Abstract Submitted
for the DAMOP10 Meeting of
The American Physical Society

Benchmark calculations for small rare gas clusters[1] VLADIMIR ROUDNEV, MICHAEL CAVAGNERO, University of Kentucky — We present detailed calculations of dimers and trimers of He and other rare gas atoms to benchmark a non-relativistic three-body code currently in development for public distribution. For these systems, uncertainties in the fundamental constants can substantially exceed the errors of numerical calculations. For example, the near-threshold bound state of the He_2 dimer is quite sensitive to small variations of the nuclear mass. Our benchmark calculations include specific estimates of the numerical accuracy of the calculations, and also explore sensitivity to fundamental constants and their uncertainties. We provide detailed analysis of both numerical and physical uncertainties for the observable characteristics of bound states of small He and other rare gas two and three-atom clusters based on widely used ab initio and model potentials.

[1]This work is supported by the NSF grant PHY-0903956

Vladimir Roudnev
University of Kentucky

Date submitted: 22 Jan 2010 Electronic form version 1.4