THE HIGH-RESOLUTION INFRA-RED SPECTRUM OF CYCLOPENTADIENYL NICKEL NITROSYL [a]

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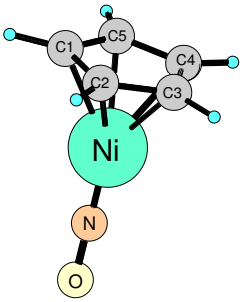

Gas Phase rotational constants for the ground and excited vibrational states have been determined for cyclopentadienyl nickel nitrosyl (C_5H_5NiNO) using a high resolution Fourier transform spectrometer (FTS) system at Kitt Peak, Arizona (KPNO). The rotationally resolved lines have been measured for the C-H symmetric stretch vibration (ν_1=3110 cm^{-1}) of cyclopentadienyl ligand. In the present analysis, twenty four lines have been assigned using a rigid rotor Hamiltonian with centrifugal distortion constants. The rotational constants measured for the ground and excited states of this prolate symmetric top molecule are A"= 0.14568(7) cm^{-1}, B"= C" = 0.04193(1) cm^{-1} and A'= 0.14324(9) cm^{-1}, B'= C' = 0.04128(3) cm^{-1} respectively. These measured parameters will be compared with the previously obtained results from microwave and infrared spectroscopy measurements. The stretching frequency and rotational constants were calculated using Density Functional Theory (DFT) calculations and these were quite helpful in resolving ambiguities in fitting procedure and initial assignments of measured lines.

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