

# Activation of Carbon-Fluorine Bonds in 2', 3', 4', 5', 6'-Pentafluoroacetophenone through a Transition Metal Complex- Manganese Pentacarbonyl

## Introduction

Fluorine forms the strongest single bond to Carbon (bond dissociation energy of about 450 kJ/mol). The great strength of this bond in conjunction with Fluorine's small size and high electronegativity give rise to the characteristic properties of fluorocarbons. Specifically, fluorocarbons are chemically inert, thermally stable, have low toxicity, dissolve gases, and repel water. Unfortunately, the unreactive components of fluorocarbons result in negative impact to the environment. Perfluorocarbons have accumulated in the atmosphere, and as potent greenhouse gases, they have entered wildlife biological systems raising concerns about ecological effects.

## Abstract

The characteristic physical properties of fluorocarbons often result in chemical compounds that are useful in industry on account of the great strength of the C-F bond. Consequently this same bond, makes fluorocarbons extremely unreactive and thus environmentally hazardous. As a result, there is a critical need to develop chemistry designed to activate C-F bonds. Transition Metal Complexes such as Manganese Pentacarbonyl anion, have proven to be a useful tool for selective C-F bond activation under mild conditions. In this synthesis, 2', 3', 4', 5', 6'-Pentafluoroacetophenone underwent a reaction with Manganese Pentacarbonyl to result in a 2', 3', 5', 6'-Tetrafluoroacetophenone compound bound to Manganese Carbonyl in place of an existing Fluorine.

## Materials

$Mn_2(CO)_{10}$  Dimanganese decacarbonyl

$KC_8$  Potassium Graphite

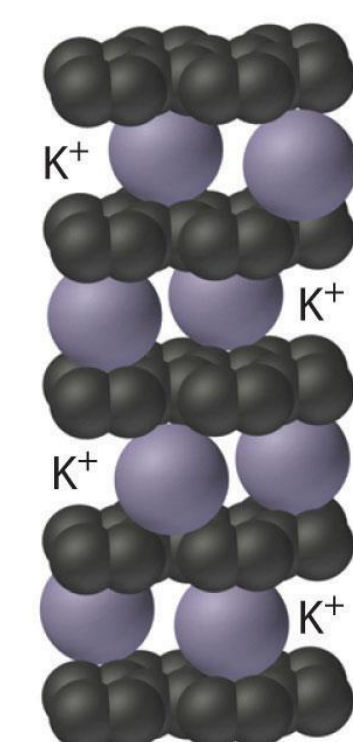
$Mn(CO)_5^-$  Manganese pentacarbonyl

$C_8H_3F_5O$   
2', 3', 4', 5', 6'-  
Pentafluoroacetophenone

THF Tetrahydrofuran

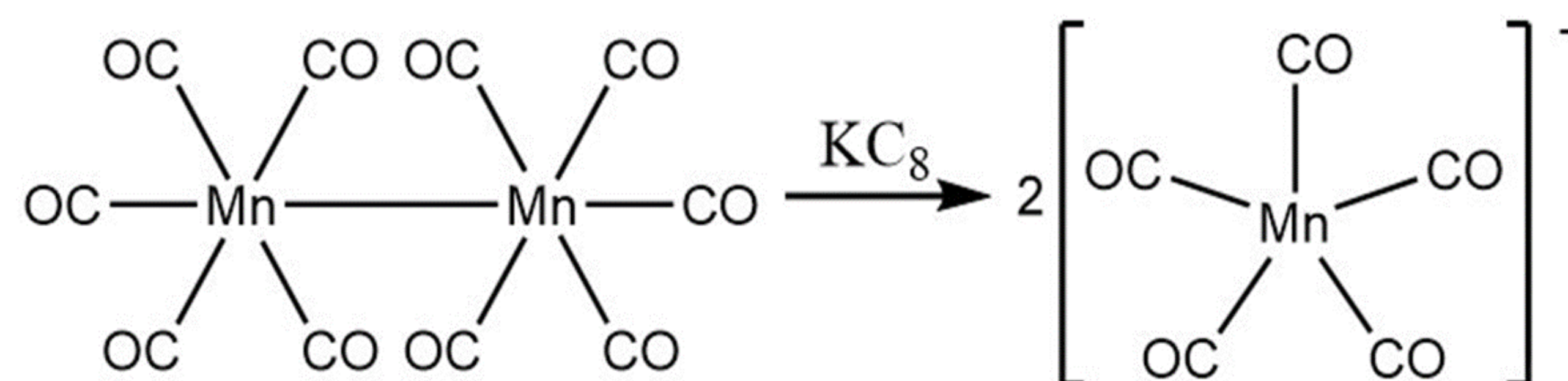
DCM Dichloromethane

$C_6H_{12}$  Cyclohexane

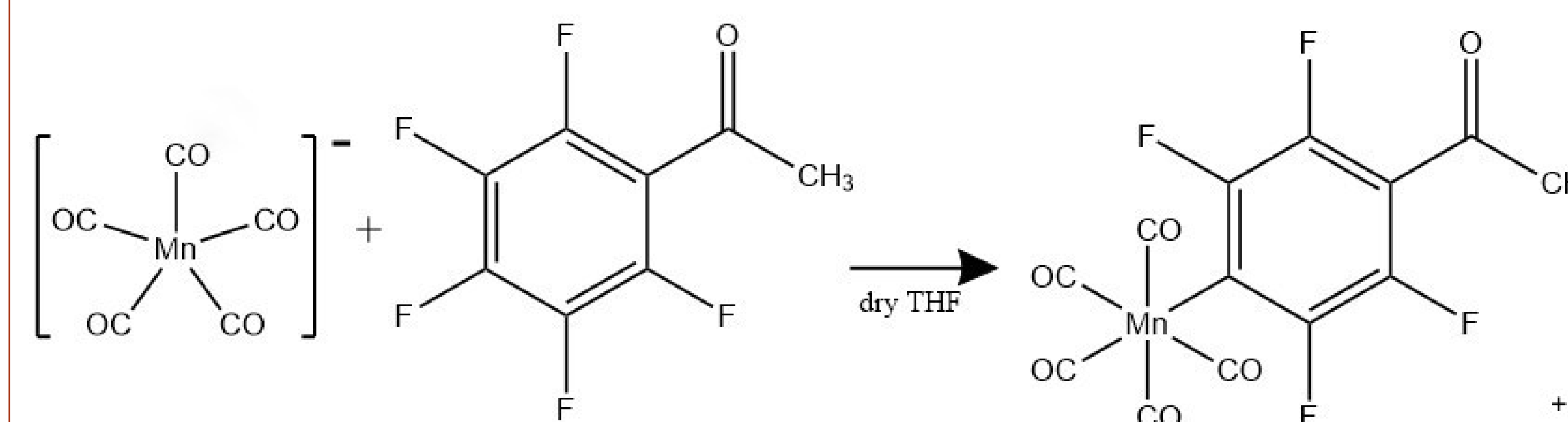


## Procedure

### Step 1



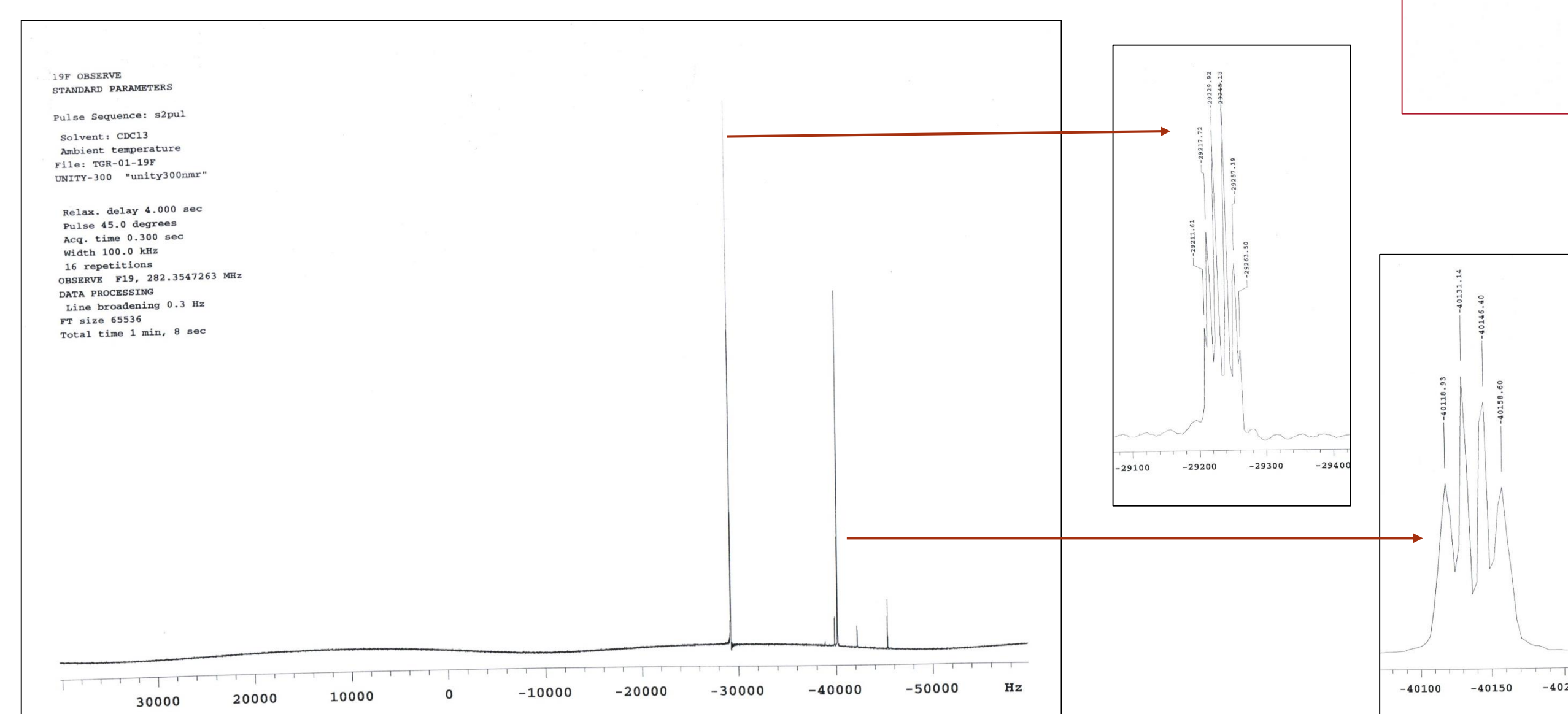
### Step 2



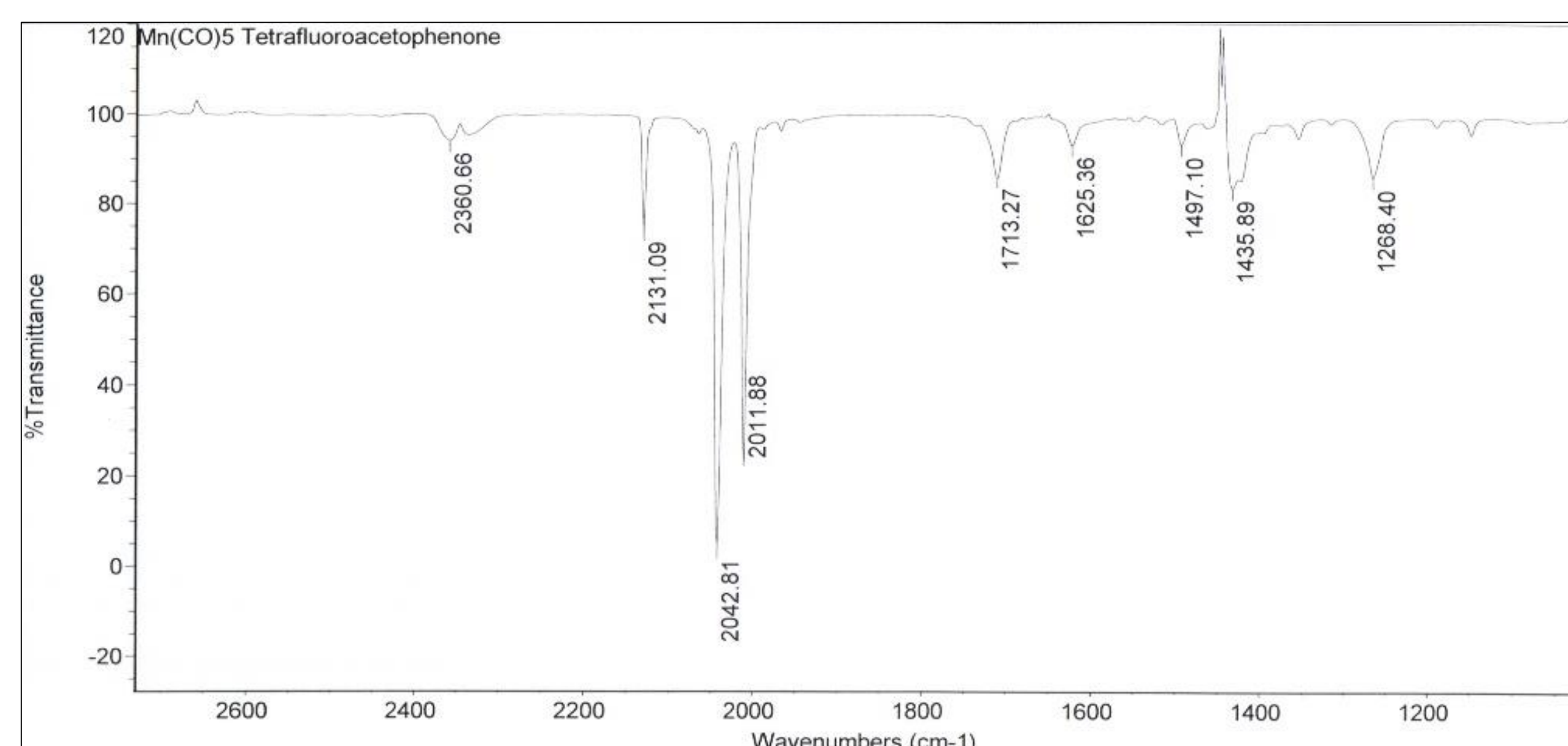
To determine structure:

- Infrared Spectroscopy
- X-ray Crystallography
- NMR- Nucleic Magnetic Resonance

## NMR



## Infrared Spectroscopy



## Data / Observations

$Mn_2(CO)_{10}$	$(OC)_5Mn-C_8H_3F_5O$	$(OC)_5Mn-C \equiv N$	$(OC)_5Mn-C_8H_2F_4O$
2042	2131	2133	2135
2013	2042	2047	2049
1982	2011	2018	2020
	1713	NA	1839

IR Peaks: • 2042, 2047, 2079 → Manganese Carbon Monoxide  $C \equiv O$

IR Peaks: • 1714, 1713 →  $C=O$  Carbonyl

Reactions of metal carbonyl anions with perfluoroarenes under a nitrogen atmosphere often result in facile C-F bond activation and displacement of halides from fluoroaromatic compounds. IR spectra was possible due to the nature of the carbonyl-metal bonding in organometallic compounds: frequency shifts depend significantly on the electron density at the metal center. The shift to higher frequencies is noticeable from the metal anions to the neutral products. The slight shift recognized in Manganese Carbon Monoxide bands suggest that the Transition Metal Complex is more or less electron rich as determined by the electron withdrawing group properties. The 2', 3', 5', 6'-Tetrafluoroacetophenone compound bound to Manganese Carbonyl has the lowest stretches in the Manganese Carbonyl Monoxide bands suggesting that group attached to the aromatic is the least electron withdrawing group.

## Works Cited

- Ahmed, S.K. H.B.S. Dissertation, University of Utah, 2009

## Acknowledgements

- Dr. Thomas G. Richmond, Associate Professor, Chemistry, University of Utah – Principal Investigator
- Dr. Rosemary Gray, Associate Professor, ACCESS program Director, University of Utah x-ray Crystallography
- Dr. Atta Arif, Adjunct Research Associate Professor, University of Utah-
- Lisa Batchelder, ACCESS program Coordinator, University of Utah
- David Baumann, Graduate Student, University of Utah
- Safia Ahmed, Richmond Group 2009, University of Utah
- Nathan Odendahl, Richmond Group, University of Utah
- R. Scott Eldredge, Richmond Group, University of Utah

