

CALIFORNIA STATE SCIENCE FAIR 2010 PROJECT SUMMARY

Name(s)

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Project Number

S0513

Project Title

Propargyl Methyl Ethers: Novel Precursors to Cobalt-Complexed Propargyl Cations

Objectives/Goals

Abstract

The generation of transition metal-stabilized organic cations under neutral conditions has long been sought after in the field of organometallic chemistry. Traditionally, unsaturated organic ligands are treated with strong Lewis acids, such as tetrafluoroboric acid (HBF4). This method, however, is inapplicable for substrates containing functional groups sensitive to acids, in particular benzyloxy and acetal groups.

Methods/Materials

The novel method for the generation of Co2(CO)6-complexed propargyl cations under neutral conditions was developed: employing the metal-bonded methyl propargyl ethers as substrates and triflic anhydride as a reagent.

Results

Ionic propargyl triflates are formed in situ as intermediates, due to successive nucleophilic substitution reactions. The transition of these reactive intermediates to the respective propargyl radicals readily occurs at 83°C (3-6 min), by way of the cluster-to-cluster and cluster-to-ligand single electron transfers. The carbon-carbon formation alpha to the metal clusters affords polysubstituted 3,4-diaryl-1,5-alkadiynes in high yields (>80%) and excellent d,l-diastereoselectivity (89-97%).

Conclusions/Discussion

The scope of the reaction was expanded by involving topologically diverse propargyl ethers, particularly those containing methoxy groups on the periphery of the aromatic nuclei.

Summary Statement

I found that, by utilizing propargyl methyl ethers instead of the traditional propargyl alcohol, I can optimize the synthesis of compounds that can potentially be used in breast cancer prevention and treatment.

Help Received

Used lab equipment at California State University, Northridge under the supervision of Dr. Melikyan. Participant in Southern California Academy of Sciences Research Training Program.