ABSTRACT

The determination of the structure of $Xe(C_6F_5)_2$ from X-ray powder diffraction data leads to the first direct proof of a xenon-compound with two xenon-carbon-bounds.

Fluoride catalyzed reaction of Xenondifluorid with Trimethylarylsilanes yields the hitherto unknown and not described xenon-compounds of the types $Xe(Ar_F)_2$ and Ar_FXeF (Ar_F = (2,3,5,6-F_4C_6H), (2,3,4,6-F_4C_6H), (2,3,4,5-F_4C_6H), (2,4,6-$F_3C_6H_2$), (2,6-$F_2C_6H_3$)), which are characterized on basis of ^{129}Xe- and ^{19}F-NMR-spectroscopy. Because of the deactivation of the silane with lower number of fluorine atoms at the aromate, this route gives the 2,6-Difluorphenyl-xenon-compound in low yield and is not suitable for synthesis of the Monofluorine- and Phenyl-xenon-compounds.

The Fluoride catalyzed reaction of Xenondifluoride with 1,4-Bis(trimethylsilyl)(2,3,5,6-tetrafluorbenzene) gives evidence for the formation of new xenon-compounds with $(Xe\text{-}C_6F_4\text{-}Xe)_n$-groups. However it is not possible to influence the composition of the different products in a sufficient way for further analysis.

The exemplary investigation of the reaction of $(CH_3)_3Si$(2,3,5,6-F_4C_6H) and $[(CH_3)_4N]F$ with the aim to proof the existence of an silicate as the postulated reactive intermediate for the arylation gives indirect proof of $[(CH_3)_4N][(CH_3)_3Si(F)$(2,3,5,6-$F_4C_6H$)].

The survey of the reaction of $F_3SiC_6H_5$ and Xenondifluoride gives NMR-spectroscopic evidence for the formation of a new non-fluorinated xenon-species, whose properties indicate the formation of $[(C_6H_5)Xe]^+$.

By reaction of [(2,6-$F_2C_6H_3$)Xe]$[BF_4]$ with $[(CH_3)_4N]F$ the new xenon-compound (2,6-$F_2C_6H_3$)XeF can be synthesized, which is characterized by its NMR-spectroscopic and chemical properties. It is shown, that (2,6-$F_2C_6H_3$)XeF reacts with silanes by exchange of the terminal fluorine atom to form new xenon-compounds of the type (2,6-$F_2C_6H_3$)XeX (X = $OCOCF_3$, Cl, Br, NCO, CN, C_6F_5, (2,3,5,6-F_4C_6H), (2,6-$F_2C_6H_3$)).

(2,6-Difluorphenyl)xenonbromine represents the first stable xenon(II)-bromine-compound, (2,6-$F_2C_6H_3$)XeNCO the first xenonisocyanate and (2,6-$F_2C_6H_3$)Xe(C_6F_5) the first assymetrical substituted xenon-aryl-compound.

Analyzing the products of the reactions of (2,6-Difluorphenyl)xenonfluoride with $(CH_3)_3SiI$ and $(CH_3)_3SiN_3$ gives evidence for postulating (2,6-$F_2C_6H_3$)XeI and (2,6-$F_2C_6H_3$)XeN_3 as reaction intermediates.

The results of the NMR-spectroscopic investigations of the reaction of 1,4-Bis(trimethylsilyl)(2,3,5,6-tetrafluorbenzene) and (2,6-Difluorphenyl)xenonfluoride indicate the formation of 1,4-Bis(2,6-difluorphenyl)xenon)(2,3,5,6-tetrafluorbenzene). The formation of 1,3-F_2-2-(CF_3)C_6H_3 as a product of the reaction of (2,6-$F_2C_6H_3$)XeF and $(CH_3)_3SiCF_3$ can be explained by the intermediate formation of (2,6-Difluorphenyl)trifluormethylxenon. Reaction of $[(CH_3)_4N][F_5Si(C_6H_5)]$ and (2,6-Difluorphenyl)xenonfluoride leads to the NMR-spectroscopic observation of a xenon-compound, whose properties allow to draw the conclusion that (2,6-$F_2C_6H_3$)Xe(C_6H_5) is formed.

By comparison of calculated structure data of $Xe(C_6F_5)_2$ with those determined by X-ray powder diffraction it is shown that on level of density functional theory (B3LYP) together witch the correlation consistent quasirelativistic *triple-ζ* basis set SDB-cc-pVTZ it is possible to determine minimal structures of xenon-compounds.

By quantum mechanical calculations predictions of structural, thermodynamic an electronic properties of carbon-xenon-compounds are made which are in good agreement with experimental results.

The calculations of electron localization function carried out for the first time on the class of xenon-carbon-compounds show to be helpful for gaining a deeper understanding of the characteristics of xenon-element-bonding.