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High precision variational calculations of five-electron systems: S-states of boron SERGIY BUBIN, Nazarbayev University, LUDWIK ADAMOWICZ, University of Arizona — We have performed benchmark variational calculations of the lowest two S-states of the boron atom. The spatial part of the wave function has been expanded in terms of all-particle explicitly correlated Gaussians, whose nonlinear variational parameters were extensively optimized. We have also computed leading relativistic corrections and various expectation values for both states. This work demonstrates that the level of accuracy achievable in calculations of five-electron atoms is now approaching the one previously seen only in three- or four-electron systems.

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