

The Determination of Radioxenon by the Study of Rotationally Inelastic Dynamics

The theoretical study of collisional excitation of LiH with rare gas shows the presence of Argon (Ar) and Xenon (Xe) in the atmosphere. The determination of ab initio potential energy surface (PES) allows the description of the interaction between the rare gas Ar or Xe and the rotating LiH molecule. The close coupling (CC) approach is used to determine the cross sections of collision. The rate coefficients are determined by averaging these cross sections over a Maxwell-Boltzmann distribution of kinetic energies. In our previous work [Niane et al. SpringerPlus 2014, 3:188 – Niane et al. Computational and Theoretical Chemistry 993 (2012) 20-25], the 11 first rotational levels of rate coefficients of rotational collision of LiH with Argon (Ar) are evaluated for temperatures ranging from 10 to 300K. The determination of rate coefficients by collisional study of LiH with radioxenon will allow us to determine its behavior in the fields of atmospherically molecules.

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