

Supplementary Material

Acetylenes from Aldehydes. Preparation of Ethynylphenols and Phenylacetylenes by Flash Vacuum Pyrolysis of Isoxazolones

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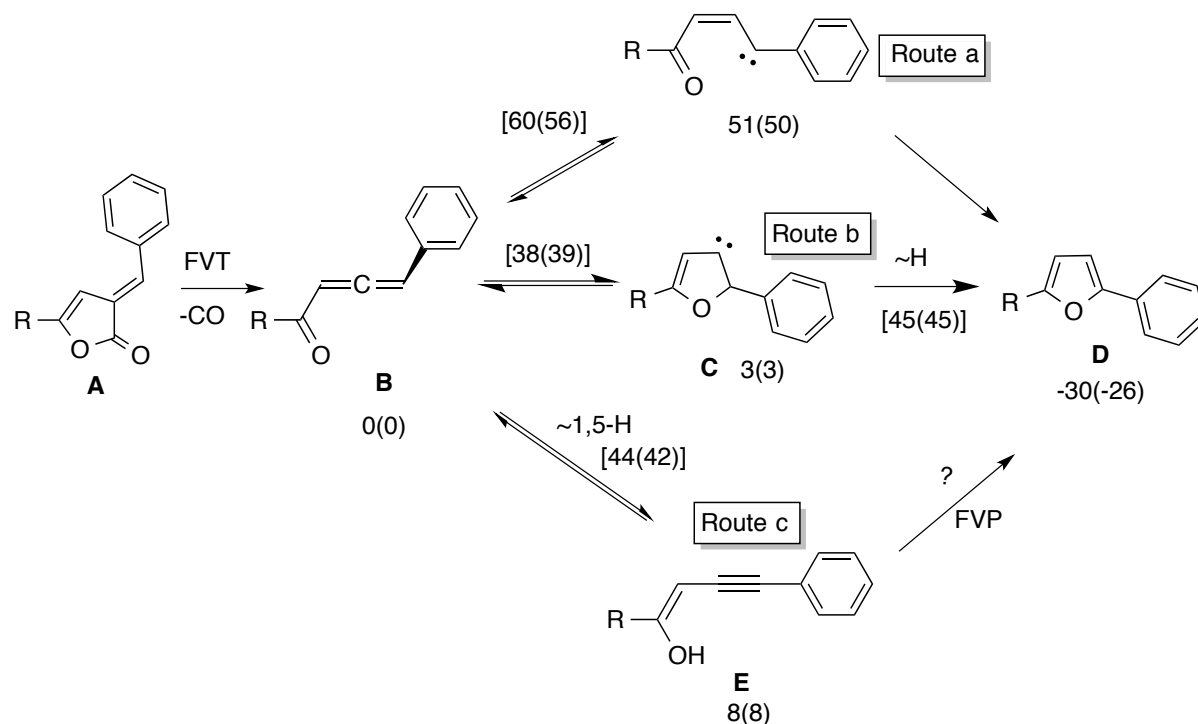
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Scheme S1. Cyclization of allenylketones to furans.¹

Potential routes for cyclization of allenylketones **B** formed by FVP of furanones **A** at 750 °C are shown. Formation of furans **D** by route b via carbene **C** is favoured energetically, but the cyclization of the 1-buten-3-yn-1-ol **E** by route c may also be a contender.¹ Calculated values of ΔE and (in parentheses) ΔG at 298.15 K are in kcal/mol at the (M06-2X/6-311+G(d,p)) level. Values in brackets are transition state energies, all relative to **B** = 0. The calculations pertain to R = H.

¹ R. Koch, H. M. Berstermann, C. Wentrup, *J. Org. Chem.* **2014**, 79, 65.