

Nonadiabatic rotational states of H₂, HD, and D₂

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We present a new computational method for the determination of energy levels in four-particle systems like H₂, HD, D₂, HeH⁺, and Ps₂ using explicitly correlated exponential basis functions and analytic integration formulas. In solving the Schrödinger equation, no adiabatic separation of the nuclear and electronic degrees of freedom is introduced. We provide formulas for the coupling between the rotational and electronic angular momenta, which enable calculations of arbitrary rotationally excited energy levels. To illustrate the high numerical efficiency of the method, we present results for various states of the hydrogen molecule. The relative accuracy to which we determined the nonrelativistic energy reached the level of 10^{-12} – 10^{-13} , which corresponds to an uncertainty of 10^{-7} – 10^{-8} cm⁻¹.

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