# STRUCTURE AND SPECTROSCOPIC CONSTANTS OF FeCN: AN *AB INITIO* MOLECULAR ORBITAL STUDY

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FeCN is one of the possible candidates for an Fe-bearing interstellar molecule. Since no experimental data is available, prediction of its structure and spectroscopic constants by *ab initio* molecular orbital (MO) calculations has been requested. The ground state FeCl is known to be $^6\Delta$, and $Cl^-$ and $CN^-$ are known to show a similar chemical behavior. Hence, we assumed $^6\Delta$ state for the ground state FeCN. Wachters' all-electron basis set augmented with Bauschlicher's f-GTO, [8s,6p,4d,1f], for Fe and Dunning's cc-pVTZ basis sets for C and N have been employed. Active space for the MR-SDCI calculations has been selected to include Fe 3d and 4s as well as CN $\pi$ and $\pi^*$ orbitals obtained by the full valence MC-SCF MO calculations. Three dimentional potential energy surface has been calculated at the MR-SDCI level, and analyzed by the Mills' 2nd order perturbation theory. The $^6\Delta$ FeCN is predicted to be a linear molecule with Fe-C and CN bond lengths of 2.066 and 1.169 Å, respectively, yielding $B_e$, $D_J$, and $B_0$ to be 3667.9, 0.0012, and 3676.1 MHz. Anharmonic vibrational frequencies $\nu_1$, $\nu_2$, and $\nu_3$ are predicted to be 2158, 185, and 450 $cm^{-1}$, respectively.