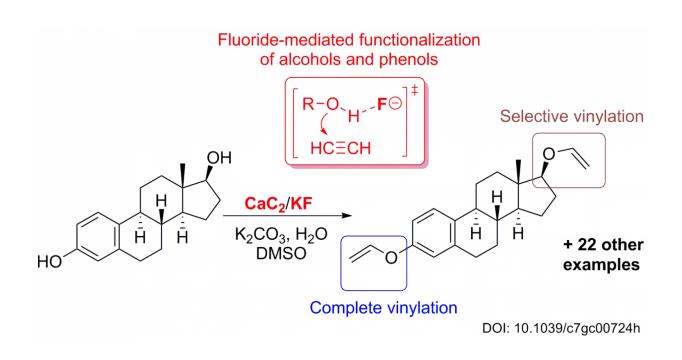


Solid acetylene reagent for laboratory applications

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Vinylation of different hydroxyl groups by CaC2/KF solid acetylene reagent. Credit: Zelinsky Institute of Organic Chemistry

Acetylene is one of the primary starting materials for chemical synthesis. However, acetylene is a highly flammable gas, dangerous and difficult to use in regular research laboratories. A novel solid acetylene regent has been developed to make chemical applications safer.

A combination of two simple compounds – calcium carbide (CaC_2) and



potassium fluoride (KF) – creates a very efficient acetylene reagent with enhanced reactivity. In the presence of water, acetylene is generated in this system, and is activated towards an in situ reaction with alcohols and phenols. Efficient vinylation converts the <u>hydroxyl group</u> (–OH) of alcohols and phenols into the H₂C=CH-O- building block. The hydroxyl group is a widespread functional group involved in a number of core organic transformations. Post-modification of drugs and <u>biologically</u> <u>active molecules</u> is an emerging area of very demanding applications of the vinylation reaction described. Biomedicine, material science and production of monomers are other well-appreciated areas of application of such vinyl monomers.

Mechanistic studies by experiment and computations have revealed two important factors: (1) the etching of the surface of CaC_2 by KF in the solid state; and (2) the fluoride-mediated activation in solution, which governs the enhanced reactivity in the developed system. The CaC_2/KF system described in the present study has crucial advantages compared to gaseous acetylene.

Acetylene is a fundamental organic molecule. However, acetylene is a flammable and explosive gas, which is very difficult to handle in laboratory. Using high-pressure acetylene requires complicated and expensive equipment with stringent safety regulations. The CaC_2/KF system described in the present study has crucial advantages compared to gaseous acetylene. This efficient CaC_2/KF solid <u>acetylene</u> reagent, a has a number of remarkable <u>applications</u>.

More information: Werner G., Rodygin K.S., Kostin A.A., Gordeev E.G., Kashin A.S., Ananikov V.P, "A solid acetylene reagent with enhanced reactivity: fluoride-mediated functionalization of alcohols and phenols", *Green Chem.*, 2017. DOI: 10.1039/c7gc00724h



Provided by Zelinsky Institute of Organic Chemistry

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