COMPUTATIONAL MOLECULAR SPECTROSCOPY OF FeCO IN THE $\tilde{X}\,^3\Sigma^-$ AND $1\,^5\Sigma^-$ ELECTRONIC STATES

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FeCO is a molecule of astrophysical interest. It also served as a bench mark molecule for testing basis sets and *ab initio* calculation methods.[a,b] We have previously reported molecular constants and relative energies of $\tilde{X}\,^3\Sigma^-$ and $1\,^5\Sigma^-$ states of FeCO, based on the two-dimensional *ab initio* potential energy surfaces (PESs) determined at the MR-SDCI+Q+$E_{\rm rel}$/[Roos ANO (Fe, C, O)] and MR-ACPF+$E_{\rm rel}$/[Roos ANO (Fe, C, O)] levels of theory.[c] We will report here molecular properties derived from the three-dimensional PESs calculated at the level of MR-SDCI+Q+$E_{\rm rel}$/[Roos ANO (Fe, C, O)]. Calculated bond lengths r_e(Fe–C), r_e(C–O), and dipole moment (with experimental r_s bond lengths[d] in parentheses) are 1.722 (1.7270) Å, 1.160 (1.1586) Å, and 3.20 D for the $\tilde{X}\,^3\Sigma^-$ state, and 1.844 Å, 1.153 Å, and 0.29 D for the $1\,^5\Sigma^-$ state, respectively. The relative energy of $1\,^5\Sigma^-$ has been calculated to be 1.27 kcal mol^{-1}, to be compared with the experimental value of 3.24 kcal mol^{-1}.[e] The general trends in low-spin/high-spin issue reported for CoH,[f] CoCN,[g] and NiCN[h] are also observed for the NiCN $\tilde{X}\,^3\Sigma^-$ and $1\,^5\Sigma^-$ state pair.

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