ANALYTICAL APPROXIMATION FOR ADIABATIC AND NONADIABATIC ELECTRONIC MATRIX ELEMENTS OF HOMONUCLEAR DIATOMIC RYDBERG STATES. APPLICATION TO SINGLET P-COMPLEX OF HYDROGEN MOLECULE

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Based on the one-channel quantum defect theory (QDT) representation of Rydberg electronic states of homonuclear diatomic molecule estimated at the standard Born-Oppenheimer approximation the simple analytical expressions to approximate adiabatic and nonadiabatic electronic matrix elements have been offered. The relations for matrix elements of radial coupling operator (first and second partial derivatives on internuclear distance R) have been obtained by applying the both diagonal and nondiagonal forms of Hellman-Feymann theorem as well as well-known scaled property of Coulomb functions at a small distance from a core r. The matrix elements of electronic coupling operator have been found in closed form based on the results of the hypervirial theorem as well as the Sidis equation. Using semiclassical approximation of QDT function formulae for integrals $\langle \nu_i | r^k | \nu_j \rangle$, where $k = 0, 2$ have been developed. It allowed for to find R-dependence matrix elements of both l and electronic coupling in an analytical form as well. The formulae have been tested on low-lying states of singlet p-complex of molecular hydrogen by comparision with "exact" ab initio results.