We have previously reported a computational molecular spectroscopic study of $^6\Delta_i$ FeNC, where we showed that the experimentally derived, too-short C-N bond length ($r_e(\text{C-N}) = 1.03(8)$ Å) can be ascribed to an inadequate treatment of the large amplitude bending motion in the experimental determination of $r_0$. Here, we report analogous calculations for $^6\Delta_i$ FeCN.

Based on the three-dimensional potential energy surface calculated at the MR-SDCI+Q+E$_{\text{ref}}$/[Roos ANO (Fe), aug-cc-pVQZ (C, N)] level of theory, the standard spectroscopic parameters of Fe$^{12}$CN and Fe$^{13}$CN are derived by perturbation methods, and ro-vibrationally averaged bond lengths $\langle r \rangle$ have been predicted as expectation values obtained with ro-vibrational wavefunctions from the MORBID program. Some of the spectroscopic constants thus determined are: $r_e(\text{Fe-C}) = 2.048$ Å and $r_e(\text{C-N}) = 1.168$ Å, $\omega_1 = 2179$ cm$^{-1}$, $\omega_2 = 173$ cm$^{-1}$, and $\omega_3 = 420$ cm$^{-1}$; dipole moment $= 4.59$ D, spin-orbit coupling constant $A_{\text{SO}} = -83$ cm$^{-1}$, $\langle r(\text{Fe-C}) \rangle_0 = 2.082$ Å, and $\langle r(\text{C-N}) \rangle_0 = 1.172$ Å. In variational MORBID calculations, rovibronic energy levels are determined, and some vibrational bands are simulated. The bending potential is shallow, and the MORBID calculations show that the zero-point averaged structure is bent with the expectation value $\langle \angle(\text{Fe-C-N}) \rangle_0 = 170(5)$° (where the number in parentheses is the quantum-mechanical uncertainty). We compare the $^6\Delta_i$ FeCN results with those obtained for $^6\Delta_i$ FeNC. Since there are no experimental spectroscopic data available for FeCN, we hope that the predictions made here may be useful in the experimental investigation of this molecule.

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