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The preferential crystallization of chiral isoxazoline cycloadducts from the (3+2) cycloaddition reaction of arylnitrile oxides and chiral monoterpenes.

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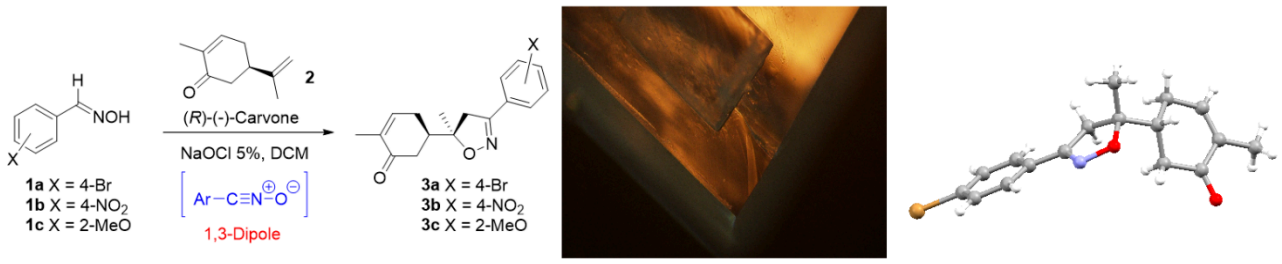
ABSTRACT

In this communication, we report our partial results on competitive crystallization process of the synthesis of 3,5-disubstituted isoxazolines solids using aryl nitrile oxides derived from **1a-c** with (*R*)-(-)- and (*S*)-(+)-carvone (**2**) in DCM and a 5% aqueous NaOCl solution. The cycloadducts are formed by the capture of the reactive intermediate arylnitrile oxide by carvone present in solution. The cycloadducts were isolated as pale white solids, and the ^{1}H and ^{13}C NMR spectra show typical signals indicating the formation of two respective diastereoisomers. For the reaction with oxime **1a**, the competitive crystallization of the cycloaddition reaction products showed interesting stereoselective results that will be discussed in detail. Scheme 1 illustrates the synthesis, appearance of the chiral single crystal of **3a** observed under light polarized optical microscope, and the crystal structure determined for diastereoisomer **3a** by single-crystal X-ray diffraction experiments (SC-XRD).



Scheme 1. Synthesis, texture of single crystal and ORTEP drawing for (*R,R*)-**3a**

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