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Two-dimensional confinement of hydrogen molecular ion

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ABSTRACT

Using the Born – Oppenheimer approximation, and considering the nuclei fixed at the foci, a study of the hydrogen molecular ion (H_2^+), confined strongly in two dimensions by ellipses of different size ξ_0 , is done. The Schrödinger equation is solved numerically in elliptic coordinates (ξ, η) , applying the separation of variables method. The equations for ξ and η are solved following an iterative process, until the energy and separation constant become consistent with the size of the confining ellipse characterized by the parameter ξ_0 and the internuclear distance R . The energies for the ion at its ground state and the equilibrium distance between the nuclei are obtained, for different values of ξ_0 , as well as the polarizability of the molecule.

Keywords: Schrödinger equation Born – Oppenheimer approximation, energies of the ion, equilibrium distance between nuclei, polarizability of the molecule.

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