EQUILIBRIUM STRUCTURES OF MOLECULES FEATURING BONDS BETWEEN SECOND-ROW ELEMENTS

SVEN THORWIRTH, *I. Physikalisches Institut, Universität zu Köln, Germany and Max-Planck-Institut für Radioastronomie, Bonn, Germany*; MICHAEL E. HARDING, *Institute for Theoretical Chemistry, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX 78712 , USA.*

Equilibrium geometries of a set of molecules containing chemical bonds between second-row elements (Al, Si, P, S, Cl) have been evaluated at the CCSD(T) level of theory in combination with large basis sets. The results of these calculations are compared against equilibrium values from experiment. Purely experimental equilibrium structures are only available for very few molecules of this kind. Consequently, empirical equilibrium structural parameters for the majority of members of the set had to be determined using ground-state rotational constants corrected for zero-point vibrational effects. The latter were obtained by second-order vibrational perturbation theory employing coupled-cluster calculations of anharmonic force fields.