**DERIVATION OF COMPLETE BASIS SET LIMIT EXTRAPOLATION FORMULAS**

We present the derivations of the three-point complete-basis set extrapolations used to compute DLPNO-CCSD(T)/CBS electronic energies using the cc-pVDZ, cc-pVTZ, and cc-pVQZ basis sets.

**INVERSE 4 – 5 POLYNOMIAL SCHEME**

The inverse 4-5 polynomial expansion is based on the formula

where is the highest angular momentum number, is the energy corresponding to the highest angular momentum basis set, and and are parameters to be determined. *N* = 2, 3, and 4 for the cc-pVDZ, cc-pVTZ, and cc-pVQZ basis sets, and give

This set of three equations can be written as

Solving the equation gives the CBS extrapolation formula