387.
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Title:Fine and hyperfine excitation of NH and ND by He: on the importance of calculating rate coefficients of isotopologues
Authors:Dumouchel, F. (1); Kłos, J. (2); Toboła, R. (3); Bacmann, A. (4); Maret, S. (4); Hily-Blant, P. (4); Faure, A. (4); Lique, F. (1)
Author affiliation:(1) LOMC, Univ. du Havre, Le Havre, France; (2) Dept. of Chem. & Biochem., Univ. of Maryland, College Park, MD, United States; (3) Fac. of Chem., Univ. of Warsaw, Warsaw, Poland; (4) Inst. de Planetologie et d'Astrophys. de Grenoble (IPAG), UJF-Grenoble 1, Grenoble, France
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Abstract:The NH and ND molecules play an important role in interstellar nitrogen chemistry. Accurate modeling of their abundance in space requires the calculation of rates for collisional excitation by the most abundant interstellar species. We calculate rate coefficients for the fine and hyperfine excitation of NH and ND by He. State-to-state rate coefficients between the first levels of NH and ND were obtained for temperatures ranging from 5 to 150 K. Fine structure resolved rate coefficients present a strong propensity rule in favor of $\Delta j = \Delta N$ transitions, as expected from theoretical considerations. The $\Delta j = \Delta F1 = \Delta F$ propensity rule is observed for the hyperfine transitions of both isotopologues. The two sets of fine structure resolved rate coefficients are compared in detail and we find significant differences between the two isotopologues. This comparison shows that specific calculations are necessary for the deuterated isotopologues of any hydride. The new rate coefficients will help significantly in the interpretation of NH and ND terahertz spectra observed with current and future telescopes, and enable these molecules to become a powerful astrophysical tool for studying the nitrogen chemistry.
Number of references:46
Inspec controlled terms:atom-molecule collisions - excited states - helium neutral atoms - hydrogenation - hyperfine structure - nitrogen compounds - potential energy surfaces - reaction rate constants
Uncontrolled terms:hyperfine excitation - NH molecules - ND molecules - interstellar nitrogen chemistry - abundance in space modeling - collisional excitation rates - state-to-state rate coefficients - fine structure resolved rate coefficients - $\Delta j = \Delta N$ transitions -$\Delta j = \Delta F_1 = \Delta F$ propensity rule - hyperfine transitions - deuterated isotopologues - NH terahertz spectra - ND

terahertz spectra - temperature 5 K to 150 K - NH - ND - He

Inspec classification codes:A3150 Excited states of atoms and molecules - A3130G Hyperfine interactions and isotope effects (atoms and molecules) - A3510F Atomic fine- and hyperfine-structure constants - A3450H Electronic excitation and ionization (atoms and molecules) - A8220P Measurements of chemical rate constants, reaction cross sections, and activation energies

Numerical data indexing:temperature 5.0E+00 1.5E+02 K

Chemical indexing:NH H N ND D/ N He

Treatment:Theoretical or Mathematical (THR)

Discipline:Physics (A)

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