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

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Spectroscopic constants and energy levels of the ground and low-lying excited states of iron carbide, FeC, have been calculated from potential energy functions obtained by the *ab initio* MR-SDCI molecular orbital approach. Investigated states are $^1\Delta$ and $^5\Pi$, both of which are proposed by DF spectra[a] as a candidate for the new $\Omega = 2$ electronic state observed above the $^3\Delta_2$ state by 3460 cm^{-1}. The character of each electronic state has been discussed theoretically. Contrary to the previous tentative assignment to $^5\Pi$, the MR-SDCI results predict that the observed $\Omega = 2$ state should be the $^1\Delta$ state and be located at 3252 cm^{-1} above $^3\Delta_2$. The spin-orbit coupling constant for $^3\Delta$ state has also been calculated.

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