G3 Electron Affinities of Silicon and Germanium Clusters

PETER DEUTSCH, Penn State Univ at Beaver Monaca, PA 15061 — We review binding energies and electron affinities for atomic silicon and germanium obtained by G3 ab initio theory with respect to potentially significant differences between what we obtain and what is in the experimental literature. We focus on the electron affinities of the five atom clusters, reviewing the impact of using different types of geometries for the higher level calculations. Specifically we review the impact on electron affinities of using geometries with more diffuse functions and more polarization functions than are employed in the G3 calculations. \(^1\) L. A. Curtiss et. al. J. Chem. Phys. 114, 9287 (2001) and references therein.