ACETYL CHLORIDE

PRODUCT IDENTIFICATION

CAS NO.	75-36-5
EINECS NO.	200-865-6
FORMULA	CH_3COCl
MOL WT.	78.50
H.S. CODE	2915.90
TOXICITY	Oral rat LD50: 910 mg/kg
SYNONYMS	Ethanoyl chloride; Acetic acid chloride;
DERIVATION	Acetic acid with a halogenating agent
CLASSIFICATION	

PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE	Clear to slightly yellow fuming liquid
MELTING POINT	112 C
BOILING POINT	51 C
SPECIFIC GRAVITY	1.104
SOLUBILITY IN WATER	rapidly hydrolysis
SOLVENT SOLUBILITY	Soluble: chloroform, glacial acetic acid, ether, benzene
pH	
VAPOR DENSITY	2.7
AUTOIGNITION	390 C
REFRACTIVE INDEX	1.3890
NFPA RATINGS	Health: 3 Flammability: 3 Reactivity: 2
FLASH POINT	4 C
STABILITY	Stable under ordinary conditions but will fume when exposed toatmospheric moisture to form HCl and acetic acid.

DESCRIPTION AND APPLICATIONS

Acyl is a radical formed from an organic acid by removal of a hydroxyl group. The general formula of acyl compound is RCO-. Acyl halide is one of a large group of organic substances containing the halocarbonyl group, have the general formula RCO·X, where X is a halogen atom (fluorine, chlorine, bromine, iodine, and astatine) and R may be aliphatic, alicyclic, aromatic, and H etc. In substitutive chemical nomenclature, their names are formed by adding '-oyl' as a suffix to the name of the parent compound; ethanoyl chloride, CH_3COCl, is an example. The terms acyl and aroyl halides refer to aliphatic or aromatic derivatives, respectively. Acyl halides are made by replacing the -OH group in carboxylic acids by halogen using halogenating agents. They react readily with water, alcohols, and amines and are widely used in organic synthetic process whereby the acyl group is incorporated into the target molecules by substitution of addition-elimination sequence called acylation reaction. Acylation reaction involves substitution by an electron donor (nucleophile) at the electrophilic carbonyl group (C=O). Common nucleophiles in the acylation reaction are aliphatic and aromatic alcohols, both of which give rise to esters and amines (RNH_2) which give amides. The carboxylic acid (X = OH) itself can function as an acylating agent when it is protonated by a strong acid catalyst as in the direct esterification of an alcohol. Two common acylation agents, with the general formula RCOX, are acid halides (X = halogen atom) and anhydrides (X = OCOR). Schotten-Baumann reaction is an acylation reaction that uses an acid chloride in the presence of dilute alkali to acylate the hydroxyl and amino group of organic compounds. There are also other acylating agents. Acid chlorides are used as very reactive intermediates to prepare carboxylic acid derivatives including anhydrides, esters and amides because of the two strong electron withdrawing chlorine and oxygen on the carbonyl compound,

and positive charge carbon accordingly. It is easy for a weak nucleophile to attack the carbon. Acid chlorides are also reactive with Gilman reagents to prepare large molecules from smal ones by replacing the halides with an organic group. Acetyl Chloride is a clear, corrosive and fuming liquid; melting point of -112 C, boiling point of 51-52 C, refractive Index of 1.3890. It undergoes violently hydrolysis in presence of atmospheric moisture. It is soluble in ether, acetone, and acetic acid. It is prepared by reacting acetic acid with a halogenating agent such as phosphorus(III or V) chloride or sulphur dichloride oxide. It is widely used as an acetylating agent in the synthesis of fine chemicals, agrochemicals and pharmaceuticals. The hydrogen atoms replace oxygen atoms in alcohols or nitrogen atoms in amines, which protects amine groups during amino acid synthesis. It is also used as an intermediate for dyes. It is also used to determine water in organic liquids and in testing cholesterol.

SALES SPECIFICATION	
APPEARANCE	Clear to slightly yellow fuming liquid
ASSAY	99.0% min
BOILING POINT	49 C min
COLOR	30 max, Hazen
TRANSPORTATION	
PACKING	190kgs in drum
HAZARD CLASS	3.2, 8 (Packing group: II)
UN NO.	1717
OTHER INFORMATION	
Hazard Symbols: F C, Risk Phrases: 11-14-20-34, Safety Phrases: 9-16-26-45	