NON-ADIABATIC ENERGIES OF THE HYDROGEN MOLECULE

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A novel perturbation theory has been developed to account for nonadiabatic effects in diatomic molecules[a]. All molecular levels can be obtained simultanously from a single nuclear equation corrected for the presence of $(m/M)^2$ terms. Comparison with the direct nonadiabatic calculations for rotationless states of H_2 demonstrates an agreement at the level of 10^{-5} cm^{-1} for the ground tone transition.

[a] K. Pachucki and J. Komasa, J. Chem. Phys. **130**, 164113 (2009)