MATRIX-ISOLATION FTIR SPECTRA OF 2-PYRONE PYROLYSIS PRODUCTS

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Cyclic, oxygenated hydrocarbons are common intermediates in the pyrolysis mechanisms for biomass used to produce biofuels and chemical feedstocks. Despite the role of these molecules in both biofuel production and combustion, there is limited understanding of their thermal decomposition pathways. In order to investigate how the chemical structure of a cyclic, oxygenated hydrocarbon affects its pyrolysis mechanism, these experiments have identified products in the gas-phase pyrolysis of 2-pyrone (2H-pyran-2-one). This molecule is commonly observed in the pyrolysate of pineapple waste, rice husks, aluminum alginate, wood chips, and cellulose, yet little research has been conducted on 2-pyrone's high-temperature chemistry. Experiments with pulsed, gas-phase pyrolysis at temperatures up to 1400 K were conducted with matrix-isolation FTIR identification of products. The FTIR spectra indicate the formation of carbon monoxide, carbon dioxide, acetylene, vinylacetylene, propyne, ethylene, and ketene, which have been observed in the pyrolysis of other cyclic, oxygenated hydrocarbons. However, several vibrational bands could not be assigned to known products in the literature and are theorized to belong to substituted ketenes such as formylketene and acryloyl ketene. Optimization and frequency calculations performed with Gaussian 09 at the B3LYP/6-311++G(d,p) support the assignments and demonstrate mechanisms consistent with the products' vibrational spectra.