Ammonia – rare gas atoms collisions

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Abstract: Collisions of ammonia with rare gas (Rg) atoms and H\textsubscript{2} have been the subject of
a large number of studies, both theoretical and experimental, mainly focusing on rotationally
inelastic scattering in an astrophysical context. Indeed, NH\textsubscript{3} is often used as a probe of the
physical conditions in various interstellar environments \cite{1}, and accurate values for the cross
sections and rate constants for NH\textsubscript{3}-He and NH\textsubscript{3}-H\textsubscript{2} collisions are required in order to interpret
observations. Recent experimental advances have renewed interest in these systems by allowing
measurements of quantum-state-resolved integral and differential cross sections in crossed
beam experiments \cite{2, 3, 4}, which can be directly compared to theoretical predictions based on
accurate potential energy surfaces and quantum-mechanical scattering calculations. The same
techniques, combined with a Stark-decelerated beam of NH\textsubscript{3}, will allow the measurement of
integral and differential cross sections at very low collision energies, where the cross section is
dominated by resonances that are very sensitive to the details of the potential energy surface
\cite{5}. Finally, inelastic collisions of NH\textsubscript{3} with He and Ne are also of interest in the simulation of
the rotational cooling of ammonia in a buffer gas cell \cite{6}.

In this context, we have recently investigated the rotationally-inelastic scattering of NH\textsubscript{3} and
ND\textsubscript{3} by rare gas atoms and H\textsubscript{2} using new potential energy surfaces obtained by means of the
coupled cluster method with single, double and perturbative triple excitations (CCSD(T)) \cite{1, 7}.
The close-coupling method is employed to compute integral and differential cross sections
at low collision energy and we compare the theoretical predictions with the experimental data.

References
\cite{1} S. Maret, A. Faure, E. Scifoni, and L. Wiesenfeld, Mon. Not. R. Astron. Soc. 399 425
(2009).
16 477 (2014).
\cite{4} O. Tkac, A. K. Saha, J. Loreau, Q. Ma, P. J. Dagdigian, D. H. Parker, A. van der Avoird,
\cite{5} Q. Ma, A. van der Avoird, J. Loreau, M. Alexander, S. Y. T. van de Meerakker, and P. J.
\cite{6} O. Schullian, J. Loreau, N. Vaeck, A. van der Avoird, B. R. Heazlewood, C. J. Rennick,