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ORIGINAL ARTICLE

Collision induced rotational excitation of AlF ($X^1\Sigma^+$) by para-H_2 ($j = 0$)

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Abstract Rotational excitation cross sections and rate coefficients of AlF collisions with para-H_2 are computed at low temperature, i.e., for $T \leq 70$ K. Prior to collisional calculations, a four-dimensional (4D) potential energy surface (PES) for the AlF-H_2 system is calculated at the *ab initio* Coupled-Cluster level of the theory with an aug-cc-pVQZ Gaussian basis set. This 4D-PES is further reduced to a two-dimensional (2D) PES based on the considerations related to collisional studies with para-H_2. The [Al-F] and [H-H] bond lengths are frozen at their experimental equilibrium value $r_e = 1.654369$ bohr and $r_e = 1.4011$ bohr respectively. The interaction energy presents a global minimum located $\sim$63 cm^{-1} below the AlF-H_2 dissociation limit. With this PES, cross sections are determined in the Close-Coupling (CC) approach and rate coefficients are inferred by averaging the cross sections over a Maxwell-Boltzman distribution of kinetic energies. These quantities are significantly magnified in comparison with their AlF-He counterparts. The already observed propensity towards $\Delta J = 1$ transitions for AlF-He remains.

Keywords PES · CC · Collision · Para-H_2 · Cross sections · Rate coefficients

1 Introduction

Collision induced rotational excitation studies have received considerable attention both experimentally and theoretically during the past three decades. This stems on one hand from the rapid development of new laser driven experimental techniques and on the other, to the improved accuracy in the calculation of the Potential Energy surface (PES) that makes it possible to perform multichannel fully converged Close Coupling (CC) calculations for closed-shell and open-shell molecules. For a review of the bibliography on collision studies, Offer et al. (1994), Alexander (1999), Wormer et al. (2005), Lique et al. (2007) and Hammami et al. (2008a, 2008b) and references therein are recommended. It should be pointed out however that to date, only a few number of molecular systems of astrophysical interest were studied with accurate methods. Indeed, the modeling of interstellar molecular emission requires excitation parameters such as cross sections, collision rates, polarization and depolarization transfer rates of the collisions between the molecules studied and the most abundant perturbers of the interstellar medium (ISM). Such data are urgently needed in the scope of the ground-based and space-based missions, such as HERSCHEL satellite or the ALMA interferometer to allow for the study in greater detail of the physical conditions of the ISM.

In the scope of the astrophysically important species, it should be pointed out that one of the most unexpected and

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