Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Exploiting explicitly correlated electronic structure methods for accurate molecular calculations involving heavy main group elements[1]
KIRK PETERSON, GRANT HILL, Washington State University, GERALD KNIZIA, HANS-JOACHIM WERNER, University of Stuttgart — Recent advances in explicitly correlated electronic structure methods, namely MP2-F12 and CCSD(T)-F12, have demonstrated significant improvements in accuracy and efficiency due to the much improved convergence with respect to the one-particle basis set. Recent work in our group involving the heavy post-d main group elements will be presented, including new F12-optimized Gaussian basis sets and benchmark molecular calculations.

[1]This work was supported by the National Science Foundation

Kirk Peterson
Washington State University

Date submitted: 20 Nov 2009 Electronic form version 1.4