

CORRELATION-CONSISTENT BASIS SETS FOR USE WITH EFFECTIVE CORE POTENTIALS

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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 1*s* 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.