

INFRARED ABSORPTION SPECTRUM OF RING-CS₂ ISOLATED IN MATRICES: INTERCONVERSION OF LINEAR-CS₂ AND RING-CS₂ BY IRRADIATION

YUAN -PERN LEE, MOHAMMED BAHOU, YU -CHANG LEE, *Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan 30043.*

Carbon disulfide (CS₂) isolated in solid argon or nitrogen at 13 K was irradiated with light at 193 nm from an ArF excimer laser. Recombination of photofragments S and CS produces ring-CS₂ that absorbs at 876.5 (881.1) and at 517.7 (522.7) cm⁻¹ in a argon matrix and 881.3, 520.9 cm⁻¹ in a nitrogen matrix; wave numbers listed parenthetically are associated with a minor site. The assignments are based on observed ³⁴S- isotopic shifts. Ab initio calculations using the MP2-FL and B3LYP density functional methods were carried out for ring-CS₂ and linear-CS₂; energies and vibrational wave numbers were predicted for each one. Observed line positions, infrared intensities and isotopic shifts fit well with those predicted for both species. Further irradiation of the matrix sample with different laser wavelengths, in the UV region with 248 and 308 nm and in the visible region with 532, 560 and 580 nm, bleached the lines corresponding to ring-CS₂ and enhanced absorption lines of linear-CS₂ Photoconversion mechanism is discussed.