CORRELATION-CONSISTENT BASIS SETS FOR USE WITH EFFECTIVE CORE POTENTIALS

J. BLAUDEAU, S. BROZELL, S. MATSIKA, Z. ZHANG, and R. M. PITZER, *Department of Chemistry, Ohio State University, 100 W. 18th Ave., Columbus OH 43210*.

For use with effective core potentials, the objectives for correlation-consistent basis sets, a series of basis sets with increasing number of contracted functions in each valence shell with efficient use of primitive functions, must be augmented with the requirement that the (pseudo-) orbitals be small in the core region. Complying with all of these requirements means that all contractions must be chosen by energy-related methods rather than the method of freeing a number of valence-shell primitives, as is done with all-electron basis sets. The additional requirement with respect to core potentials principally affects s atomic shells. Primitive orbitals of the $1s$ type have their maxima at the nucleus and can only describe pseudo-orbitals by means of substantial differencing. Several methods of choosing contraction coefficients were investigated and the atomic natural orbital choice was found to be the most effective. The polarized double-zeta and triple-zeta basis sets for the oxygen atom are described, as are the exponent-collapse problems for heavier atoms.