AN *AB INITIO* MOLECULAR ORBITAL STUDY OF ELECTRONIC EXCITED STATES OF FeC

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There has been a continuing effort to investigate the electronic states of iron carbide, FeC, by several research groups in the gas phase spectroscopy, but only electronic ground states have been established as $^3\Delta_i$ state arising from the configuration ...$8\sigma^2 3\pi^4 1\delta^3 9\sigma^1$. In this study, we have focused on characterizing the electronic excited states observed by LIF[a], R2PI[b] and DF[c] spectra. Spectroscopic constants and energy levels of the excited states have been calculated from the *ab initio* multireference singles and doubles configuration interaction (MR-SDCI) molecular orbital method using all-electron large basis sets. Both relativistic and spin-orbit coupling effects were taken into account.

Many electronic states which are of complicated nature were found to populate densely in the low energy region. The lowest excited states for each spin and spatial symmetry, except the $^1\Delta$ state, were approximately described as the excited states derived by the promotion of one electron from the ground state. The excited states higher than these were found to be of completely multiconfigurational character. Each electronic state has been discussed in terms of electronic configuration, dipole moment, charge distribution, spin-orbit coupling constant, and spectroscopic constants.

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[a] W. J. Balfour, J. Cao, C. V. V. Prasad, and C. X. W. Qian *J. Chem. Phys.* **103**, 4046, (1995)

[b] D. J. Brugh and M. D. Morse *J. Chem. Phys.* **107**, 9772, (1997)

[c] K. Aiuchi, K. Tsuji, and K. Shibuya *Chem. Phys. Lett.* **309**, 229, (1999)