MR-SDCI + Q \textit{ab initio} molecular orbital calculations of FeCO: importance of well-contrived SA-MCSCF wave functions and 8-10\textit{e} electron correlations

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FeCO has been used as a benchmark molecule to evaluate the basis functions for Fe\textit{a,b} and the methods of calculation since it is known to be difficult to reproduce the energy difference between the \(\tilde{a}\pi^2\Sigma^-\) and the \(X^3\Sigma^-\) states as well as the experimentally observed bond lengths of the \(X^3\Sigma^-\) state by \textit{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 8-10\textit{e} electrons with the active space consisting of Fe 3\(d\), 4\(a\) orbitals and CO \(\pi\), \(\pi^*\) orbitals. Our predicted term value of the \(\tilde{a}\pi^2\Sigma^-\) state, bond lengths \(r_{\text{Fe-C}}\) and \(r_{\text{CO}}\) of the \(X^3\Sigma^-\) state are 0.87 kcal mol\(^{-1}\), 1.720 Å, and 1.159 Å with relativistic energy corrections, which are to be compared with the corresponding experimental values of 3.24 kcal mol\(^{-1}\),\(\text{c}\) 1.7270 Å \([r_{\text{Fe-C}}]\),\(\text{d}\) and 1.1586 Å \([r_{\text{CO}}]\),\(\text{d}\) respectively. Similar results have also been obtained by the MR-ACPF methods.