MICROWAVE SPECTROSCOPIC MEASUREMENTS OF THE ROTATIONAL SPECTRUM OF METHYL CYCLOPENTADIENYL IRON DICARBONYL

CHAKREE TANJAROON and STEPHEN G. KUKOLICH[a], *Department of Chemistry, The University of Arizona, Tucson, Arizona 85721*.

The rotational spectra of the methyl cyclopentadienyl iron dicarbonyl complex (namely methyl-Fip) were measured using a pulsed molecular beam Fourier transform microwave spectrometer. Methyl-Fip is an asymmetric top complex with a single methyl rotor bound to iron. The complex is challenging to study experimentally in the gas phase because it is unstable and exhibits methyl internal rotation. We report here the first measurements of the *a*-type rotational spectrum and determination of a methyl torsional barrier height. Analysis of the observed doublet splittings of low J and K lines yielded a barrier height of 8.7(8) kJ. The observed rotational constants for the parent (^{56}Fe) complex are A = 1431.74(13), B = 1062.263(84), and C = 828.016(15) MHz. Assignment of the measured rotational spectrum, quantum chemical calculations, and the molecular structure of methyl-Fip will be discussed.

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