

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

SACHIKO S. ITONO and TSUNEO HIRANO, *Department of Chemistry, Faculty of Science, Ochanomizu University, Tokyo 112-8610, Japan*; UMPEI NAGASHIMA, *Tsukuba Advanced Computing Center, National Institute of Advanced Industrial Science and Technology, Ibaraki 305-8562, Japan*.

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  $^2\Delta$ . Coincidence between the predicted spectroscopic constants and those observed by Aiuchi et al.<sup>a</sup> and Ziurys et al.<sup>b</sup> shows that the state they observed is the  $X^2\Delta \Omega = 2/5$  spin substate. The equilibrium bond length  $r_e$ , rotational constant  $B_0$ , centrifugal distortion constant  $D_J$ , harmonic frequency  $\omega_e$ , 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<sup>-1</sup>, 1.17 x 10<sup>-6</sup> cm<sup>-1</sup>, 890 cm<sup>-1</sup>, 8.2 cm<sup>-1</sup>, and -362 cm<sup>-1</sup>, respectively.

---

<sup>a</sup>K. Aiuchi and K. Shibuya, *J. Mol. Spectrosc.* **204**, 235, (2000).

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