ACCURATE COUPLED CLUSTER CALCULATIONS OF MOLECULAR PROPERTIES: ELECTRON AFFINITIES AND POLARIZABILITIES OF O_2 AND CN AND THE SECOND HYPERPOLARIZABILITY OF O_2.

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We have calculated molecular properties of the title compounds by using the spin adapted ROHF CCSD(T) method. Electron affinity of the molecular oxygen represents benchmark results. Considering the complete basis set extrapolations based on the three series of ANO, aug- and d-aug cc-pVXZ (up to X=6) basis sets, relativistic, vibration and core correlation corrections we have arrived at EA=0.457 eV, well within the error bars of the experimental value. Electron affinity of the CN radical is a bit less accurate due to more significant difference between iterative CCSDT method and its noniterative counterpart. Details of the spin adaptation in ROHF CCSD(T) and various aspects of the selection of denominators in noniterative triples are analyzed as well. Most demanding is the second hyperpolarizability of the molecular oxygen. Satisfactory agreement of $< \gamma >$ obtained from the Sadlej and Pluta HPOL basis set, 1069 a.u. with Shelton's experimental value of 962, is a bit plagued by the fact that aug- and d-aug-basis sets with X up to Q still show bad convergence towards the final value. Another issue is our observation of serious numerical problems in calculations with lower symmetry due to the external electric field in the finite field approach. Limits of capability of obtaining accurate molecular properties from ROHF CCSD(T) calculations are based on the analysis of largest CCSD excitation amplitudes.