MILLIMETER-WAVE SPECTROSCOPY OF THE IRON CARBONYL RADICAL(FeCO) IN THE ν_2 BENDING VIBRATIONAL STATE

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The rotational spectrum of iron carbonyl radical FeCO in the ν_2 bending vibrational state of the ground $X^3\Sigma^-$ electronic state was observed in the millimeter-wave region. The radical was produced by a dc discharge of iron pentacarbonyl $Fe(CO)_5$. Seven rotational lines, split into sextet by the electron spin-spin interaction and Λ-type dobling, were identified in the frequency region of 154-254 GHz. Molecular constants derived, the rotational and centrifugal distortion constants, the spin-spin coupling constant $\lambda_0 = 679.37(291)$GHz and the spin-rotation coupling constant $\gamma_0 = -1180.0(19)$ MHz, are reasonably similar to those of the ground state [a]. Although the electronic state is $^3\Sigma^-$, a large spin-orbit coupling constant $A = 14.0746(57)$ GHz was derived, indicating the vibronic coupling with the $^3\Pi$ electronic state located about 6500 cm^{-1} above the ground state. From the Λ-type doubling, large interaction constants, $o = -18.2899(55)$ GHz, $p = -355.36(64)$ MHz, and $q = 9.5167(69)$ MHz, were determind, where the figures in parentheses are a standard error to be attached to the last digits.

[a] K. Tanaka, M. Shirasaka and T. Tanaka, J. Chem. Phys. 106, 6820 (1997)