DOI: https://doi.org/10.5281/zenodo.14688610

REACTION OF VINYLATION OF PHENOL AND PHENOL DERIVATIVES

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Annotation. *Based on quantum-chemical and molecular-dynamic calculations of monoatomic phenols and their vinyl derivatives, the regularities of their structure dependence on reactivity have been determined. Research into the conditions and development of the technology for vinylation of phenols and their derivatives with vinylacetylene in the presence of highly basic systems.*

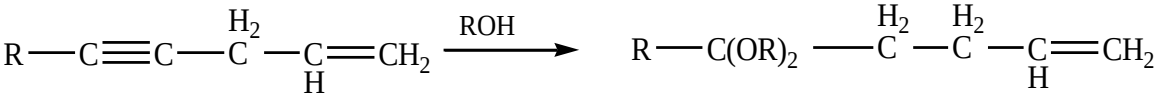
Keywords: *Phenol, vinylacetylene, vinylalkylacetylene, formyloxy-butadiene, cresol, alcohol. In our country, currently, organic synthesis products, especially unsaturated vinyl derivatives of compounds containing various functional groups, are widely used in various sectors of the economy, agriculture, pharmaceuticals, chemical industry, textile, paint and varnish, and oil and gas chemistry.*

Vinylacetylene production is currently the most effective technology for acetylene processing. In recent years, the processing of natural, oil and associated gases has shown significant positive results in the development of this technology. On this basis, the production of vinylacetylene derivatives can also be organized. At the same time, not all the possibilities for the use of vinylacetylene hydrocarbons in the chemical industry have yet been sufficiently studied. This is clearly demonstrated, first of all, by the information on the ethylenes in the literature of recent years [1].

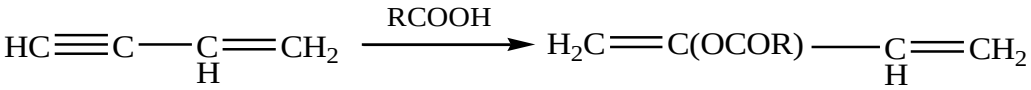
In some scientific works, vinylalkylacetylenes under the influence of acidic catalysts (boron fluoride) undergo analogous coupling with alcohols. However, these

data require verification in the light of new studies on the coupling of water and alcohols to vinylalkylacetylenes in the presence of alcoholates.

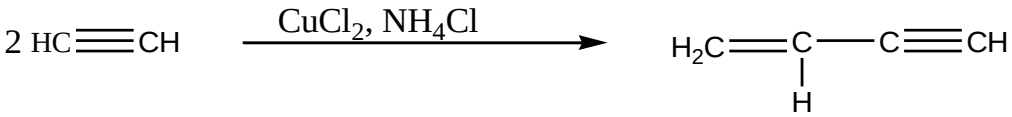
Allylacetylenes undergo analogous coupling with alcohols:



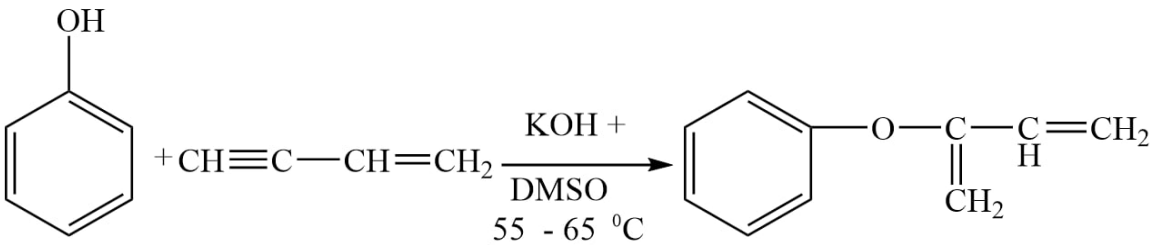
The addition of acids to vinylacetylene proceeds according to the following scheme, with the formation of only divinyl β-acyloxy derivatives.



In the presence of a boron fluoride-based catalyst, formyloxybutadiene is produced in 60% yield, and acetoxybutadiene in 30% yield. In the presence of mercuric sulfate, the yield is much lower. The addition of benzoic acid to vinylacetylene has not yielded any practical results. In our experiments, phenol was reacted with vinylacetylene in a highly basic system at normal pressure and at various temperatures. Initially, vinylacetylene was obtained as a result of the following reaction and was absorbed into cresol and stored.



Vinylacetylene absorbed into cresol begins to desorb and release with increasing temperature and is introduced into the phenol reaction mixture. Under the influence of phenol on vinylacetylene, the reaction proceeds in the following direction.



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