6

I-7

MULTINUCLEAR NMR STUDIES ON CF$_3$ SUBSTITUTED SULFUR, SELENIUM AND TELLURIUM COMPOUNDS

W. Gombler

Ruhr-Universität Bochum, Anorganische Chemie II, D-4630 Bochum (F.R.G.)

A systematic investigation of thirty-four CF$_3$Se(II, IV) and eight CF$_3$Te(II, IV) compounds by ^{13}C, ^{19}F, ^{77}Se and ^{125}Te NMR spectroscopy resulted in some general features for chemical shifts and coupling constants which agree with the trends of reported ^{19}F and new ^{13}C NMR data of CF$_3$S(II, IV) compounds. Moreover, the NMR spectra of molecules of the type E=CXY (E = chalcogen, X, Y = halogen) and substances containing a C=Se double bond have been studied. From the comparison of these NMR data with those of CF$_3$ substituted chalcogen compounds, a partial double bond character of the carbon-fluorine and carbon-chalcogen bond in CF$_3$ substituted chalcogen compounds can be derived:

$$F_3C-E-R \; \rightleftharpoons \; F^- \left[\begin{matrix} F \\ \diagdown \\ \diagup \\ F \end{matrix} C \cdots E-R \right]^+$$

I-8
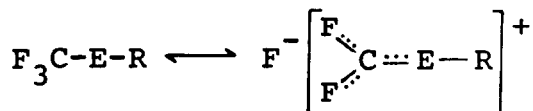
TRIFLUORMETHYLISONITRILE CF$_3$NC, VERSATILE LIGAND IN METAL ORGANIC CHEMISTRY

D. Lentz

Institut f. Anorganische und Analytische Chemie, Freie Universität Berlin, Fabeckstrasse 34–36, 1000 Berlin 33 (F.R.G.)

Although isonitriles and their transition metal complexes have been discovered about one century ago, the first synthesis of Trifluoro-methylisonitrile has been published in 1967 by Makarov et al. But except for the ←addition of bromine no further reactions have been investigated.

The high yield synthesis of CF$_3$NC will be described in detail. Preparation and structural investigations on the new complexes (CO)$_5$CrCNCF$_3$, (CO)$_5$WCNCF$_3$, Ni(CNCF$_3$)$_4$ are given. Especially the vibrational spectra of (CO)$_5$Cr(CNCF$_3$) and (CO)$_5$WCNCF$_3$ differ very much from those of the nonfluorinated species. They are nearly identical to those of the hexacarbonyls and thus give a strong hint that trifluoromethylisonitrile as a ligand