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Variational calculations of the H^+_2 and HD^+ rovibrational energies

Monday, 15 April 2019 15:00 (15 minutes)

We use the exponential explicitly correlated variational basis set of the type exp(−α_n*R*−*β*_*n*r_1−γ_n*r_2) to calculate systematically the nonrelativistic bound-state energies for the hydrogen molecular ion H^+_2 and HD^+.We perform calculations for the states of the total orbital angular momentum L=0-4 with the complete
set of vibrational quantum numbers v=0–10.

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