Theoretical study of $^{1,3}\Delta$ Rydberg states of HeH$^+$ ion using the Halfium model

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The Halfium code was developed to determine the excited states of diatomic molecules with two active electrons [1]. The theoretical method is based on the combination of the R-matrix variational method and the multichannel quantum defect theory. The first applications of the model focused on the hydrogen molecule H_2 [1]. Recently, the code was improved to study the states of symmetry Σ^- [1] and calculating rovibronic levels with spectroscopic precision. [2]. The aim of our work is to generalize the halfium code to study Rydberg states of heteronuclear diatomic molecular systems with two active electrons. Indeed, it is necessary to take into account the *gerage/ungerade* symmetry breakdown, which requires a substantial update of the code. In this contribution, we present the results of our calculations of the symmetries $^{1,3}\Delta$ for internuclear distances R ranging from 1 to 5 a.u. For the first three bound states of these symmetries and when comparing our results with those obtained by quantum chemical calculations of reference [3-4], we found a good agreement. The energy difference is about 230 cm^{-1} for $^1\Delta$ symmetry and 260 cm^{-1} for $^3\Delta$ symmetry. These differences are comparable to those obtained for the H_2 molecule for the same symmetries. For even more excited Rydberg states, we have made predictions in terms of quantum defects for both symmetries and internuclear distances R from 1 to 5 a.u. The results are summarized in an article that has been recently submitted for publication [5].

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