How accurate are „gold standard“ CCSD(T)/CBS interaction energies?

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The CCSD(T) method stands out among various coupled-cluster (CC) approximations as the “golden standard” in computational chemistry and is widely and successfully used in the realm of covalent and noncovalent interactions. The CCSD(T) method provides reliable interaction energies, but their surprising accuracy is believed to arise partially from the error compensation. The convergence of the CC expansion has been investigated up to fully iterative pentuple excitations (CCSDTQP); for the smallest 8 electron complexes the full CI calculations have further been performed. We conclude that the convergence of interaction energy for the complexes studied is reached already at CCSDTQ or CCSDT(Q) levels. When even higher accuracy is required, then the non-iterative CCSDTQ(P) method is recommended.