

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Benchmark calculations of low-lying triplet states of Be atom¹

SERGIY BUBIN, Nazarbayev University — Benchmark variational calculations of several lowest triplet states of the beryllium atom are reported. The wave functions of the states were expanded in terms of highly optimized explicitly correlated Gaussian basis sets and accurate energies are determined assuming finite nuclear mass of the atom. These wave functions were used to compute various expectation values, including those that appear in the leading relativistic and QED corrections. Density distributions and pair correlation functions are analyzed for both electrons and nucleus.

¹This work has been supported by the Ministry of Education and Science of Kazakhstan

Sergiy Bubin
Nazarbayev University

Date submitted: 10 Nov 2016

Electronic form version 1.4