P&M-Invest Ltd.
Contact to: http://www.fluorine1.ru
Tel: +7 (499)135-64-94, Fax: +7 (499)135-65 -09
E-mail: igumnov@fluorine1.ru

4,4,4-Trifluorocrotononitrile (abb.FMCN)

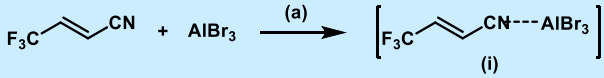
(4,4,4-トリフルオロクロトノニトリル)

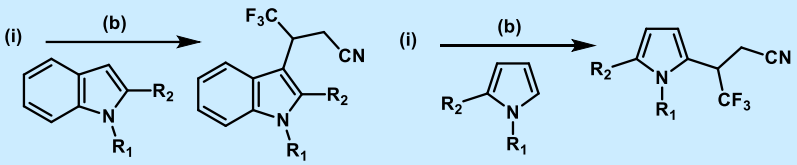
$CF_3CH=CHCN$

Purity	97%
CAS Number	406-86-0
Molecular Formula	C4H2F3N
Molecular Weight	121.06

Application

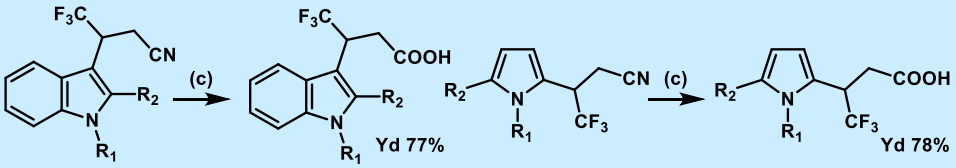
They proposed a method for introducing functional trifluoroalkyl groups into heterocycles. In a study of C-alkylation of N-alkylpyrrole and N-alkylindole, FMCN did not show any C-alkylation reactivity toward the π donor ring like dicyanoethylene, even in various solvents and at high temperatures. Furthermore, even with a common Friedel-Crafts catalyst, C-alkylation remained in low yield (25%).
It was found that C-alkylation of N-alkylpyrrole and N-alkylindole can proceed in good yield by mixing FMCN and AlBr3 in advance to form a homogeneous catalyst. It was also shown that this trifluoromethyl-alkylated nitrile can be easily converted to the corresponding carboxylic acid.





(a) CH2Br2, 20℃, (b) CH2Br2, 5℃*1hr*20℃*6hr, NaHCO3/H2O

No.	R1	R2	Yields Indoles	Yields Pyrroles
1,4	CH3	H	73%	70%
2,5	H	H	55%	58%
3,6	H	H	62%	72%



(c) H2O 25%KOH 75℃*2hr+HCl/H2O,EA

Fluorine Notes, August 2023, by A.L.Sigan et al.

Properties:

Appearance	Liquid
Boiling point, °C	84-85

Packing:

UN, PG:	-