

POLARIZED MATRIX INFRARED SPECTRA OF CYCLOPENTADIENONE - AN IMPORTANT REACTIVE INTERMEDIATE IN COMBUSTION AND BIOMASS PYROLYSIS

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A detailed vibrational analysis of the infrared spectra of cyclopentadienone ($C_5H_4=O$ and $C_5D_4=O$) in rare gas matrices has been carried out. Ab initio coupled-cluster anharmonic force field calculations were used to guide the assignments. Flash pyrolysis of o-phenylene sulfite ($C_6H_4O_2SO$ and $C_6D_4O_2SO$) was used to provide a molecular beam of cyclopentadienone entrained in the rare gas carrier. The beam was interrogated with time-of-flight photoionization mass spectrometry (TOF-PIMS), confirming the clean, intense production of $C_5H_4=O$. Matrix isolation infrared spectroscopy was coupled with 355 nm polarized UV for photo-orientation and linear dichroism experiments to determine the symmetries of the vibrations.