MOLECULAR PROPERTIES OF THE "ANTI-AROMATIC" SPECIES CYCLOPENTADIENONE, C_5H_5=0

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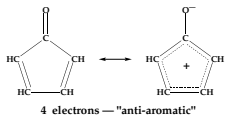

A common intermediate in the high temperature combustion of benzene is cyclopentadienone, C_5H_4=O. Cyclopentadienone is considered to be an "anti-aromatic" molecule. It is certainly a metastable species; samples persist at LN_2 temperatures but dimerize upon warming to -80°C. It is of great interest to physically characterize this "anti-aromatic" species. The microwave spectrum, the infrared spectrum, the ionization energy, and the electron affinity of cyclopentadienone have been measured. Flash pyrolysis of o–phenylene sulfite ($C_6H_4O_2SO$) provides molecular beams of C_5H_4=O entrained in a rare gas carrier. The beams are interrogated with time-of-flight photoionization mass spectrometry, confirming the clean, intense production of C_5H_4=O. a) Chirped-pulse Fourier transform microwave spectroscopy and CCSD(T) electronic structure calculations have combined to determine[a] the r_e molecular structure of C_5H_4=O. b) Guided by CCSD(T) electronic structure calculations, the matrix infrared absorbance spectrum of C_5H_4=O isolated in a 4 K neon matrix has been used[b] to assign 20 of the 24 fundamental vibrational frequencies. c) Imaging photoelectron photoion coincidence (iPEPICO) spectra[c] of cyclopentadienone establishes the ionization energy, IE(C_5H_4=O), to be 9.41 $\pm$ 0.01 eV. d) Prof. A. Sanov's group[d] has reported the electron affinity, EA(C_5H_4=O), to be 1.06 $\pm$ 0.01 eV.

[a] Kidwell *et al.* J. Phys. Chem. Letts. 2201 (2014)

[b] Ormond *et al.* J. Phys. Chem. A **118**, 708 (2014)

[c] Ormond *et al.* Mol. Phys. **in press** (2015)

[d] Khuseynov *et al.* J. Phys. Chem. A **118**, 6965 (2014)