Theoretical study of collisions of NH by H_2 in the interstellar medium

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Introduction

- Since the last decades, the nitrogen abundance is still subject to debate [1]
- Accurate models of NH abundance is of great interest as NH is involved in many reactions of chemical networks [2]
- H_2 is the dominant collider in the ISM
- Previous theoretical studies focused on NH colliding with He [3, 4] and Ar [5]
- There is no collisional data for the NH-H_2 system

This work: Calculations of fine structure resolved excitation cross sections and rate coefficients for the NH-H_2 collisional complex

Computational methodology

Potential energy surface (PES)

- New 4D potential energy surface
- CCSD(T)-F12 approach
- aVTZ atomic basis set using the MOLPRO code [7]
- PES expressed in terms of bispherical harmonics

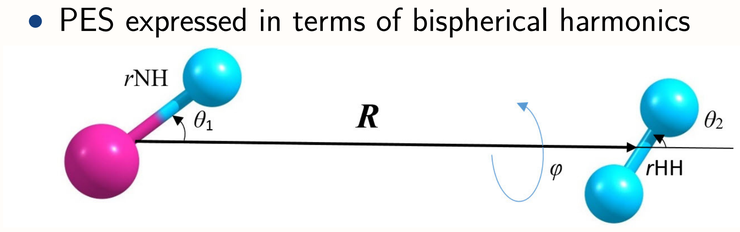


Figure 1: Representation of the NH-H_2 complex in Jacobi coordinates

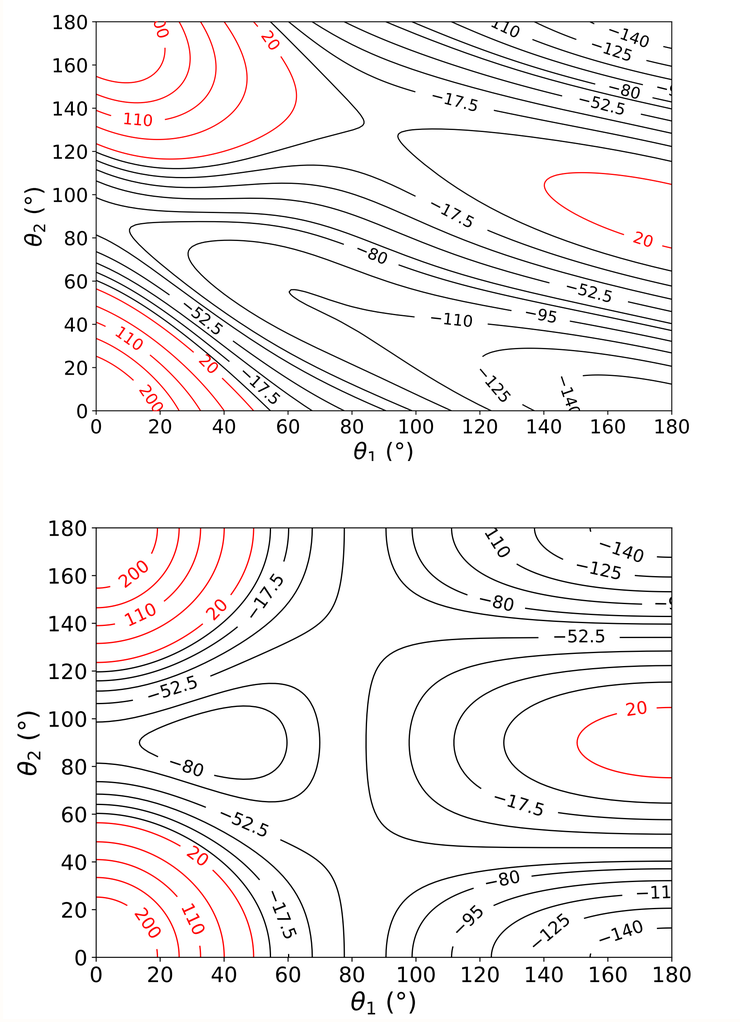


Figure 2: Contour plots of the PES (in cm^{-1}) for $\varphi = 0°$ (upper panel) and $\varphi = 90°$ (lower panel) at R = 3.33Å, corresponding to the distance where the global minimum is found

Scattering calculations

Fine structure of NH in its electronic ground state is due to spin-rotation coupling. Energy levels can be written in the intermediate coupling scheme.

- Collisions of NH are studied with both *ortho*-H_2 and *para*-H_2 collisional partners in their j_2 rotational ground state
- Close-coupling approach using the HIBRIDON code [8]
- Extraction of fine structure cross sections and rate coefficients

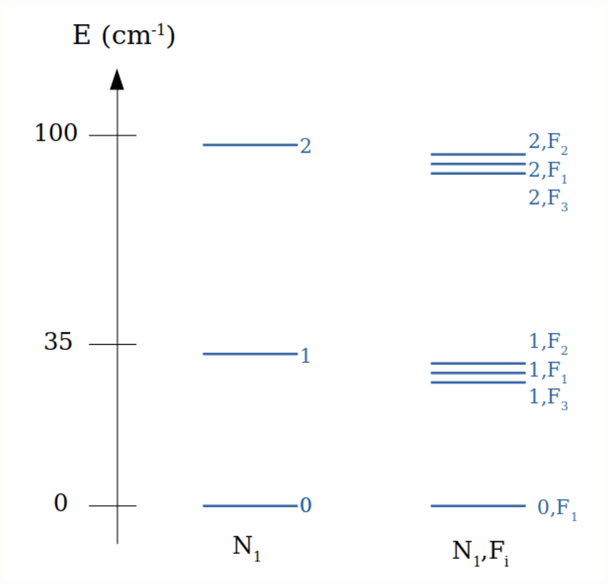


Figure 3: Rotational and fine structure energy levels of NH

Results

Fine structure resolved cross sections

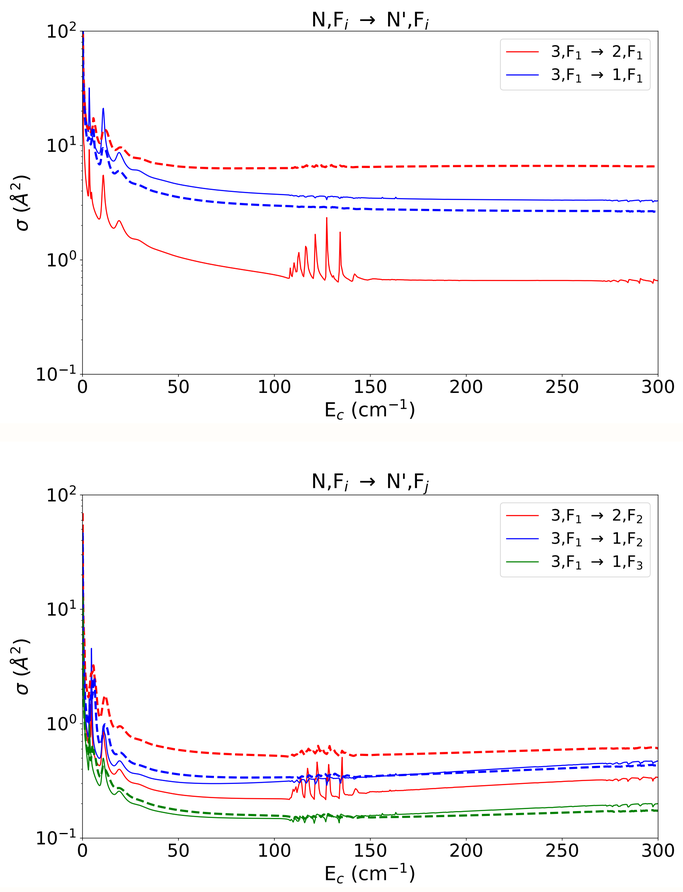
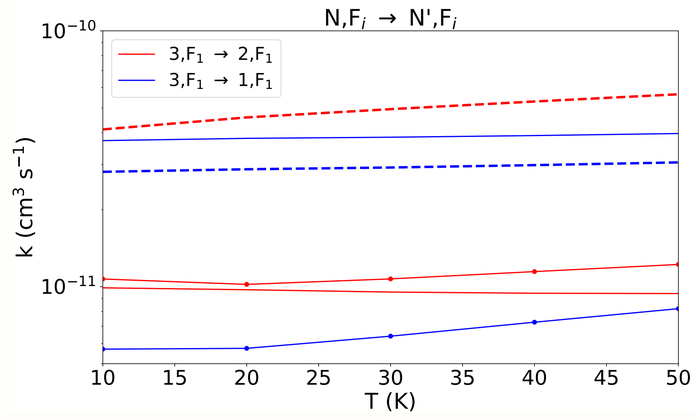


Figure 4: State-to-state desexcitation of NH by *ortho*-H_2 (dashed lines) and by *para*-H_2 (solid lines) as a function of the collisional energy for F-conserving transitions (upper panel) and for F-changing transitions (lower panel)

1. Feshbach and shape resonances are found for small collisional energies
2. Propensity rule is in favor of F-conserving transitions, which is predicted by the theory [6]
3. Cross sections are larger for collisions of NH with *ortho*-H_2
4. Results show a propensity rule in favor of $\Delta N = 1$ transitions for NH in collision with *ortho*-H_2 whereas a propensity rules in favor of $\Delta N = 2$ is observed for collisions with *para*-H_2. This is a consequence of the strong anisotropies of the PES

Rate coefficients



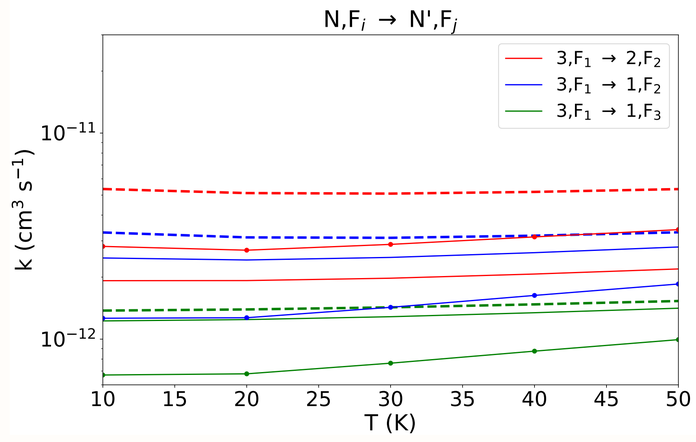


Figure 5: State-to-state rate coefficients for NH in collisions with *ortho*-H_2 (dashed lines), with *para*-H_2 (solid lines), and with He (doted lines) as a function of the temperature for F-conserving transitions (upper panel) and for F-changing transitions (lower panel)

1. Differences up to an order of magnitude are found between rate coefficients for NH in collisions with H_2 and He
2. Propensity rules are different for NH collisions with *para*-H_2 and He at low temperatures

Summary and conclusions

- First collisional data for NH-H_2 system
- Different general behavior for NH collisions with *ortho*-H_2 and *para*-H_2
- NH can be a tracer of the *ortho* to *para*-H_2 ratio in the ISM
- He is not a good proxy for H_2 in astrophysical models

References

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