AN *AB INITIO* MOLECULAR ORBITAL STUDY OF THE GROUND AND LOW-LYING ELECTRONIC EXCITED STATES OF FeN: PREDICTION TOWARD MOLECULAR SPECTROSCOPY

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To answer the long-standing debate which state is the electronic ground state of FeN, highly correlated $ab\ initio$ molecular orbital calculations with or without relativistic corrections and spin-orbit coupling interaction have been carried out for several low-lying electronic states including the $^2\Delta$, $^4\Pi$, $^4\Phi$, $^2\Pi$, $^2\Phi$, and $^6\Sigma^+$ states. The MR-ACPF calculations as well as the MR-SDCI + Q calculations showed that the electronic ground state of FeN is $^2\Delta$. Coinsidence between the predicted spectroscopic constants and those observed by Aiuchi et al.[a] and Ziurys et al.[b] shows that the state they observed is the $X^2\Delta$ Ω =2/5 spin substate. The equilibrium bond length r_e, rotational constant B_0, centrifugal distortion constant D_J, harmonic frequency ω_e, anharmonicity constant $\omega_e x_e$, and spin-orbit coupling constant A predicted for the $X^2\Delta$ state at the MR-ACPF level are 1.5752 Å, 0.60334 cm^{-1}, 1.17 x 10^{-6} cm^{-1}, 890 cm^{-1}, 8.2 cm^{-1}, and -362 cm^{-1}, respectively.

[a] K. Aiuchi and K. Shibuya, *J. Mol. Spectrosc.* **204**, 235, (2000).

[b] P. M. Sheridan, M. A. Brewster, and L. M. Ziurys, *Proc. of 56th Ohio State Univ. Int. Symp. Molec. Spectrosc.* **FB06**, 207, (2001).