

Theoretical study of Rydberg states of HeH⁺ ion using the Halfium model

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It is well known that hydrogenic systems as H₂, HeH and their molecular ions H₂⁺, H₃⁺, HeH⁺ are present in interstellar medium and intervene in several molecular processes. Very precise calculations on electronic excited states and rovibronic ones of these systems are required. These last years, our team under the leadership of professor Mourad Telmini and in collaboration with professor Christian Jungen from Aimé Cotton Laboratory in Orsay France, developed a new code to investigate the excited states of diatomic molecules with two active electrons called the Halfium code. The theoretical method is based on the combination of the R-matrix variational method and the multichannel quantum defect theory. The initial applications of the theory focused on the hydrogen molecule H₂ [1].

We report here the first application of the Halfium code to study Rydberg states of heteronuclear diatomic molecular ion HeH⁺. In this contribution [2, 3], we present systematic study of the Rydberg spectrum of HeH⁺ ion for the 1,3 Λ ($\Lambda = 0 - 4$) symmetries over the bond length interval [1-5] a.u. . Furthermore, we compare our results with those of other authors [4, 5, 6] and discuss the agreements/disagreements with them. In addition to that, we will present our preliminary results on doubly excited states of HeH⁺ which intervene in the DR process of HeH⁺⁺ ion.

References:

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