

Trifluoroacetyl Chloride
CAS No. 354-32-5

INTRODUCTION

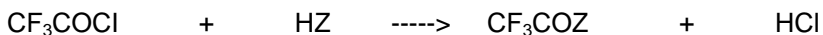
Gaseous trifluoroacetyl chloride (TFAC) provides a way to introduce trifluoromethyl groups into more complex molecules. This compound has been used in the production of pharmaceutical and agricultural chemicals, as well as in many other specialized applications. Halocarbon is proud to have been the first to manufacture this compound and remains the leading producer.

PROPERTIES

CAS Number	354-32-5
Molecular Formula	CF ₃ COCl
Molecular Weight	132.45
Freezing Point, °C	-146
Boiling Point, °C	-28
Density, g/ml, 25°C	1.384 (20°C)
Heat of Vaporization, kJ/mol (Btu/lb)	20 (65)

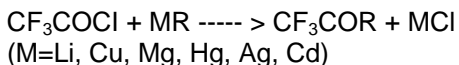
CHEMISTRY

TFAC reacts with active hydrogen (HZ, such as hydroxy and amino groups):



TFAC works in nonaqueous systems producing anhydrous hydrogen chloride as the coproduct. Because HCl can be readily removed from neutral systems, this is usually the most practical commercial route.

The chlorine in TFAC is readily replaced by many anions; I, F, CN, NCO and NCS are examples. TFAC also reacts smoothly with many metal alkyls:



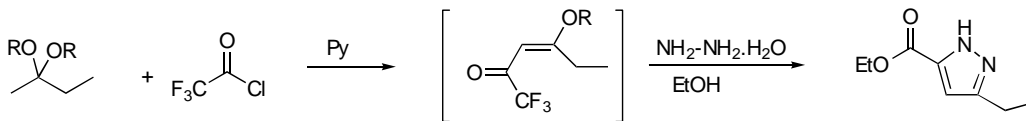
The reaction of TFAC with ketene followed by esterification yields trifluoroacetoacetate esters:



The acetoacetic ester, with two functional sites, is useful in forming heterocyclic compounds for both agricultural and pharmaceutical uses. Some other reactions of TFAC from the recent patent literature which demonstrate its potential as a useful intermediate are shown below.

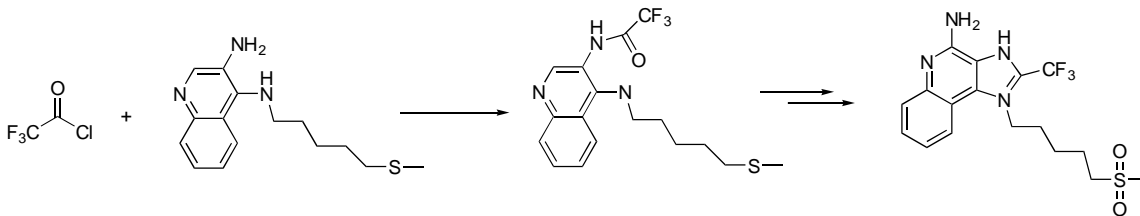
Process for the preparation of pyrazoles

U.S. 6,407,259, 2002, Pfizer, Inc.



Thioether substituted imidazoquinolines

U.S. 6,667,312, 2003, 3M Innovative Properties Company



HANDLING AND SAFETY

Materials of Construction

TFAC is a gas under ambient conditions so it is shipped as a liquid under pressure in cylinders, ton containers and larger steel containers.

Safety

TFAC will cause severe burns to the skin, eyes, mucous membranes and other exposed tissues because of its strong acidity and fast tissue penetration. Special precautions and protective clothing, including rubber gloves and face masks, should be worn when handling this material. The best treatment for spills on the skin is immediate and continuous flooding with water on the affected area.

This compound does not exhibit poisoning due to fluoride ion or any toxicity resembling that of monofluoroacetic acid.

For additional safety information, refer to our Material Safety Data Sheets. The information given above is intended for general reference only.