

## PYROLYSIS REACTIONS OF OXOLAN-3-ONE STUDIED VIA MATRIX-ISOLATION FTIR

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Oxolan-3-one is a cyclic, oxygenated hydrocarbon that occurs frequently in the pyrolysis of many forms of biomass and is thus an important intermediate in the production of biofuels. In order to identify thermal decomposition products of oxolan-3-one, an approximately 0.4% mixture in argon was subject to pyrolysis in a resistively heated SiC microtubular reactor at 800-1400 K. Matrix-isolation FTIR spectroscopy was used to identify pyrolysis products. The products observed include ethylene, carbon monoxide, formaldehyde, ketene, acetylene, and propyne. A comprehensive computational study of the unimolecular decomposition mechanism shows reactions consistent with these products and suggests the appearance of hydroxyketene in the mechanism. Efforts were undertaken to pyrolytically generate and characterize hydroxyketene via matrix-isolation FTIR to confirm the assignment. The experimental and computational results combined provide clues to the overall mechanism of thermal decomposition of oxolan-3-one and are important in relating the molecule's structure to the mechanism.