IN PURSUIT OF THE AB INITIO LIMIT - CASE STUDIES

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The convergence of *ab initio* predictions to the one- and *n*-particle limits has been systematically explored for several conformational energy prototypes: the inversion barrier of ammonia, the barrier to linearity of water, isocyanic acid, and silicon dicarbide, the torsional barrier of ethane, and the *E/Z* rotamer separation of formic acid. In particular, for the case of water attention is given to the degree of accord among extrapolations of conventional MP2, CCSD, and CCSD(T) energies to the complete basis set (CBS) limit and corresponding linear R12 schemes for these correlation methods. Small corrections to the barriers due to core correlation effects, the diagonal Born-Oppenheimer correction (DBOC), and one- and two-particle relativistic terms have also been investigated.