MR-SDCI + Q *AB INITIO* MOLECULAR ORBITAL CALCULATIONS OF FeCO: IMPORTANCE OF WELL-CONTRIVED SA-MCSCF WAVE FUNCTIONS AND 8-10σ ELECTRON CORRELATIONS

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FeCO has been used as a benchmark molecule to evaluate the basis functions for Fe[a,b] and the methods of calculation since it is known to be difficult to reproduce the energy difference between the $\tilde{a}^5\Sigma^-$ and the $\tilde{X}^3\Sigma^-$ states as well as the experimentally observed bond lengths of the $\tilde{X}^3\Sigma^-$ state by *ab initio* molecular orbital calculations. We carried out the MR-SDCI + Q and MR-ACPF calculations, based on the state-averaged MCSCF orbitals, taking into account the electron-correlation of 8-10σ electrons with the active space consisting of Fe 3*d*, 4*s* orbitals and CO π, π^* orbitals. Our predicted term value of the $\tilde{a}^5\Sigma^-$ state, bond lengths r_e(Fe-C) and r_e(CO) of the $\tilde{X}^3\Sigma^-$ state are 0.87 kcal mol^{-1}, 1.720 Å, and 1.159 Åwith relativistic energy corrections, which are to be compared with the corresponding experimental values of 3.24 kcal mol^{-1},[c] 1.7270 Å [r_s(Fe-C)],[d] and 1.1586 Å [r_s(CO)],[d] respectively. Similar results have also been obtained by the MR-ACPF methods.

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