Trichloroacetonitrile as a Source of Positive Chlorine Ion for Trapping the Huisgen’s Zwitterions

Samira Nasiri-Gheidari, Issa Yavari

Department of Chemistry, Tarbiat Modares University, P.O. Box 14115-175, Tehran, Iran
yavarisa@modares.ac.ir

Activated nitriles are highly reactive reagents that have found application in organic synthesis [1], among them trichloroacetonitrile is a unique compound in which, both the cyano group and the trichloromethyl group acquire high reactivities as a result of their mutual effect [2]. In spite of extensive applications of trichloroacetonitrile in organic synthesis [3], there has been no published report on its use as a source of positive chlorine ion.

As part of our current studies on the development of new routes in heterocyclic synthesis [4], we report the results of our studies involving trapping of the Huisgen’s zwitterions derived from isoquinoline (1) and acetylenic esters 2 with trichloroacetonitrile (3), which constitutes a synthesis of dialkyl 2-chloro-3-([dichloro(cyano)methyl]-1,2-dihydroisoquinolin-2(1H)-yl)maleates 4 in good yields.

The reactions proceeded spontaneously in CH₂Cl₂ at room temperature. The structures of compounds 4 were deduced from their IR, ¹H-NMR and ¹³C-NMR spectra.

The structures of compounds 4 were deduced from their IR, ¹H-NMR and ¹³C-NMR spectra.

```
N + CO₂R
CO₂R
CO₂R
|| + Cl₃C-CN
CH₂Cl₂ r.t. →
Cl

1 2 3 4
\  a \ Me \ b \ Et \ Yield %
\ a \ Me \ 90 \ b \ Et \ 80
```

REFERENCES