

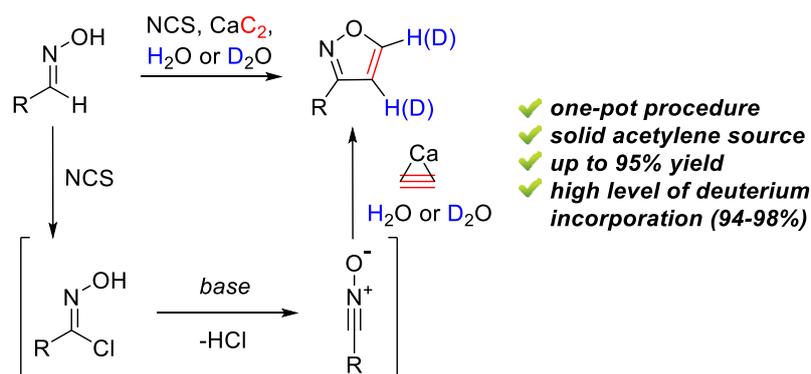
Calcium carbide in the synthesis of isoxazoles and 4,5-dideuteroisoxazoles

Maria S. Ledovskaya

Institute of Chemistry, Saint Petersburg State University,
Universitetsky prospect 26, Peterhof, 198504, Russia
maria.s.ledovskaya@gmail.com

Acetylene is an outstanding building block that undergoes a variety of chemical reactions, including addition to its triple bond or terminal hydrogen cleavage (to form acetylides) and substitution.¹ For example, acetylene is a raw material for an industrial synthesis of acetic acid, acetaldehyde, ethanol, vinyl chloride, benzenes, *etc.* In spite of acetylene is inexpensive and widely available it is a highly flammable gaseous material that requires additional measuring equipment to provide high safety level. Therefore, the development of alternatives for the gaseous acetylene is an important problem of modern chemistry. One of the simplest analogs of gaseous acetylene is calcium carbide.²

A novel synthetic methodology for the *one pot* preparation of isoxazoles directly from the reaction of calcium carbide with aldoximes and *N*-chlorosuccinimide (NCS) was developed.³ By this way, the chloraldoxime precursors of the active nitrile oxide species are generated *in situ* from the corresponding aldoxime and NCS. And the calcium carbide acts as a safe and inexpensive acetylene source and as a source of base ($\text{Ca}(\text{OH})_2$) that enable to generate nitrile oxide from the chloraldoxime released. Various 3-substituted isoxazoles are synthesized from the corresponding aldoximes in good to excellent yields under the optimized conditions. 4,5-Dideuteroisoxazoles were firstly synthesized by this methodology using deuterium oxide instead of water.



1. a) B.A. Trofimov, *Curr. Org. Chem.*, **2002**, *6*, 1121; (b) H. Schobert, *Chem. Rev.*, **2014**, *114*, 1743; (c) I.-T. Trotuş, T. Zimmermann, F. Schüth, *Chem. Rev.*, **2014**, *114*, 1761.
2. K. S. Rodygin, G. Werner, F. A. Kucherov, V. P. Ananikov, *Chem. Asian J.*, **2016**, *11*, 965.
3. M. S. Ledovskaya, K. S. Rodygin, V. P. Ananikov, *Org. Chem. Front.*, **2018**, *5*, 226.

Acknowledgements

This work was supported by the Russian Science Foundation (Project No 16-13-10301).