Equation-of-motion coupled cluster method for high spin calculations

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The equation-of-motion (EOM) coupled cluster (CC) approach in the version applicable for the double electron attachment (DEA) has been formulated for high spin components of the triplets and quintets states. The DEA EOM-CC scheme is based on the restricted Hartree-Fock reference and the standard amplitude equations as used in the Davidson based diagonalization procedure yield the singlet states. The triplet and higher spin components require separate amplitude equations. In the case of quintets the relevant equations are much simpler and easier to solve. Out of 21 diagrammatic terms contributing to the R_2 and R_3 equations in the case of quintets only R_3 equation survives with four diagrammatic terms present. In addition all the terms engaging threebody elements of the similarity transformed hamiltonian, i.e. $\bar{H}$ dissapear. This indicates substantial simplification of the theory. The implemented method has been applied in the study of the triplet and quintets states of the Carbon and Silicon atoms and potential energy curves for the Na-Na bond dissociation.