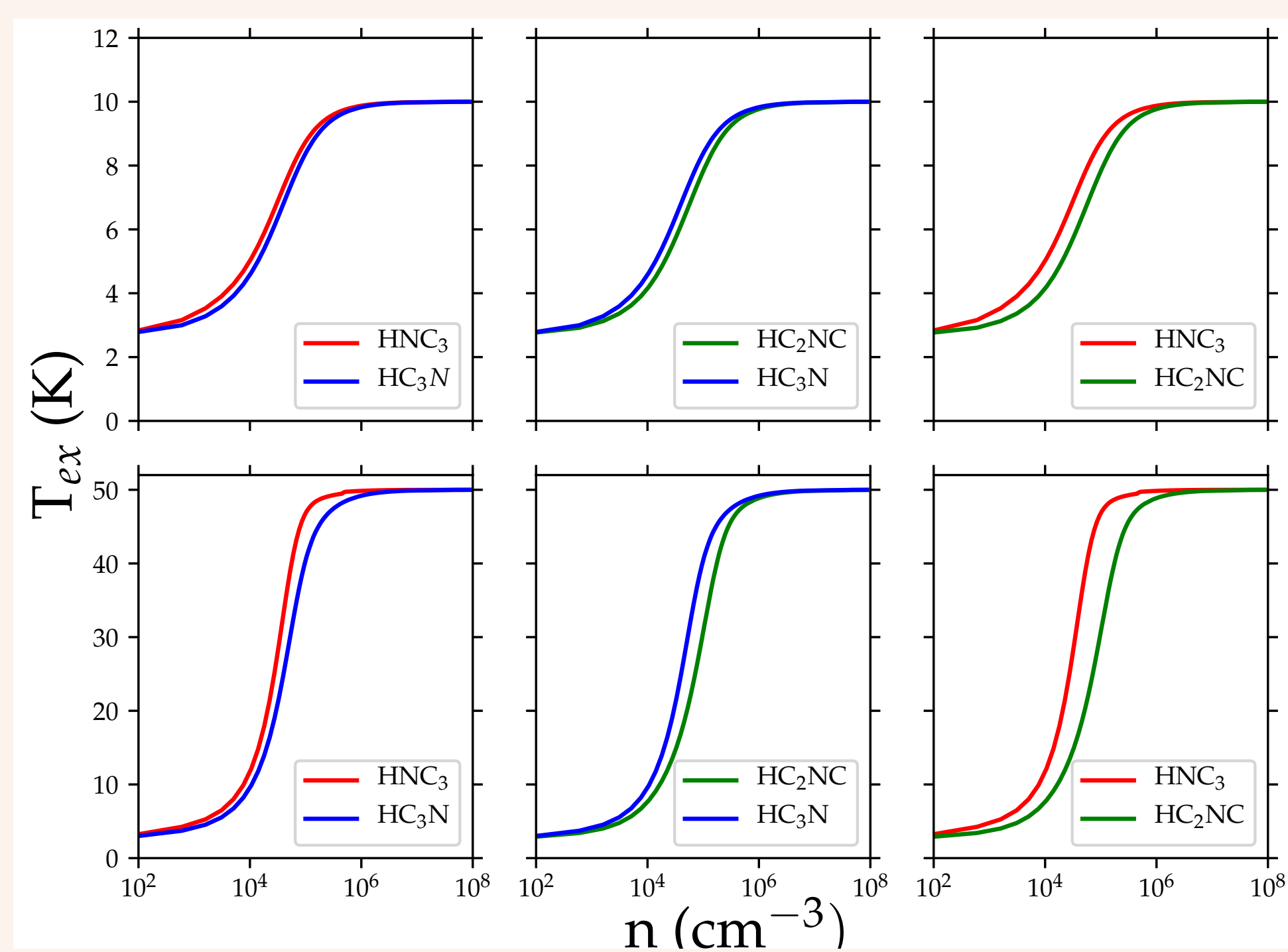


Fig. 2: Excitation temperature for the $j_1 = 8 - 7$ line of HC_3N , HC_2NC and HNC_3 calculated for temperatures $T_k = 10$ K (top panels) and 50 K (bottom panels) and a fixed column density of 10^{13} cm^{-2} , for all isomers.

BRIGHTNESS TEMPERATURE

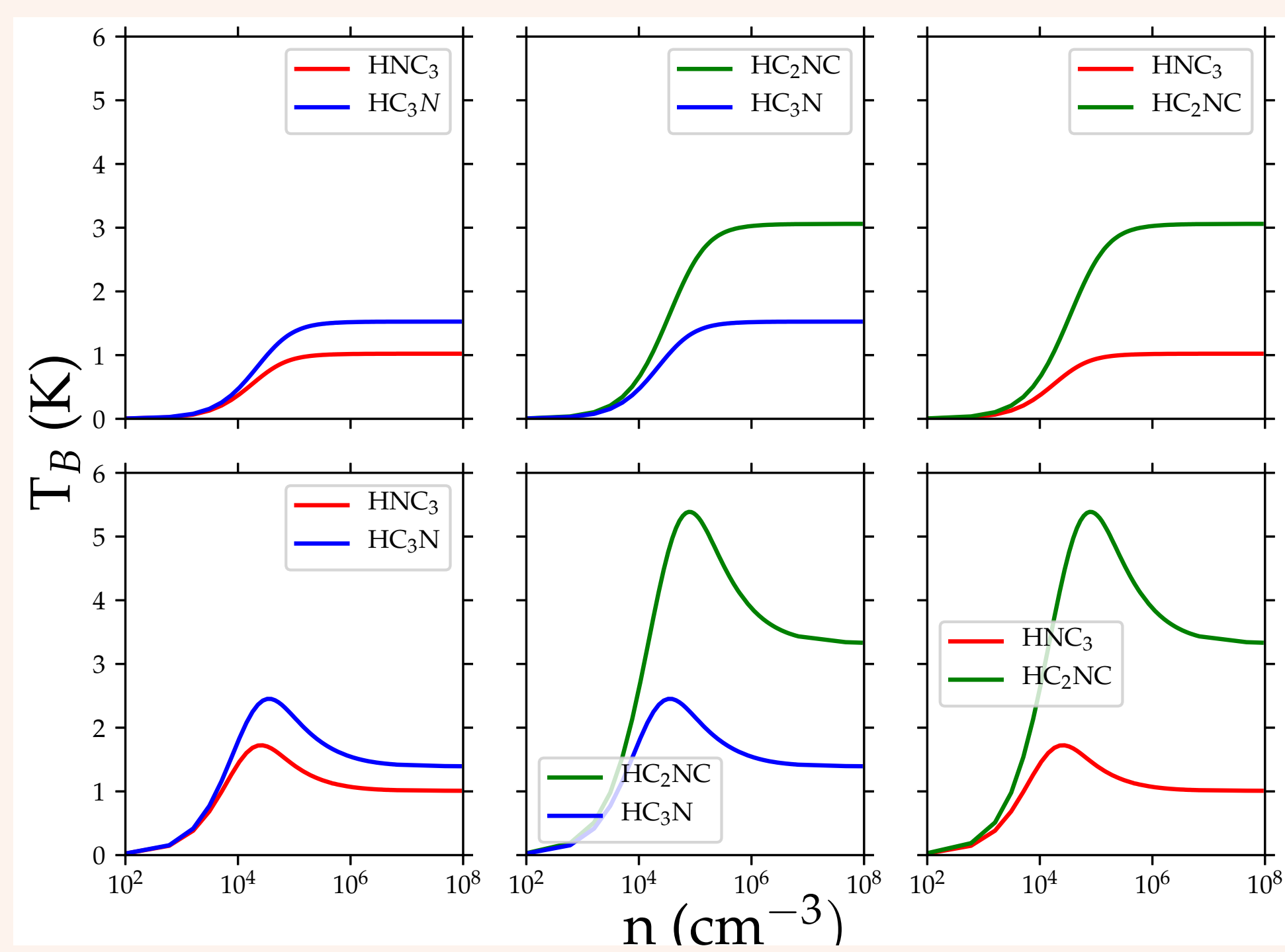


Fig. 3: Brightness temperature for the $j_1 = 8 - 7$ line of HC_3N , HC_2NC and HNC_3 calculated for temperatures of $T_k = 10$ K (top panels) and 50 K (bottom panels) and a fixed column density of 10^{13} cm^{-2} , for all isomers.

LINE INTENSITY RATIO

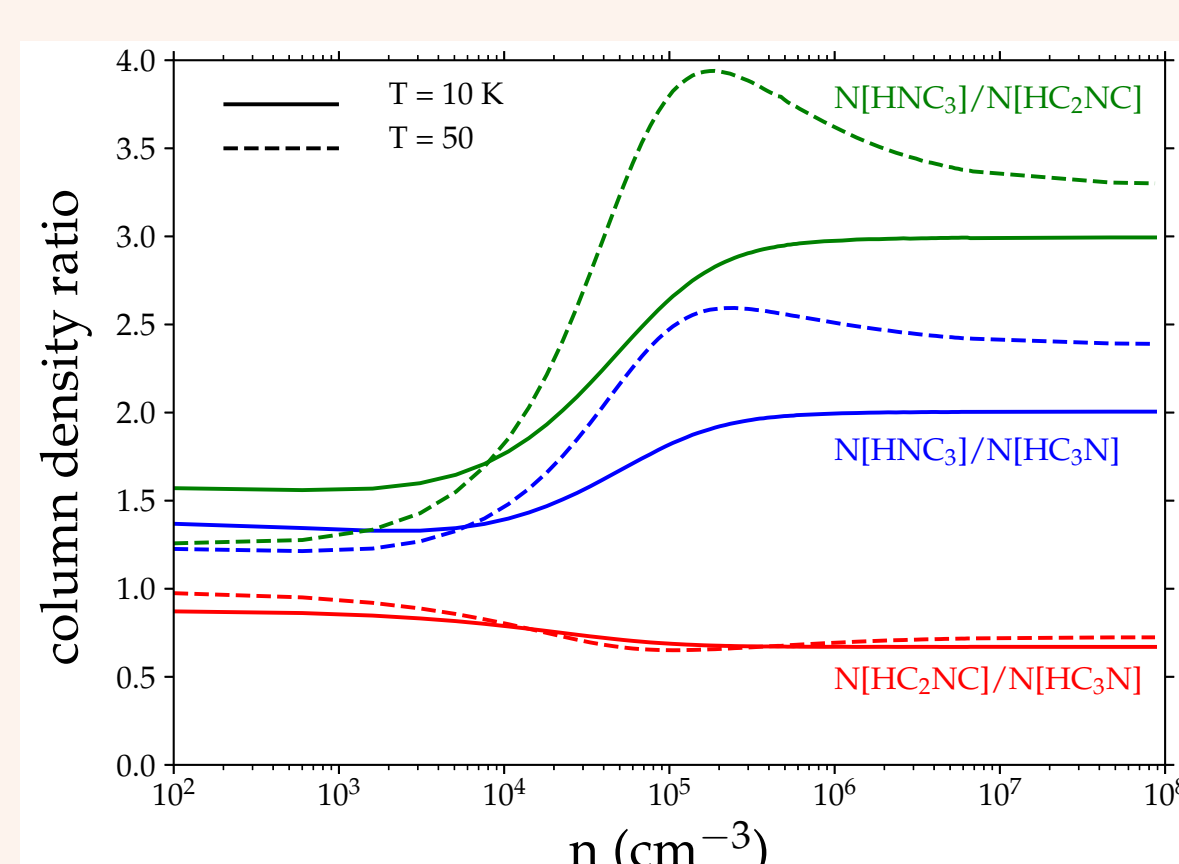


Fig. 4: Comparison of line intensities.

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