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Radiative stabilization and photodissociation of HeH^+ in its two lowest $^3\Sigma^+$ states

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Synopsis Although it is thought to play an important role in the chemistry of some extra-terrestrial environments, the HeH^+ cation has not been detected in space so far. We suggest it could be observed in its triplets rather than singlet states and we study the formation by radiative stabiliation and the destruction by photodissociation of the two lowest states of this symmetry.

The HeH^+ cation is predicted to the first molecular species to have formed in the universe, by radiative association of H^+ and He [1]. Although models predict HeH^+ to be abundant in certain planetary nebulae, stars formed from primordial material or Helium-rich white dwarves, every attempt of extra-terrestrial observation of this cation has so far proven inconclusive [2]. It is proposed here that the HeH^+ ion could be detected in its $a\ ^3\Sigma^+$ metastable state, as it has a long lifetime (> 100 s). The first superior electronic state of the same symmetry, the $b\ ^3\Sigma^+$ state, has a much shorter lifetime ($\approx 10^{-8}$ s) and will thus populate the a state radiatively.

Using time-dependent quantum dynamics, we investigate the formation of HeH^+ in the a and $b\ ^3\Sigma^+$ states by radiative association and its destruction by photodissociation. The partial photodissociation cross-sections from all vibrational levels of the a and b states towards the ten $^3\Sigma^+$ and the six $^3\Pi$ superior states are calculated, from which the corresponding radiative stabilization cross-sections are then inferred.

The rate constants for both processes are estimated in the range of temperature and of radiative energy distribution found in planetary nebulae. It is shown that the vibrational dependence of the radiative stabilization cross-section, usually neglected in the estimation of the rate constant, has a significant impact at low temperature.

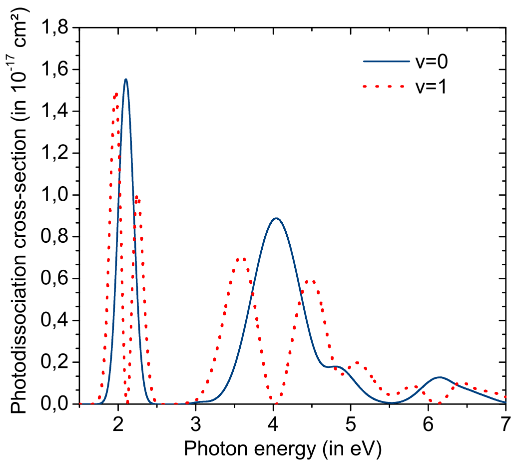

Figure 1. Total photodissociation cross-sections from the $v = 0$ and the $v = 1$ level of the $b\ ^3\Sigma^+$ state

References

[1] J. Loreau *at al* 2010 *J. Phys. B* **43** 065101

[2] E. A. Engel *at al* 2005 *Astron. Astrophys.* **357** 471

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