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Static Properties and Stark Effect of the Ground State of the HD Molecular Ion

By -

Bibliogov, United States, 2013. Paperback. Book Condition: New. 246 x 189 mm. Language: English . Brand New Book ***** Print on Demand *****.We have calculated static properties of the ground state of the HD(+) ion and its lowest-lying P-state without making use of the Born-Oppenheimer approximation, as was done in the case of H₂(+) and D₂(+) [Phys. Rev. A 58, 2787 (1998)]. The ion is treated as a three-body system whose ground state is spherically symmetric. The wavefunction is of generalized Hylleraas type, but it is necessary to include high powers of the internuclear distance to localize the nuclear motion. We obtain good values of the energies of the ground S-state and lowest P-state and compare them with earlier calculations. Expectation values are obtained for various operators, the Fermi contact parameters, and the permanent quadrupole moment. The cusp conditions are also calculated. The polarizability was then calculated using second-order perturbation theory with intermediate P pseudostates. Since the nuclei in HD(+) are not of equal mass there is dipole coupling between the lowest two rotational states, which are almost degenerate. This situation is carefully analyzed, and the Stark shift is calculated variationally as a function of the applied electric field.



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