

# Modelling the emission of HNCO towards IRAS16293-2422 using a new set of collisional coefficients

Hernández-Gómez A.<sup>1,2</sup>, Sahnoun E.<sup>3</sup>, Caux E.<sup>2</sup>, Wiesenfeld L.<sup>4</sup>,  
Loinard L.<sup>1</sup>, Bottinelli S.<sup>2</sup> and Hammami K.<sup>3</sup>

<sup>1</sup>Instituto de Radioastronomía y Astrofísica, Universidad Nacional Autónoma de México,  
Morelia 58089, Mexico

<sup>2</sup>IRAP, Université de Toulouse, CNRS, UPS, CNES, Toulouse, France

<sup>3</sup>Université de Tunis El Manar, Tunisia

<sup>4</sup>Université Grenoble Alpes, CNRS, IPAG, F-38000 Grenoble, France

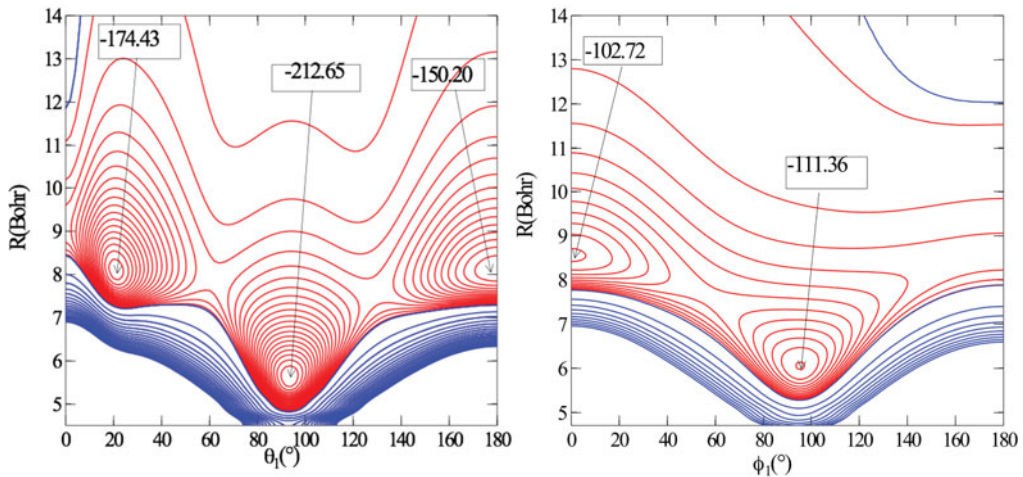
**Abstract.** Isocyanic acid (HNCO) is a simple molecule containing the four main atoms essential for life and can be considered as a prebiotic molecule. To model the HNCO emission in the IRAS16293-2422 class 0 low-mass protostar, we used a new set of HNCO collisional coefficients with ortho-H<sub>2</sub> and para-H<sub>2</sub>, computed from a set of rotational excitation quenching rates between HNCO and H<sub>2</sub> based on a novel potential energy surface for the rigid molecules interactions. We present here the HNCO Potential Energy Surface used to compute this new set of collisional coefficients and the result of the IRAS16293-2422 HNCO spectrum modelling using them.

**Keywords.** Protostars, molecular emission, non-LTE modelling.

---

## 1. Introduction

Isocyanic acid (HNCO) has been observed in different physical environments in the interstellar medium and in external galaxies. As a simple molecule containing the four main atoms essential for life as we know it, isocyanic acid can be considered as a prebiotic molecule. Modelling the emission of HNCO in star-forming regions is therefore of prime importance. IRAS16293-2422, the Class 0 low-mass protostar with the richest line spectrum is the template source for astrochemistry and has been the subject of many spectroscopic studies. We have in hands the broadest spectral surveys conducted towards this source with single-dish instruments, the TIMASSS survey (Caux *et al.* 2011) (with IRAM, JCMT and APEX in the 80 – 500 GHz range), and the CHESS survey (Ceccarelli *et al.* 2010) (in the 0.5 – 1 THz range with the HIFI instrument onboard the ESA Herschel Observatory). Because in star-forming environments the HNCO emission is not always at LTE, collisional coefficients are needed to use non-LTE transfer codes as RADEX to predict the line emission. The HNCO-He system has been calculated by Green (1996), but the published collisional coefficients fail to reproduce the observed emission in IRAS16293-2422. To model the HNCO lines observed in this source, we used new collisional coefficients of HNCO with ortho-H<sub>2</sub> and para-H<sub>2</sub>, computed from a set of rotational excitation quenching rates between HNCO and H<sub>2</sub> based on a novel potential energy surface for the rigid molecules interactions (Sahnoun *et al.* 2017; in prep.).



**Figure 1.** *Left.* Planar configuration with  $\text{H}_2$  along the intermolecular axis, and on the side opposite to  $\text{H}(\text{NCO})$  ( $\phi = 180^\circ$ ). Dependence on the angle  $\theta$  in the  $\text{HNCO}$  plane. PES extrema in  $\text{cm}^{-1}$ . *Right.* Planar configuration with  $\text{H}_2$  perpendicular to the intermolecular axis. Dependence on the angle  $\phi$  perpendicular to the  $\text{HNCO}$  plane.  $\theta = 0^\circ$ . PES extrema in  $\text{cm}^{-1}$ .

## 2. Potential energy surface (PES) and scattering

The interaction of  $\text{HNCO}$  and  $\text{H}_2$  has been computed for both molecules taken as rigid.  $\text{HNCO}$  is planar, with the angles  $\langle \text{HNC} \rangle = 128.0^\circ$  and  $\langle \text{CNO} \rangle = 170.0^\circ$ . It is thus an asymmetric rotor. Interaction energies were computed in the supermolecule approach, with the help of the MOLPRO ab initio suite. We made use of the CCSD(T)-F12 method, with the moderately large basis set augcc-pAVDZ/AVTZ. Basis set superposition error has been corrected. The potential is highly anisotropic and fitting procedures required up to 2500 points per distance. A view of the PES is given in Figure 1, with attractive part in red and repulsive part in blue. Subsequent fits in terms of hyperspherical functions lead to 509 terms in the expansion, with angular terms up to  $l = 15$ . The complex structure in the PES reveals itself by the multiple extrema.

Scattering computations were performed from threshold to  $E_{\text{tot}} = 500 \text{ cm}^{-1}$  (for para- $\text{H}_2$ ). For para- $\text{H}_2$  (basis set  $J = 0, 2$ ), computations were performed at the coupled-channel (CC) level up to  $20 \text{ cm}^{-1}$  and at the coupled states (CS) level above. For ortho- $\text{H}_2$ , computations were performed at the CS level. Rotational basis for  $\text{HNCO}$  is up to  $J = 21$ , maximum rotational energy is  $600 \text{ cm}^{-1}$ . Examples of cross-sections are given in Figure 2. The computations cover all rotational  $\text{HNCO}$  levels up to  $144 \text{ cm}^{-1}$ , and  $T \leq 205 \text{ K}$ , still an incomplete set for a full spectral simulation.

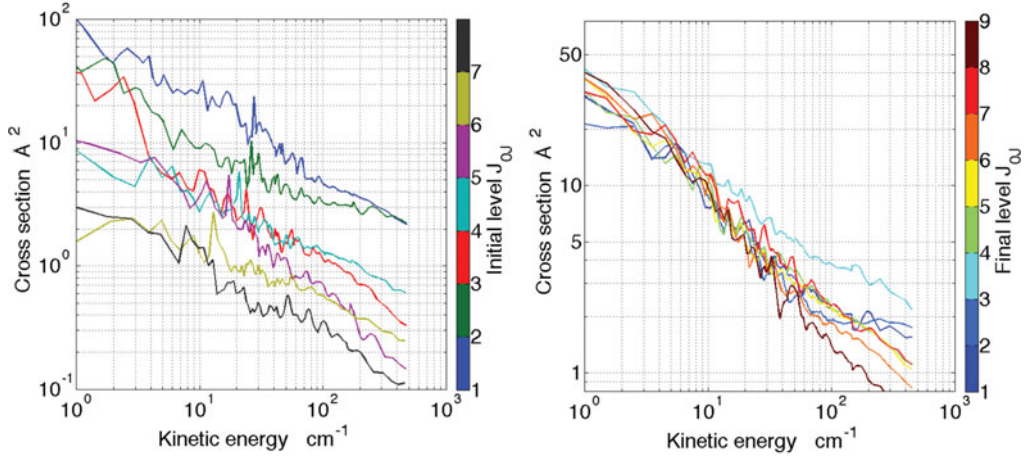
## 3. IRAS16293-2422 HNCO model

To model the  $\text{HNCO}$  emission of IRAS16293-2422, we used the CASSIS<sup>†</sup> code with RADEX (van der Tak *et al.* 2007) for a two-component model, one originating from the warm internal part of the envelope and one originating from the cold external part of the envelope. We performed a MCMC minimisation computing synthetic spectra with 3 free parameters for each component (size,  $T_{\text{kin}}$ , FWHM). The best fitted physical parameters are shown in Table 1.

<sup>†</sup> <http://cassis.irap.omp.eu>

**Table 1.** Best fitted physical parameters obtained from the CASSIS-RADEX MCMC minimisation.

Component	$N(\text{HNC0})$ ( $\text{cm}^{-2}$ )	$T_{kin}$ (K)	FWHM ( $\text{km s}^{-1}$ )	$V_{LSR}$ ( $\text{km s}^{-1}$ )	Size ( $''$ )	$n(\text{H}_2)$ ( $\text{cm}^{-3}$ )	$X$
Inner envelope	$(6.3 \pm 0.9) \times 10^{14}$	$75.0 \pm 3.0$	$5.5 \pm 0.1$	$3.7 \pm 0.1$	$3.5 \pm 0.2$	$1.0 \times 10^8$	$1.0 \times 10^{-9}$
Outer envelope	$(6.2 \pm 0.9) \times 10^{12}$	$14.0 \pm 1.0$	$1.3 \pm 0.1$	$4.1 \pm 0.1$	60.0	$4.0 \times 10^5$	$1.4 \times 10^{-10}$

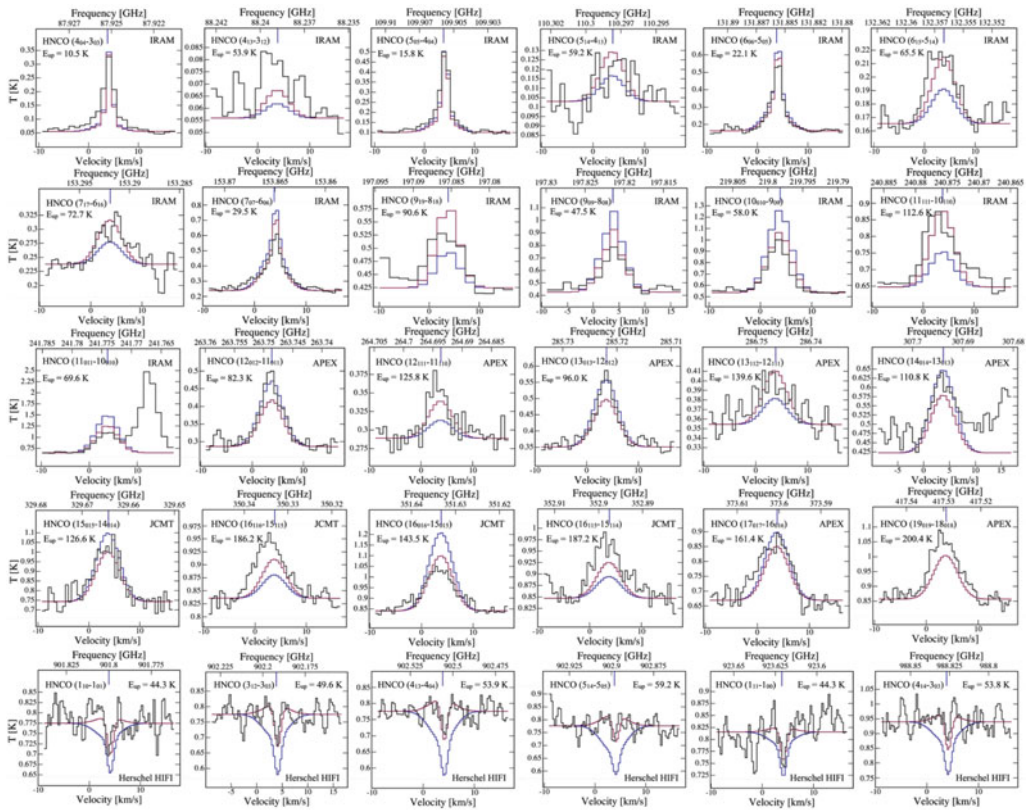
**Figure 2.** **Left.** Rotational quenching cross sections HNC0 – ortho-H<sub>2</sub> ( $J = 1$ ). Initial state as shown. Final state, ground state  $0_{00}$ . **Right.** Rotational quenching cross sections HNC0 – ortho-H<sub>2</sub> ( $J = 1$ ). Initial state  $1_{01}$ . Final state as shown.

We assumed a H<sub>2</sub> ortho/para ratio of 3 for both components, but we checked that smaller values do not change the results. We could not find such a good agreement with the old collisional coefficients with He from Green (1996).

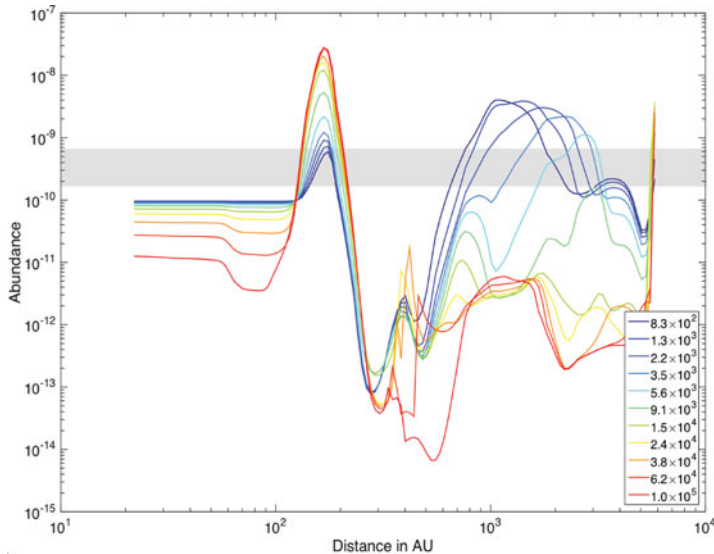
## 4. Results

In Figure 3 we show the spectra computed with the physical parameters obtained with our model and we compare them directly with the observations from IRAM, APEX, JCMT and HIFI. We are able to reproduce most of the line profiles at all frequencies. In particular, the absorption features observed with HIFI are much better reproduced with our new computed collisional coefficients. In order to understand the distribution of HNC0 along the envelope of IRAS16293, we have estimated the radial abundance profile of HNC0 using the Nautilus chemical model (Ruard *et al.* 2016) and the static physical structure computed by Crimier *et al.* (2010). The obtained abundances are shown as a grey rectangle in Figure 4. We note that the abundance corresponding to the obtained sizes in our model for both inner and outer envelopes are consistent with the Nautilus model.

To have a better idea of the structure of IRAS16293-2422 and to refine the results we have obtained, we plan to use the LIME 3D radiative transfer code (Brinch & Hogerheijde) to model the line emission using a three-dimensional structure. To achieve this, we will use GASS (Quénard *et al.* 2017), which will allow us to define a physical 3D structure with several components to be used as input for LIME.



**Figure 3.** Observed HNC lines (black) and modelled ones with new collisional coefficients (red) and Green collisional coefficient (blue). HNC line frequencies are from CDMS (Müller *et al.* 2001).



**Figure 4.** HNC abundance profiles computed with Nautilus.

**References**

- Brinch, C. & Hogerheijde, M. R. 2010, *A&A*, 523, A25
- Caux, E., Kahane, C., Castets, A., *et al.* 2011, *A&A*, 532, A23
- Ceccarelli, C., Bacmann, A., Boogert, A., *et al.* 2010, *A&A*, 521, L22
- Crimier, N., Ceccarelli, C., Maret, S., *et al.* 2010, *A&A*, 519, A65
- Green 1986, NASA Tech. Memo. TM 87791
- Müller, H. S. P., Thorwirth, S., Roth, D. A., & Winnewisser, G. 2001, *A&A*, 370, L49
- Quénard, D., Bottinelli, S., & Caux, E., 2017, *MNRAS*, 468, 685
- Rnaud, M., Wakelam, V., & Hersant, F., 2016, *MNRAS*, 459, 3756
- Sahnoun *et al.* 2017, in preparation
- van der Tak, F. F. S., Black, J. H., Schöier, F. L., Jansen, D. J., & van Dishoeck, E. F., 2007, *A&A*, 468, 627