

MILLIMETER-WAVE SPECTROSCOPY OF THE FeCO($X^3\Sigma^-$) AND FeNO($X^2\Delta_i$) RADICALS IN THE VIBRATIONAL EXCITED STATES

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Rotational spectra of the FeCO and FeNO radicals produced by UV laser photolysis in the vibrational excited states were measured in the millimeter-wave region with the conventional absorption cell at room temperature.

The rotational transitions of the FeCO radical in the ground and ν_2 states have been observed by millimeter-wave spectroscopy^a, and the ν_1 fundamental band and hot band from ν_2 state also have been studied by infrared diode laser spectroscopy. In the present work, the rotational transitions ($J = 33 - 32 \sim 37 - 36$) in the ν_3 state of the $X^3\Sigma^-$ state were observed to split into 3 components due to the spin-rotation and spin-spin interactions. Molecular constants including rotational constant and centrifugal distortion constant were determined by a least squares fitting. The equilibrium rotational constant B_e was calculated to be 4373.405(72) MHz from the vibration rotation constant $\alpha_3 = 20.2051(42)$ MHz, and previously reported α_1 and α_2 . The bond length between Fe and C, calculated to be 1.725 Å assuming $r_{CO} = 1.159$ Å, agrees well with the *ab initio* result, $r_{FeC} = 1.722$ Å^b. The $2\nu_2$ state split into 9 substates due to the vibronic interaction, and the rotational transitions in the $P = 0$ component were observed.

The rotational transitions of the FeNO radical in the ground and ν_2 states^c, and the ν_1 band have been observed in the millimeter-wave and infrared region, respectively. The rotational transitions ($J = 28.5 - 27.5 \sim 32.5 - 31.5$) in the $2\nu_2$ state of the $X^2\Delta_i$ state were observed in the present study. The $2\nu_2$ state ($\Omega = 5/2$) splits into 3 substates, $^2\Gamma_{P=9/2}$, $^2\Delta_{P=5/2}$ and $^2\Sigma_{P=1/2}$, due to the vibronic interaction. The absorption lines in the $^2\Sigma_{P=1/2}$ state split into two components because of the *p*-type doubling. The transition in the ν_3 state is now under survey to determine the constant α_3 and the equilibrium rotational constant.

^aK. Tanaka, M. Shirasaka, T. Tanaka, *J. Chem. Phys.*, 106, 6820-6824 (1997)

^bU. Nagashima, R. Okuda, T. Hirano, *Molecular Spectroscopy Symposium*, Tokyo (2005)

^cS. Ikeda, M. Nakashima, M. Hayashi, K. Harada and K. Tanaka, 60th Ohio Meeting (2005)