QED corrections to the Born Oppenheimer energy curve of H_2

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Until recently the need for computation of QED effects for chemical molecules has been restricted to the ones containing heavy nuclei. Recent advances in molecular spectroscopy and in the theoretical calculations for few-electron molecules made it necessary to include the radiative correction for H_2, D_2 and other light molecules as well, as they, together with the nonadiabatic corrections, constitute the biggest source of theoretical uncertainty.

For H_2 molecule, just as for light atoms, the most convenient way of computing the QED effects is based on the expansion of energy in powers of the fine structure constant:

$$E = E_0 + \alpha^2 E_2 + \alpha^3 E_3 + \alpha^4 E_4 + \dots$$

Techniques for computing the nonrelativistic energy and wavefunctions, in particular the method of Exponentially Correlated Gaussian functions are well developed for few-electron molecules in both the Born-Oppenheimer and nonadiabatic cases. Large progress have also been made on the field of computing the expectation values of singular operators constituting the Breit-Pauli Hamiltonian [1, 2]. While the contribution of the α^3-order QED terms could be estimated to be of similar magnitude as that of the α^2 terms, its complete computation has been limited because of computational difficulty of evaluating the Bethe logarithm. Using the new integral representation of the Bethe logarithm [4] and a new integration routine we evaluated $\ln k_0$ for a number of internuclear distances. We also derived the large-distance $(1/R)$ expansion of Bethe logarithm and the total α^3-order QED correction, and computed its coefficients.

Our main result is the QED corrections to the potential energy curve of hydrogen molecule, including the region of large distances, where they join the retardation regime [3]. We also present the radiative corrections to ionization and dissociation energy and to the energies of rovibrational levels in H_2.

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