Contribution ID: **110** Type: **Poster (Student, Not in Competition) / Affiche (Étudiant(e), pas dans la compétition)**

Variational Calculation of Hydrogen Molecular Ion

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We have performed a benchmark calculation of non-relativistic energy level of H_2^+, using Hylleraas coordinates containing three non-linear parameters so that three inter-particle radial coordinates r_1, r_2 and r_{12} can be described independently. Rayleigh-Ritz variational principle is used to find out minimum of the expectation value of Hamiltonian of this system. Configuration of base varies according to the total angular momenta J of the system, the bigger J is, the more blocks are needed. To solve the matrix equation, the Power Method is used to identify the ground state as well as some other excited states. The non-relativistic ground state energy of H_2^+ has been calculated to a few parts in 10^{34}, which represents the best energy level reported so far.enter code here

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