PRE-BORN–OPPENHEIMER ENERGIES, LEADING-ORDER RELATIVISTIC and QED CORRECTIONS FOR ELECTRONICALLY EXCITED STATES OF MOLECULAR HYDROGEN

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For rovibronic states corresponding to the B and B' Σ_u^+ electronic states of the hydrogen molecule, the pre-Born–Oppenheimer (four-particle) non-relativistic energy is converged to a 1–3 parts-per-billion relative precision. The four-particle non-relativistic energy is appended with leading-order relativistic, leading- and estimated higher-order quantum-electrodynamics corrections [1]. The resulting term values referenced to the rovibronic ground state are obtained in an excellent agreement with the experimental results [2]. Further results are reported and discussed for other rovibronic states assignable to the $C\ ^1\Pi_u$ and the EF, GK, and HH Σ_g^+ electronic states.

References

[1] E. Saly, D. Ferenc, and E. Mátyus, *Mol. Phys.* e2163714 (2023).
[2] D. Bailly, E. J. Salumbides, M. Vervloet, and W. Ubachs, *Mol. Phys.* **108,** 827 (2010).

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