CALIFORNIA STATE SCIENCE FAIR
2014 PROJECT SUMMARY

Name(s)

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Project Number

S0607

Project Title

Generating TMSOCF3 from TMSCF3: A Synthetic Attempt

Abstract

Objectives/Goals

If TMSCF3 transfers the trifluoromethyl anion to carbonyls in presence of trimethyl-N-oxide, which was proposed to proceed though a pentavalent silicon intermediate, then it should be possible for the trimethyl anion to do a 1-2 shift from Si to O in order to form TMSOCF3.

Methods/Materials

In a typical procedure, trimethyl-N-oxide and initiator were weighed in a microwave vial under an Argon atmosphere, and then tightly sealed with a stir vane. Solvent and TMSCF3 were added to the vial and stirred at room temperature. Then, TMSCF3 was added and the reaction mixture was allowed to come to room temperature. All the reactions were analyzed by 19F NMR, using trifluorotoluene as an internal standard.

Results

The first experimental method developed was to add the N-oxide and TMSCF3 with various solvents and temperatures to set a baseline for our understanding of the reaction. Considering lower solubility, Trimethylamine-N-oxide forms a pentavalent intermediate where the geometry of the sigma orbital of the O-N bond is not in place for the trimethyl anion to undergo a 1, 2 shift (not antiperiplanar geometry), we decided to alter this geometry by adding more silophilic species such as F- in the form of TBAT or TMAF. In these reactions, we were expecting to see a signal between -70 to -75 ppm(s) in 19F NMR, which was based on other OCF3 signals in the literature. We observed 20% with respect to internal standard, a signal around -73 ppm in 19F NMR. After screening several conditions, we saw that none of the reactions improved the signal at -73 ppm significantly. However, ample amounts of CF3H were created in the process. Given that each experiment had some amount of CF3H remaining in the mixture, this was considered a product of a side reaction. Our understanding was that the CF3 was cleaved off, as it was supposed to be, but abstracted a proton from a variety of sources, such as a solvent. This potentially explains why we obtained a large amount of CF3H in the reaction mixture.

Conclusions/Discussion

In summary, we attempted to develop TMSOCF3, a compound that was hypothesized to be stable compared to other trifluoromethoxide transfer reagents. To suppress the formation of CF3H, other non-acidic N-oxide reagents need to be explored. In order to confirm the product formation, different approaches are being studied along with computational calculations of the product#s stability (energies) and NMR chemical shifts.

Summary Statement

The OCF3 subgroup is believed to bolster the current medication for Alzheimer's Disease to make it more effective, so the project involves the creation of TMSOCF3 from a known compound, TMSCF3.

Help Received

Used lab equipment at University of Southern California under the supervision of Dr. G. K. Surya Prakash and Sankarganesh Krishnamoorthy