

Different ways to compute the ground state of electronic energy of ion hydrogen molecule confined via variational method

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Abstract: The electronic energy can be calculated by two ways [1,2]. We want to compare two methods of calculate the ground state of electronic energy of H_2^+ confined in impenetrable cavities. One way is using the mean value of the electronic energy of the atomic orbital [1] and the other way is computing the atomic electronic energy [2]. There is a discussion about this subject in literature [3,4]. We conclude that both methods are appropriated to describe confined molecules. But, the method that uses the mean value of the atomic orbital affords energy eigenvalues less than the energy eigenvalues of the other method.

Key-words: ground state, electronic energy, ion hydrogen molecule, confined system, variational method.

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