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C_6F_5XeY Molecules (Y = F and Cl): New Synthetic Approaches. First Structural Proof of the Organoxenon Halide Molecule C_6F_5XeF

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Abstract

The arylxenonium salt $[C_6F_5Xe][BF_4]$ reacts with different sources of nucleophiles, Y (naked fluoride, $[N(CH_3)_4]F$, the silanes, $(CH_3)_3SiCl$ and $(C_2H_5)_3SiH$, and the cadmiumorganyl, $Cd(C_6F_5)_2$), in coordinating solvents (C_2H_5CN, CH_3CN, CD_3CN). While the products C_6F_5XeF, C_6F_5XeCl, and $(C_6F_5)_2Xe$ are well defined molecules, in reactions with $(C_2H_5)_3SiH$ only decomposition products presumably derived from <C_6F_5XeH> and <$C_6F_5XeC_2H_5$> are found. Molecular parameters and intermolecular contacts in the single crystal X-ray structure of C_6F_5XeF are discussed.

Keywords: Arylxenonium tetrafluoroborate, organylxenon molecules, reactions with nucleophiles in coordinating solvents, pentafluorophenylxenon fluoride crystal structure

1. Introduction

The chemistry of organylxenonium salts [RXe][Z] is comprehensively treated in several reviews.[1] The majority of available information concerns the salt $[C_6F_5Xe][BF_4]$ with an electrophilic cation and a moderately to weakly coordinating anion. The most frequently used procedure to obtain ArXeY started from ArXeF (Ar = C_6F_5, $C_6H_nF_{5-n}$) which were reacted with alkylsilanes, Alk_3SiY, (Y = Cl,[2,3] Br, NCO[2], CN,[2,3,4,5] $CF_3C(O)O$, $CF_3S(O)_2O$,[2] C_6F_5,[2,3,4,5] 2,6–$C_6H_3F_2$[2]) in the weakly coordinating solvent CH_2Cl_2. The strong Si–F bond of the co-product was the driving force (Eq 1).

$$\mathrm{ArXeF} + \mathrm{Alk_3SiY} \xrightarrow{CH_2Cl_2/-78\ ^\circ C} \mathrm{ArXeY} + \mathrm{Alk_3SiF} \qquad (1)$$

Thus, ArXeF can be regarded as a key substrate in the syntheses of ArXeY molecules. It was prepared by two routes: (a) the F^- catalyzed F/Ar substitution with Me_3SiAr in XeF_2[6] (the product contained an admixture of $(C_6F_5)_2Xe$) and (b) in the very slow surface reaction of $[ArXe]^+$ salts with $[N(CH_3)_4]F$ in CH_2Cl_2.[4]

In the current work we offer a useful modification of route (b) and a fast homogeneous synthesis of C_6F_5XeF. Furthermore, we investigate the direct reaction of $[C_6F_5Xe][BF_4]$ with Alk_3SiY (Y = Cl, H) to C_6F_5XeY molecules. In case of Y = Cl, we discuss the results which differ from that obtained previously with $[C_6F_5Xe][AsF_6]$.[7] Furthermore, it will be shown that the electrophilic cation of $[C_6F_5Xe][BF_4]$ can directly interact with the carbon nucleophile of the organometallic compound, $Cd(C_6F_5)_2$.

2. Results and Discussion

2. 1. Synthesis of C_6F_5XeF

In 2000, we reported the surface reaction of insoluble $[C_6F_5Xe][AsF_6]$ with equimolar amounts of dissolved $[N(CH_3)_4]F$ in CH_2Cl_2 at –78 °C.[4] That reaction required more than 2 days for complete conversion and was accompanied by the partial decomposition of the product, C_6F_5XeF. A modified reaction using 1.5 equiv of $[N(CH_3)_4]F$ in CH_2Cl_2 is described in the present work. The excess of $[N(CH_3)_4]F$ can act as a HF scavenger. Finally, *n*-pentane was added to reduce the density of the solvent and to precipitate all $[N(CH_3)_4]^+$ salts. After distilling off the solvent mixture from C_6F_5XeF, the latter remained as a white powder (66% yield) which was dissolved in CH_2Cl_2 at –50 °C. Crystals suitable for single crystal X-ray structural determination having a plate morphology with right angles were obtained by a very slow partial removal of the solvent under vacuum.

An alternative fast synthesis of C_6F_5XeF started from a cold (–78 °C) C_2H_5CN solution of $[C_6F_5Xe][BF_4]$ which was added to a cold (–78 °C) CH_2Cl_2 solution of $[N(CH_3)_4]F$. Monitoring the reaction after 20 min revealed the total conversion of the xenonium salt with the formation of C_6F_5XeF (95%), C_6F_5H (5%), and traces of C_6F_6 (Eq 2).

$$[C_6F_5Xe][BF_4]/C_2H_5CN + [N(CH_3)_4]F/CH_2Cl_2 \xrightarrow{-78\ ^\circ C} C_6F_5XeF + [N(CH_3)_4][BF_4] \quad (2)$$

2. 2. The Molecular Structure of C_6F_5XeF and Important Intermolecular Contacts in the Solid State Structure

The compound, C_6F_5XeF crystallizes in the monoclinic space group $P2_1/n$ (a = 12.2038(3) Å, b = 9.9596(3) Å, c = 13.0904(4) Å, β = 101.140(1)°) with eight molecules in the unit cell and two molecules in the asymmetric unit. The crystallographic data are given in Table 1. The molecular parameters of both molecules are similar and mainly differentiated by their intermolecular contacts. The C-Xe-F arrangement of C_6F_5XeF is linear with a C1-Xe1-F1 angle in molecule 1 of 178.67(6)° (the analogous angle in molecule 2: 179.46(7)°). The Xe-C distance in molecule 1 is 2.132(2) Å (2.128(2) Å in molecule 2) and is longer than in the xenonium cations of $[C_6F_5Xe][AsF_6]$ (2.079(5) and 2.082(6) Å),[8] $[C_6F_5Xe][B(CN)_4]$ (2.081(3) Å),[9] $[C_6F_5Xe][B(CF_3)_4]$ (2.104(5) Å),[9] in the acetonitrile adducts of the xenonium cation in $[C_6F_5Xe \cdot NCCH_3]$ $[B(CF_3)_4]$ (2.100(6) Å) and $[C_6F_5Xe \cdot NCCH_3][B(C_6F_5)_4]$ (2.100(10) Å),[9] and only slightly longer than in $C_6F_5XeOC(O)C_6F_5$ (2.122(4) Å).[10] On the other hand, the Xe-F distance in C_6F_5XeF (2.172(1) Å (molecule 1) and 2.182(1) Å (molecule 2)) is significantly shorter than the Xe-F cation–F contacts (F from the counterion) in $[C_6F_5Xe][AsF_6]$ (2.714(5) and 2.672(5) Å),[8] $[C_6F_5Xe][B(CF_3)_4]$ (2.913(4) Å).[9] Thus, bonding in the C-Xe-F fragment is best described as an asymmetrical hypervalent bond. The C-Xe distance is shorter than in $(C_6F_5)_2Xe$ (2.394(9) and 2.35(1) Å)[11] and the Xe-F distance longer than in XeF_2 (2.00(1) Å.[12] In addition to arguments based on experimental distances, the asymmetry is also supported by the partial charges on the C_6F_5 group and F ("Natural Population Analysis" charges (DFT method SVWN, basis set SDD): C_6F_5 –0.33 e^-, F –0.64 e^-, Xe 0.97 e^-; (RHF method, basis set LANL2DZ): C_6F_5 –0.37 e^-, F –0.77 e^-, Xe 1.13 e^-. The calculated gas phase structure depends on the applied method and basis set. Using the DFT method SVWN and the basis set SDD the C-Xe distance is overestimated (2.18 Å) and the Xe-F distance underestimated (2.08 Å) when compared with the solid state experimental parameters. With the RHF method and the basis set LANL2DZ, the C-Xe distance was 2.20 Å (overestimated) and Xe-F distance was 2.13 Å (underestimated). In comparison with the symmetrical parent molecules (values from the [DFT method, SVWN and basis set SDD] and the {RHF method and basis set LANL2DZ} XeF_2 [Xe-F 2.03 Å, Xe 1.10 e^-, F –0.55 e^-], {Xe-F 2.03 Å, Xe 1.33 e^-, F –0.67 e^-} and $(C_6F_5)_2Xe$ [Xe-C 2.30 Å, Xe 0.81 e^-, C_6F_5 –0.40 e^-], {Xe-C 2.34 Å, Xe 0.98 e^-, C_6F_5 –0.49 e^-}, the molecule C_6F_5XeF can also be described as a close ion pair. The distribution of partial charges allows also to interpret the observed intermolecular interactions of C_6F_5XeF in the solid state: Xe-bonded fluorine and Xe^{II} interact in a donor acceptor manner. Two symmetry equivalent molecules 2 are arranged head to tail in a side-on mode and form a Xe2-F11–Xe2'-F11' parallelogram (Figure 1). In addition, each Xe2 of the parallelogram acts as acceptor of F1 and each F11 of the parallelogram as donor to Xe1. It is worth stressing, that the donor property of F11, which donates to two Xe^{II}, namely Xe1 and Xe2', leads to one shorter contact than in the single contact of F1''' to Xe2.

2. 3. Synthesis of C_6F_5XeCl

In 1999, we investigated the conversion of $[C_6F_5Xe][AsF_6]$ into C_6F_5XeCl.[7] We were only successful when insoluble $[C_6F_5Xe][AsF_6]$ was reacted with soluble

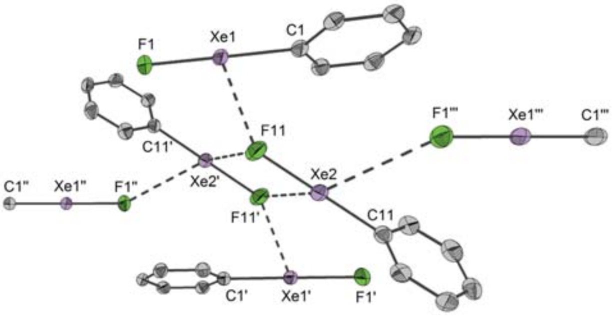

Figure 1. The molecular structure of C_6F_5XeF (fluorine atoms of the C_6F_5 group are not depicted) showing the most significant intermolecular contacts. The thermal ellipsoids are drawn at the 50% probability level.
Selected distances / Å and angles / °: Xe1–C1 2.132(2), Xe1–F1 2.172(1), C1–Xe1–F1 178.67(6), Xe2–C11 2.128(2), Xe2–F11 2.182(1), C11–Xe2–F11 179.46(7).
Significant intermolecular contacts / Å and angles / °: Xe1–F11 3.036(1), Xe2–F1''' 3.261(1), Xe2–F11' 3.288(1), F11-Xe2–F11' 78.65(4), Xe2-F11–Xe2' 101.35(5), Xe2-F11–Xe1 146.97(6), Xe2'–F11–Xe1 90.95(4), F1-Xe1–F11 108.06(4), C1-Xe1–F11 72.38(6)

Table 1. Crystallographic and refinement data for C_6F_5XeF

Compound	C_6F_5XeF
Empirical formula	C_6F_6Xe
Crystal size	0.32 mm × 0.26 mm × 0.16 mm
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 12.2038(3) Å
	b = 9.9596(3) Å
	c = 13.0904(4) Å
	β = 101.140(1)°
Volume	1561.09(8)Å^3
Z (molecules/unit cell)	8
Density (calculated)	2.701 g cm^{-3}
Temperature	173 ± 2 K
Radiation	Mo K$_\alpha$ (λ = 0,71073 Å)
F(000)	1152
Theta range for data collection	2.09–30.46 °
Final R indices	R_1 = 0.0180, wR_2 = 0.0431

4-$ClC_5H_4N \cdot HCl$ in weakly coordinating CH_2Cl_2 at –78 °C. When CH_3CN solutions of $[C_6F_5Xe][AsF_6]$ and $[N(CH_3)_4]Cl$ were combined at ≤ –20 °C, no reaction proceeded and at 0 °C, C_6F_5Cl was formed along with Xe^0. When $(CH_3)_3SiCl$ was used as a source of chlorine in CH_2Cl_2 at –78 °C, 3 equiv of the silane were required for the total conversion of $[C_6F_5Xe][AsF_6]$. Instead of C_6F_5XeCl, the salt with the chlorine bridged bis(pentafluorophenylxenonium) cation, $[(C_6F_5Xe)_2Cl][AsF_6]$, was isolated and established from its crystal structure.[7] Under these conditions, the $[AsF_6]^-$ anion also underwent F/Cl substitution followed by the elimination of chlorine from the proposed intermediate, $AsCl_5$ (Eq 3).

$$2\,[C_6F_5Xe][AsF_6] + 6\,(CH_3)_3SiCl \xrightarrow{CH_2Cl_2/-78\ ^\circ C} [(C_6F_5Xe)_2Cl][AsF_6] + 6\,(CH_3)_3SiF + AsCl_3 + Cl_2 \tag{3}$$

In contrast to Eq 3, the presence of CH_3CN avoided F/Cl substitution on AsF_5 (Eq 4).

$$2\,[C_6F_5Xe][AsF_6] + (CH_3)_3SiCl + CH_3CN \xrightarrow{CH_2Cl_2/-78\ ^\circ C} [(C_6F_5Xe)_2Cl][AsF_6] + (CH_3)_3SiF + AsF_5{\cdot}NCCH_3 \tag{4}$$

In the present work, we report a different mode of reactivity for $[C_6F_5Xe][BF_4]$ with $(CH_3)_3SiCl$. In CH_2Cl_2 at –40 °C (heterogeneous reaction), only 8% conversion into soluble C_6F_5XeCl occurred within 3 h (Eq 5), whereas in the homogenous reaction in CH_3CN at –40 °C the total conversion took place in less than 20 min (Eq 6). In C_2H_5CN solution at –78 °C, only a slow reaction was observed, but at –55 °C the conversion proceeded in less than 5 min.

$$\underset{\text{8\% conversion/3 h}}{[C_6F_5Xe][BF_4] + (CH_3)_3SiCl} \xrightarrow{CH_2Cl_2/-40\ ^\circ C} C_6F_5XeCl + BF_3 + (CH_3)_3SiF \tag{5}$$

$$\underset{\text{100\% conversion/≤20 min}}{[C_6F_5Xe][BF_4] + (CH_3)_3SiCl} \xrightarrow{CH_3CN/-40\ ^\circ C} C_6F_5XeCl + BF_3{\cdot}NCCH_3 + (CH_3)_3SiF \tag{6}$$

Eqs 5 and 6 show that the $[BF_4]^-$ anion was involved in the reaction with $(CH_3)_3SiCl$ and that another Xe^{II} product resulted that differs from that formed in the presence of the $[AsF_6]^-$ anion. To elucidate the interaction of the $[BF_4]^-$ anion with $(CH_3)_3SiCl$, the reaction of $[N(n\text{-}C_4H_9)_4][BF_4]$ with $(CH_3)_3SiCl$ was investigated at 20 °C in CH_3CN and only 17% conversion of $[BF_4]^-$ to $[BClF_3]^-$ within 1.5 h was found. That result underlines the participation of the electrophilic $[C_6F_5Xe]^+$ cation in F/Cl-substitution (Eq 6) in the presence of CH_3CN. It was reported that the $[BF_4]^-$ anion was also involved in the very slow reaction (4 d) of $[2,6\text{-}C_6H_3F_2Xe][BF_4]$ with $(CH_3)_3SiOSO_2CF_3$ in a CH_3CN/CH_2Cl_2 mixture at –20 °C.[13] A forthcoming paper will exemplify the general character of the participation of electrophilic cations of tetrafluoroborate salts in nucleophilic substitution reactions.

2. 4. The Reaction of $[C_6F_5Xe][BF_4]$ with $(C_2H_5)_3SiH$ in CD_3CN and C_2H_5CN Solutions

The reaction of $[C_6F_5Xe][BF_4]$ with $(C_2H_5)_3SiH$ in CD_3CN at –40 °C proceeded almost quantitatively within 20 min. The $[BF_4]^-$ anion was converted into $BF_3 \cdot NCCD_3$. C_6F_5H resulted as the main product (61%) besides traces of C_6F_5D (2%) only. Over and above that, five C_6F_5 compounds were formed: $(C_6F_5)_2Xe$ (5%), $(C_6F_5)_2$ (1%), $C_6F_5CH_2CH_3$ (5%), $C_6F_5Si(C_2H_5)_3$ (2%), and $[C_6F_5C(CD_3) = N(H,D)_2]^+$ (19%) The above products and their molar ratio allow some reasonable conclusions. (a) C_6F_5H can result from the short living (not NMR spectroscopically proven) compound C_6F_5XeH by Xe^0 elimination or, as the in cage product of $C_6F_5^\bullet$ and $H^\bullet$ radical combination, after oxidation of H^- by $[C_6F_5Xe]^+$ and subsequent Xe^0 elimination from the $[C_6F_5Xe]^\bullet$ radical. Abstraction of deuterium by $C_6F_5^\bullet$ (out of cage) proceeded only by a minor route. (b) $(C_6F_5)_2Xe$, $(C_6F_5)_2$, and $C_6F_5C_2H_5$ may result from the intermediate $<C_6F_5XeC_2H_5>$: $(C_6F_5)_2Xe$ as one product of the equilibration, $C_6F_5C_2H_5$ by the direct elimination of Xe^0 from $C_6F_5XeC_2H_5$ and $(C_6F_5)_2$ by Xe^0 elimination from

$(C_6F_5)_2Xe$. The latter route is described in the literature.[4] (c) The formation of large amounts of $[C_6F_5C(CD_3)=N(H,D)_2]^+$ presumably results from the addition of $C_6F_5^{\bullet}$ radicals to the C-N triple bond of the solvent, followed by H or D scavenging and $(H,D)^+$ addition to the imino nitrogen atom). The high-frequently *p*-fluorine resonance (–141.5 ppm) is a strong indicator of the cationic nature. The ^{19}F NMR shift values are in good agreement with that of the only related structure in the literature $[C_6F_5C(CH_3)=N(C_2H_5)_2]Br$.[14] A Xe-C structure can be rejected despite the high-frequently *p*-F resonance, which is typical for Xe-C_6F_5 cations, because neither a ^{129}Xe resonance nor ^{129}Xe satellites in ^{19}F signals were found nor did the compound decompose after heating to 20 °C for 1 h.

When the reaction of $[C_6F_5Xe][BF_4]$ with $(C_2H_5)_3SiH$ was performed in C_2H_5CN solution at –90 °C, a similar mixture of products resulted, but at a slower rate. The main difference derives from the $C_6F_5^{\bullet}$ radical interaction with the solvent, namely the formation of the $[C_6F_5C(C_2H_5)=NH_2]^+$ cation.

Based on RHF/LANL2DZ calculations the assumed intermediate, C_6F_5XeH, should be described in the gas phase as H-Xe–C_6F_5 with a very weak Xe-C bond (2.54 Å) and a Xe-H bond of 1.74 Å and "Natural Population Analysis" charges of 0.80 e^- (Xe), –0.08 e^- (H), and –0.72 e^- (C_6F_5).

2. 5. The Reaction of $[C_6F_5Xe][BF_4]$ with $Cd(C_6F_5)_2$ in C_2H_5CN Solution

When $[C_6F_5Xe][BF_4]$ was reacted with $Cd(C_6F_5)_2$ in the coordinating solvent C_2H_5CN at –78 °C the $[BF_4]^-$ anion was involved in a metathesis reaction and in contrast to reactions with Alk_3SiY, it did not serve as a source of fluoride for the acidic Cd^{II} center. $(C_6F_5)_2Xe$ was precipitated within less than 2 h along with small amounts of $Cd[BF_4]_2$, which could be removed by washing with cold C_2H_5CN (Eq 7).

$$2\,[C_6F_5Xe][BF_4] + Cd(C_6F_5)_2 \xrightarrow{C_2H_5CN/-78\ ^{\circ}C} 2(C_6F_5)_2Xe\downarrow + Cd[BF_4]_2 \qquad (7)$$

It is worth mentioning that $(C_6F_5)_2Xe$ was found to decompose when pressure was exerted on the solid, e.g., with a spatula, even in a C_2H_5CN suspension at –78 °C. After decomposition, $(C_6F_5)_2$ and C_6F_5H were found in the molar ratio of 83 to 17.

3. Experimental Section

3. 1. General

The NMR spectra were recorded on a Bruker AVANCE 300 spectrometer (^1H at 300.13 MHz; ^{19}F at 282.40 MHz; ^{11}B at 96.29 MHz, ^{129}Xe at 83.02 MHz, and ^{13}C at 75.47 MHz). The chemical shifts were referenced to TMS (^1H and ^{13}C), CCl_3F (^{19}F, with C_6F_6 as secondary reference (–162.9 ppm)), $BF_3 \cdot OEt_2/CDCl_3$ (15% v/v) (^{11}B), and $XeOF_4$ (^{129}Xe, with XeF_2 in CH_3CN (extrapolated to zero concentration) as secondary external reference (–1818.3 ppm)[15], respectively. The composition of the reaction mixtures was determined by ^{19}F NMR spectroscopy using internal standards for integration.

X-ray diffraction data were collected at 173 ± 2 K using a diffractometer equipped with a Siemens SMART three axis goniometer and an APEX II area detector system. Crystal structure solution by Direct Methods and refinement on *F*2 were performed using the Bruker AXS SHELXTL software suite Version 6.12 after data reduction, and empirical absorption correction was performed using the Bruker AXS SAINT program Version 6.0. For crystallographic and refinement details see Table 1.

Crystal structure data have been deposited at the Cambridge Crystallographic Data Centre (CCDC). Enquiries for data can be directed to Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, U.K., CB2 1EZ or (e-mail) deposit@ccdc.cam.ac.uk or (fax) +44 (0) 1223 336033. Any requests sent to the Cambridge Crystallographic Data Centre for this material should quote the full literature citation and the reference number CCDC 889108.

$[C_6F_5Xe][BF_4]$ was prepared according to literature.[16] CH_3CN, C_2H_5CN, *n*-C_5H_{12}, and CH_2Cl_2 were purified and dried as described in ref 17. $(C_2H_5)_3SiH$ (Merck, >99%) was used as supplied. $(CH_3)_3SiCl$ (Merck, >99%) was freshly distilled and $[N(n\text{-}C_4H_9)_4[BF_4]$ (Fluka, >99%) was dried under vacuum before use. $Cd(C_6F_5)_2$ and $[N(CH_3)_4]F$ were prepared according to refs 18 and 19, respectively.

All reactions were performed in FEP (a block copolymer of tetrafluoroethylene and hexafluoropropylene) or PFA (a block copolymer of tetrafluoroethylene and perfluoroalkoxytrifluoroethylene) vessels under an atmosphere of dry argon.

3. 2. Synthesis of C_6F_5XeF in CH_2Cl_2

An excess of $[N(CH_3)_4]F$ (143.1 mg; 1.537 mmol) was partially dissolved in cold CH_2Cl_2 (10 mL; –78 °C) in an FEP trap (inner diameter = 23 mm). Solid $[C_6F_5Xe][BF_4]$ (386.4 mg; 1.003 mmol) was added and the suspension was intensively stirred for 2 d at –78 °C. Because of the lower density of the solid relative to the solution, the solid remained on the surface. *n*-Pentane (10 mL; –78 °C) was added till the solid precipitated. A sample (250 µL; –78 °C) was taken and analyzed by ^{19}F NMR spectroscopy.

^{19}F NMR (CH_2Cl_2/*n*-C_5H_{12} at –80 °C) δ(ppm): –129.0 (m, $^3J(F^{2,6}\text{-}^{129}Xe)$ = 81 Hz, 2F, *o*-C_6F_5), –146.6 (t, $^3J(F^4\text{-}F^{3,5})$ = 20 Hz, 1F, *p*-C_6F_5), –156.2 (m, 2F, *m*-C_6F_5),

–2.2 (s, $\Delta\nu_{1/2}$ = 153 Hz, $^{1}J(^{19}\mathrm{F}\text{-}^{129}\mathrm{Xe})$ = 4030 Hz, 1F, Xe*F*), C_6F_5XeF; –139.3 (m, 2F, *o*-C_6F_5), –154.5 (t, $^{3}J(\mathrm{F}^{4}\text{-}\mathrm{F}^{3,5})$ = 21 Hz, 1F, *p*-C_6F_5), –162.7 (m, 2F, *m*-C_6F_5), C_6F_5H; –141.3 (m, 2F, *o*-C_6F_5), –150.9 (m, 1F, *p*-C_6F_5), –161.4 (m, 2F, *m*-C_6F_5), C_6F_5Cl; molar ratio related to the sum of C_6F_5 compounds: C_6F_5XeF (66%); C_6F_5H (33%); C_6F_5Cl (1%).

$[N(CH_3)_4]F$ and $[N(CH_3)_4][BF_4]$ are insoluble in CH_2Cl_2/*n*-pentane (1:1) at –78 °C and could be separated from the C_6F_5XeF solution by centrifugation at –78 °C. After removal of the solvents under vacuum (1.5 h; –55 to –50 °C; $8 \cdot 10^{-2}$ hPa) a white powder remained, which was dissolved in CH_2Cl_2 (3 mL; –50 °C) in an FEP trap (inner diameter = 8 mm). For growing single crystals, the solution was slowly concentrated in vacuum (8 h; –55 to –45 °C; $8 \cdot 10^{-2}$ hPa). After 8 h colorless transparent crystals (right angular plates; dimensions: 1 to 2 mm) were grown and stored under the mother liquor at –78 °C. The crystallographic data are compiled in Table 1.

3. 3. Synthesis of C_6F_5XeF in C_2H_5CN/CH_2Cl_2

A cold solution of $[N(CH_3)_4]F$ (8.9 mg; 0.096 mmol) in CH_2Cl_2 (450 μL; –78 °C) was added to a cold solution of $[C_6F_5Xe][BF_4]$ (20.0 mg; 0.0519 mmol) in C_2H_5CN (50 μL; –78 °C) in an FEP inliner. A suspension resulted. After 20 min the total conversion into C_6F_5XeF (95% yield) was confirmed by ^{19}F NMR spectroscopy. Only 5% of C_6F_5H and traces of C_6F_6 were present. The co-product $[N(CH_3)_4][BF_4]$ was insoluble.

^{19}F NMR (C_2H_5CN at –80 °C) δ(ppm): –129.4 (m, $^{3}J(\mathrm{F}^{2,6}\text{-}^{129}\mathrm{Xe})$ = 81 Hz, 2F, *o*-C_6F_5), –147.1 (t, $^{3}J(\mathrm{F}^{4}\text{-}\mathrm{F}^{3,5})$ = 21 Hz, 1F, *p*-C_6F_5), –156.7 (m, 2F, *m*-C_6F_5), –4.0 (s, $\Delta\nu_{1/2}$ = 60 Hz, $^{1}J(^{19}\mathrm{F}\text{-}^{129}\mathrm{Xe})$ = 4007 Hz, 1F, Xe*F*), C_6F_5XeF; –139.8 (m, 2F, *o*-C_6F_5), –155.1 (t, $^{3}J(\mathrm{F}^{4}\text{-}\mathrm{F}^{3,5})$ = 21 Hz, 1F, *p*-C_6F_5), –163.1 (m, 2F, *m*-C_6F_5), C_6F_5H; –162.9 (s, $\Delta\nu_{1/2}$ = 5 Hz, 6F), C_6F_6; –94.4 (s, $\Delta\nu_{1/2}$ = 44 Hz, 1F), F^-; molar ratio related to the sum of C_6F_5 compounds: C_6F_5XeF (95%); C_6F_5H (5%); C_6F_6 (<1%); F^- (82%).

3. 4. Synthesis of C_6F_5XeCl in CH_3CN

$(CH_3)_3SiCl$ (7.1 mg; 0.065 mmol; 8.2 μL) was added to a suspension of $[C_6F_5Xe][BF_4]$ (22.6 mg; 0.0588 mmol) in cold CH_2Cl_2 (350 μL; –78 °C) in an FEP inliner. The starting materials were intensively mixed and the progress of the reaction was monitored by ^{19}F NMR spectroscopy. After 1 h at –78 °C only traces of C_6F_5XeCl, BF_3, and $(CH_3)_3SiF$ were formed. Even after 3 h at –40 °C the conversion reached 8% only. The mother liquor was separated from unreacted $[C_6F_5Xe][BF_4]$. The salt was washed twice with cold CH_2Cl_2 (each 300 μL; –78 °C) and dried in vacuum (3 h; –78 to –50 °C; $4 \cdot 10^{-2}$ hPa). Recovered $[C_6F_5Xe][BF_4]$ was dissolved in cold CH_3CN (300 μL; –45 °C) and $(CH_3)_3SiCl$ (6.9 mg; 0.064 mmol; 8.0 μL) was added. After 20 min the total conversion was confirmed by NMR.

^{19}F NMR (CH_3CN at –40 °C) δ(ppm): –130.3 (m, $^{3}J(\mathrm{F}^{2,6}\text{-}^{129}\mathrm{Xe})$ = 91 Hz, 2F, *o*-C_6F_5), –146.7 (tt, $^{3}J(\mathrm{F}^{4}\text{-}\mathrm{F}^{3,5})$ = 20 Hz, $^{4}J(\mathrm{F}^{4}\text{-}\mathrm{F}^{2,6})$ = 3 Hz, 1F, *p*-C_6F_5), –156.4 (m, 2F, *m*-C_6F_5), C_6F_5XeCl; –156.2 (dec, $^{3}J(\mathrm{F}\text{-}\mathrm{H})$ = 7 Hz, $^{1}J(^{19}\mathrm{F}\text{-}^{29}\mathrm{Si})$ = 273 Hz, 1F), $(CH_3)_3SiF$; –141.6 (s, $\Delta\nu_{1/2}$ = 31 Hz, 3F), $BF_3 \cdot NCCH_3$; molar ratio related to C_6F_5XeCl: C_6F_5XeCl (100%); $(CH_3)_3SiF$ (100%); $BF_3 \cdot NCCH_3$ (100%). ^{1}H NMR (CH_3CN at –40 °C) δ(ppm): 0.4 (s, $\Delta\nu_{1/2}$ = 2 Hz, 9H), $(CH_3)_3SiCl$; 0.2 (d, $^{3}J(\mathrm{H}\text{-}\mathrm{F})$ = 7 Hz, 9H), $(CH_3)_3SiF$; molar ratio: $(CH_3)_3SiCl$ (18%); $(CH_3)_3SiF$ (100%)

3. 5. Synthesis of C_6F_5XeCl in C_2H_5CN

A solution of $(CH_3)_3SiCl$ (11.3 mg; 0.104 mmol) in cold C_2H_5CN (200 μL; –78 °C) was added to a solution of $[C_6F_5Xe][BF_4]$ (28.5 mg; 0.0739 mmol) in cold C_2H_5CN (200 μL; –78 °C) in an FEP inliner. At –78 °C only 6% conversion proceeded within 80 min. After 5 min at –55 °C and following storage at –78 °C ^{19}F NMR spectroscopy confirmed the total conversion. At –50 °C $(CH_3)_3SiF$ was removed from C_6F_5XeCl in vacuum without decomposition of the latter.

^{19}F NMR (C_2H_5CN at –80 °C) δ(ppm): –131.1 (m, $^{3}J(\mathrm{F}^{2,6}–^{129}\mathrm{Xe})$ = 94 Hz, 2F, *o*-C_6F_5), –147.3 (t, $^{3}J(\mathrm{F}^{4}\text{-}\mathrm{F}^{3,5})$ = 21 Hz, 1F, *p*-C_6F_5), –157.1 (m, 2F, *m*-C_6F_5), C_6F_5XeCl; –139.5 (m, 2F, *o*-C_6F_5), –154.6 (tm, $^{3}J(\mathrm{F}^{4}\text{-}\mathrm{F}^{3,5})$ = 21 Hz, 1F, *p*-C_6F_5), –162.5 (m, 2F, *m*-C_6F_5), $C_6F_5H^{*}$; –157.1 (dec, $^{3}J(\mathrm{F}\text{-}\mathrm{H})$ = 7 Hz, $^{1}J(^{19}\mathrm{F}\text{-}^{29}\mathrm{Si})$ = 273 Hz, 1F), $(CH_3)_3SiF$; –142.2 (s, $\Delta\nu_{1/2}$ = 5 Hz, 3F), $BF_3 \cdot NCC_2H_5$; –151.1 (br, $\Delta\nu_{1/2}$ = 19 Hz, 4F), $[BF_4]^-$; molar ratio related to the sum of C_6F_5 compounds: C_6F_5XeCl (98%), C_6F_5H (2%), $(CH_3)_3SiF$ (100%), $BF_3 \cdot NCC_2H_5$ (92%), $[BF_4]^-$ (3%). * C_6F_5H (2%) resulted during the dissolution of $[C_6F_5Xe][BF_4]$ in C_2H_5CN already and did not increase after addition of $(CH_3)_3SiCl$.

^{1}H NMR (C_2H_5CN at –80 °C) δ(ppm): 7.4 (t, $^{3}J(\mathrm{H}\text{-}\mathrm{F}^{2,6})$ = 8 Hz, 1H), C_6F_5H; 0.4 (s, $\Delta\nu_{1/2}$ = 4 Hz, 9H), $(CH_3)_3SiCl$; 0.2 (d, $^{3}J(\mathrm{H}\text{-}\mathrm{F})$ = 7 Hz, 9H), $(CH_3)_3SiF$; 0.1 (s, $\Delta\nu_{1/2}$ = 4 Hz, 18H), $((CH_3)_3Si)_2O^{**}$; molar ratio: C_6F_5H (2%), $(CH_3)_3SiCl$ (38%), $(CH_3)_3SiF$ (100%), $((CH_3)_3Si)_2O$ (2%); ** $(CH_3)_3SiCl$ contained 1% $((CH_3)_3Si)_2O$.

C_6F_5XeCl

^{19}F NMR (C_2H_5CN at –80 °C) δ(ppm): –131.1 (m, $^{3}J(^{19}\mathrm{F}^{2,6}\text{-}^{129}\mathrm{Xe})$ = 94 Hz, 2F, *o*-C_6F_5), –147.3 (t, $^{3}J(\mathrm{F}^{4}\text{-}\mathrm{F}^{3,5})$ = 21 Hz, 1F, *p*-C_6F_5), –157.1 (m, 2F, *m*-C_6F_5); (cf., ref 7 (CH_2Cl_2 at –60 °C) δ(ppm): –130.8, –146.2, –155.5, (C_2H_5CN/CH_3CN (3:1) at –60 °C) δ(ppm): –131.0, –147.5, –157.0). ^{13}C{^{19}F} NMR (C_2H_5CN at –80 °C) δ(ppm): 144.2 (s, C^4), 143.8 (s, $C^{2,6}$), 138.7 (s, $C^{3,5}$), 103.5 (s, $^{1}J(^{13}\mathrm{C}^{1}\text{-}^{129}\mathrm{Xe})$ = 231 Hz, C^1); (cf., ref 7 (CH_2Cl_2 at –60 °C) δ(ppm): 143.3, 142.6, 137.6, 101.6). ^{129}Xe NMR (C_2H_5CN at –80 °C) δ(ppm): –4077 (br, $\Delta\nu_{1/2}$ = 206 Hz); (cf., ref 7 (CH_2Cl_2 at –60 °C) δ(ppm): –4117).

3. 6. Interaction of $[N(n\text{-}C_4H_9)_4][BF_4]$ with $(CH_3)_3SiCl$ in CH_3CN

$(CH_3)_3SiCl$ (16.8 mg; 0.155 mmol; 19.6 μL) was added into an FEP inliner which contained $[N(n\text{-}C_4H_9)_4][BF_4]$ (50.8 mg; 0.154 mmol) dissolved in CH_3CN (500 μL). $C_6H_5CF_3$ (11.0 mg; 0.0752 mmol; 9.2 μL) was added as internal standard for integration. The progress of the reaction was monitored by ^{19}F NMR at 24 °C. After 1.5 h the amount of $[BF_4]^-$ was reduced by 17% and after 1 d by 19% only. Besides $(CH_3)_3SiF$, $[BClF_3]^-$ was formed (broad singlet at –123.5); (cf., ref 20). The anions $[BCl_2F_2]^-$ ($^1J(^{19}F\text{-}^{11}B)$ = 54 Hz) and $[BCl_3F]^-$ ($^1J(^{19}F\text{-}^{11}B)$ = 79 Hz) with significant larger $^1J(^{19}F\text{-}^{11}B)$ coupling constants than $[BClF_3]^-$ ($^1J(^{19}F\text{-}^{11}B)$ = 25 Hz) and smaller quantities were not observed.[20]

^{19}F NMR (CH_3CN at 24 °C) δ(ppm): –123.5 (s, $\Delta\nu_{1/2}$ = 177 Hz, 3F), $[BClF_3]^-$; –149.8 (s, $\Delta\nu_{1/2}$ = 20 Hz, 4F), $[BF_4]^-$; –155.9 (dec, ^3J(F-H) = 7 Hz, 1F), $(CH_3)_3SiF$; molar ratio after 1.5 h: $[BClF_3]^-$: $[BF_4]^-$: $(CH_3)_3SiF$ = 14 : 83 : 20, after 1 d: $[BClF_3]^-$: $[BF_4]^-$: $(CH_3)_3SiF$ = 8 : 81 : 31.

^1H NMR (CH_3CN at 24 °C) Δ(ppm): 3.1 (m, $^1J(H\text{-}^{13}C)$ = 143 Hz, 8H, C^1H_2), 1.6 (tm, $^3J(H^2\text{-}H^3)$ = 7 Hz, 8H, C^2H_2), 1.4 (tq, $^3J(H^3\text{-}H^2)$ = 7 Hz, $^3J(H^3\text{-}H^4)$ = 7 Hz, 8H, C^3H_2), 1.0 (t, $^3J(H^4\text{-}H^3)$ = 7 Hz, $^1J(H\text{-}^{13}C)$ = 125 Hz, 12H, C^4H_3), $[N(n\text{-}C_4H_9)_4]^+$; 0.4 (s, $\Delta\nu_{1/2}$ = 1 Hz, 9H), $(CH_3)_3SiCl$; 0.2 (d, ^3J(H-F) = 7 Hz, 9H), $(CH_3)_3SiF$; molar ratio after 1.5 h: $[N(n\text{-}C_4H_9)_4]^+$ (100%); $(CH_3)_3SiCl$ (73%); $(CH_3)_3SiF$ (20%); after 1d: $[N(n\text{-}C_4H_9)_4]^+$ (100%); $(CH_3)_3SiCl$ (63%); $(CH_3)_3SiF$ (31%)

^{11}B NMR (CH_3CN at 24 °C) δ(ppm): 1.7 (s, $\Delta\nu_{1/2}$ = 121 Hz), $[BClF_3]^-$; –1.3 (s, $\Delta\nu_{1/2}$ = 15 Hz), $[BF_4]^-$.

3. 7. Reaction of $[C_6F_5Xe][BF_4]$ with $(C_2H_5)_3SiH$ in CD_3CN

$(C_2H_5)_3SiH$ (9.5 mg; 0.082 mmol; 13 μL) was added to a solution of $[C_6F_5Xe][BF_4]$ (24.5 mg; 0.0636 mmol) in cold CD_3CN (500 μL; –40 °C) in an FEP inliner. The mixture was intensively shaken and after 20 min analyzed by ^{19}F and ^{11}B NMR spectroscopy.

^{19}F NMR (CD_3CN at –40 °C) δ(ppm): –131.8 (m, $^3J(F^{2,6}\text{-}^{129}Xe)$ = 43 Hz, 4F, *o*-C_6F_5),–153.8 (t, $^3J(F^4\text{-}F^{3,5})$ = 21 Hz, 2F, *p*-C_6F_5), –158.7 (m, 4F, *m*-C_6F_5), $(C_6F_5)_2Xe$;[4] –139.3 (m, 2F, *o*-C_6F_5), –154.8 (t, $^3J(F^4\text{-}F^{3,5})$ = 21 Hz, 1F, *p*-C_6F_5), –162.5 (m, 2F, *m*-C_6F_5), C_6F_5H; –139.6 (m, 2F, *o*-C_6F_5), –154.8 (t, $^3J(F^4\text{-}F^{3,5})$ = 21 Hz, 1F, *p*-C_6F_5), –162.6 (m, 2F, *m*-C_6F_5), C_6F_5D; –138.3 (m, 4F, *o*-C_6F_5), –151.0 (t, $^3J(F^4\text{-}F^{3,5})$ = 21 Hz, 2F, *p*-C_6F_5), –160.6 (m, 4F, *m*-C_6F_5), $(C_6F_5)_2$; –142.7 (m, 2F, *o*-C_6F_5), –155.8 (tm, $^3J(F^4\text{-}F^{3,5})$ = 21 Hz, 1F, *p*-C_6F_5), –161.9 (m, 2F, *m*-C_6F_5), $C_6F_5CH_2CH_3$; –134.9 (m, 2F, *o*-C_6F_5), –141.5 (tt, $^3J(F^4\text{-}F^{3,5})$ = 21 Hz, $^4J(F^4\text{-}F^{2,6})$ = 8 Hz, 1F, *p*-C_6F_5), –159.6 (m, 2F, *m*-C_6F_5), $[C_6F_5C(CD_3)=N(H,D)_2]^+$ [a]; –127.2 (m, 2F, *o*-C_6F_5), –152.7 (tt, $^3J(F^4\text{-}F^{3,5})$ = 20 Hz, $^4J(F^4\text{-}F^{2,6})$ = 3 Hz, 1F, *p*-C_6F_5), –161.9 (m, 2F, *m*-C_6F_5), $C_6F_5Si(C_2H_5)_3$ [b]; –174.4 (sep, ^3J(F-H) = 6 Hz, $^1J(^{19}F\text{-}^{29}Si)$ = 286 Hz, 1F), $(C_2H_5)_3SiF$ [c]; –180.5 (dquin, ^2J(F-H) = 53 Hz, ^3J(F-H) = 7 Hz, 1F), $(C_2H_5)_2SiFH$; –142.9 (quin, ^3J(F-H) = 5 Hz, 2F), $(C_2H_5)_2SiF_2$ [d]; –141.7 (br, $\Delta\nu_{1/2}$ = 212 Hz, 3F), $BF_3 \cdot NCCD_3$; –149.4 (br, $\Delta\nu_{1/2}$ = 438 Hz, 4F), $[BF_4]^-$; molar ratio after 20 min related to the sum of C_6F_5 compound: $(C_6F_5)_2Xe$ (5%), C_6F_5H (61%), C_6F_5D (2%), $(C_6F_5)_2$ (1%), $C_6F_5CH_2CH_3$ (5%), $[C_6F_5C(CD_3)=N(H,D)_2]^+$ (19%), $C_6F_5Si(C_2H_5)_3$ (2%), $(C_2H_5)_3SiF$ (52%), $(C_2H_5)_2SiFH$ (7%), $(C_2H_5)_2SiF_2$ (6%), $BF_3 \cdot NCCH_3$ (94%), $[BF_4]^-$ (6%).

([a] cf., ref 14 ($CDCl_3$) δ(ppm): –136.2, –143.9, –155.1 $[C_6F_5C(CH_3)=N(C_2H_5)_2]^+$; [b] cf., ref 21 ($CCl_4$) δ(ppm): –127.2, –152.6, –162.0; [c] cf., ref 22 (C_6D_6) δ(ppm): –175.2; [d] cf., ref 23 (CCl_4) δ(ppm): –145.7). ^{11}B NMR (CH_3CN at –40 °C) δ(ppm): –1.4 (s, $\Delta\nu_{1/2}$ = 10 Hz), $[BF_4]^-$; –2.2 (s, $\Delta\nu_{1/2}$ = 37 Hz), $BF_3 \cdot NCCD_3$.

3. 8. Reaction of $[C_6F_5Xe][BF_4]$ with $(C_2H_5)_3SiH$ in C_2H_5CN

A solution of $[C_6F_5Xe][BF_4]$ (59.5 mg; 0.1546 mmol) in cold C_2H_5CN (200 μL; –90 °C) was transferred to a solution of $(C_2H_5)_3SiH$ (19.2 mg; 0.165 mmol; 26 μL) in cold C_2H_5CN (150 μL; –90 °C) and vigorously mixed before the reaction was monitored by ^{19}F NMR spectroscopy. After 20 min at –90 °C 63% of the $[C_6F_5Xe]^+$ cation and 44% of $[BF_4]^-$ was reacted. All reaction products are comparable with that in CD_3CN, except the product deriving from the $C_6F_5^{\bullet}$ radical attack on the solvent. In C_2H_5CN the cation $[C_6F_5C(C_2H_5)=NH_2]^+$ (δ(ppm): –136.7 (br, $\Delta\nu_{1/2}$ = 45 Hz, 2F, *o*-C_6F_5), –142.4 (br, 1F, *p*-C_6F_5), –160.1 (br, $\Delta\nu_{1/2}$ = 51 Hz, 2F, *m*-C_6F_5)) was formed. Molar ratio of products related to the sum of B-F compounds after 20 min: $[C_6F_5Xe]^+$ (37%); $(C_6F_5)_2Xe$ (4%); C_6F_5H (37%), $(C_6F_5)_2$ (traces), $[C_6F_5C(C_2H_5)=NH_2]^+$ (9%), $C_6F_5Si(CH_3CH_2)_3$ (1%), $(CH_3CH_2)_3SiF$ (31%); $(CH_3CH_2)_2SiFH$ (4%); $(CH_3CH_2)_2SiF_2$ (6%); $BF_3 \cdot NCC_2H_5$ (44%); $[BF_4]^-$ (56%). The ratio stayed nearly constant after 100 min at –90 °C, but changed after 5 d at –70 °C: $(C_6F_5)_2Xe$ (2%), C_6F_5H (58%), $(C_6F_5)_2$ (1%), $[C_6F_5C(C_2H_5)=NH_2]^+$ (17%), $C_6F_5Si(CH_3CH_2)_3$ (2%), $(CH_3CH_2)_3SiF$ (44%), $(CH_3CH_2)_2SiFH$ (2%), $(CH_3CH_2)_2SiF_2$ (8%), $BF_3 \cdot NCC_2H_5$ (65%), $[BF_4]^-$ (35%).

^{129}Xe NMR (CH_3CH_2CN at –90 °C after 55 min) δ(ppm): –3971; (m) $[C_6F_5Xe]^+$; –4134 (m) $(C_6F_5)_2Xe$.

3. 9. Synthesis of Bis(pentafluorophenyl) Xenon(II) in C_2H_5CN

Solid $Cd(C_6F_5)_2$ (25.6 mg; 0.0574 mmol; –78 °C) was deposited in an FEP inliner. A cold solution of $[C_6F_5Xe][BF_4]$ (41.2 mg; 0.107 mmol) in C_2H_5CN (400 μL; –78 °C) was added and the mixture was intensively shaken at –78 °C. A white suspension resulted which was characterized by ^{19}F NMR spectroscopy after 2.5 h at –80 °C: δ/ppm –131.8 (m, $^3J(F^{2,6}\text{-}^{129}Xe)$ = 43 Hz, 4F, *o*-C_6F_5),

–153.5 (t, $^3J(F^4\text{-}F^{3,5})$ = 20 Hz, 2F, *p*-C_6F_5), –158.6 (m, 4F, *m*-C_6F_5). After separation (–78 °C), the solid fraction was repeatedly washed with cold C_2H_5CN (4 x 400 μL; –78 °C) and incorporated $Cd(C_6F_5)_2$ and $Cd[BF_4]_2$ were removed. The product $(C_6F_5)_2Xe$ (almost quantitative yield) was only slightly soluble in C_2H_5CN (–78 °C) and shock-sensitive even in suspension. Decomposition proceeded also when pressure was exerted on the solid in suspension, e.g., with a spatula, and a yellow solution resulted which contained $(C_6F_5)_2$ and C_6F_5H in the molar ratio 83 : 17.

4. Conclusion

Strongly coordinating nitrile molecules (CH_3CN, C_2H_5CN) can be replaced in the coordination sphere of the electrophilic Xe^{II} centre of the $[C_6F_5Xe]^+$ cation by anions which are stable against oxidation such as F^-.

More oxidizable anions such as Cl^- can be introduced into the $[C_6F_5Xe]^+$ moiety with support of $[BF_4]^-$ as the counterion using $(CH_3)_3SiHal$. Fluoride in the coproduct, $(CH_3)_3SiF$, originates from the $[BF_4]^-$ anion. The latter is transformed into the solvent adduct $BF_3 \cdot NCAlk$. Anions which are sensitive to oxidation can be protected by interaction with Lewis acids such as H^+ or BF_3.

The reaction of $[C_6F_5Xe]^+$ with $(C_2H_5)_3SiH$ in nitrile solvents is complex. From the observed products, two intermediates C_6F_5XeH and $C_6F_5XeC_2H_5$ can be deduced. Alternatively to C_6F_5XeH, a one-electron transfer in cage from H^- to $[C_6F_5Xe]^+$ as main reaction channel cannot be excluded.

Oxidation resistant organyl groups of organometallic compounds such as $Cd(C_6F_5)_2$ are nucleophilic enough to replace nitrile solvent molecules coordinated at Xe^{II} in $[C_6F_5Xe]^+$. The carbon nucleophile does not interact with the $[BF_4]^-$ anion. Formally, a metathesis of the $[BF_4]^-$ anion by the carbanion $[C_6F_5]^-$ proceeds. The reaction of organylxenonium salt solutions in nitrile solvents with organometallic compounds which possess a very polar M-C bond promises an interesting access to new organylxenon compounds, $R^1\text{-Xe-}R^2$.

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6. References

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Povzetek

Soli $[C_6F_5Xe][BF_4]$ regirajo z različnimi viri nukleofilnih zvrsti Y (»goli« fluorid, $[N(CH_3)_4]F$, silani, $(CH_3)_3SiCl$ in $(C_2H_5)_3SiH$ ter $Cd(C_6F_5)_2$) v koordinirajočih topilih (C_2H_5CN, CH_3CN, CD_3CN). Produkte C_6F_5XeF, C_6F_5XeCl in $(C_6F_5)_2Xe$ smo uspeli jasno določiti. V primeru reakcije s $(C_2H_5)_3SiH$ pa smo uspeli določiti le produkte razgradnje, ki lahko izvirajo iz $<C_6F_5XeH>$ in $<C_6F_5XeC_2H_5>$. Spojino C_6F_5XeF smo karakterizirali z rentgensko strkturno analizo monokristalov.