Abstract

The isolation and NMR spectroscopic characterization of phenylethynylxenon(II) trifluoromethanesulfonate and phenylethynylxenon(II) methanesulfonate was successful at lower temperatures. Phenylethynylxenon(II) methanesulfonate appears to be the first isolated organoxenon-compound containing no halogen atoms. The compounds were isolated in form of powders which explode at temperatures above -20 °C and are poor soluble in organic solvents. Both compounds were characterized by ^{1}H NMR respectively ^{19}F NMR , ^{13}C{^{1}H} NMR and ^{129}Xe NMR spectroscopy.

The complete NMR data set of the molecule fragment -C≡CXeF for the thermally highly unstable compounds (1-hexynyl)xenon(II) fluoride and (propynyl)xenon(II) fluoride was determined by 2D ^{19}F-^{13}C{^{1}H} HMQC NMR spectra. These results unambiguiously prove the existence of these moiety in the prepared compounds. The sign of the $^{1}J(^{13}C-^{129}Xe)$ coupling was determined for both compounds.

The thermal stability of (phenylethynyl)- und (1-hexynyl)xenon(II) fluoride in solution was investigated by NMR spectroscopy: It could be verified that (phenylethynyl)xenon(II) fluoride is the more stable neutral compound.

The reactions of XeF_2 with bis(trimethylsilyl)diynes, which were substituted with aliphatic or aromatic groups between the alkynyl functional groups, gave reference to the possible synthesis of (alkynyl)xenon(II)-compounds with several (alkynyl)xenon(II) ligands.

The NMR spectroscopic investigation of the reaction of ((trimethyl)(phenylethynyl)silane with $[(CH_3)_4N]F$ gave ^{19}F NMR spectroscopic reference to the formation of a hypervalent (phenylethynyl)fluorosilicate. The detection of signals for these silicate in ^{29}Si NMR spectra failed.

The investigation of alternative synthetic pathways for the formation of (alkynyl)xenon(II) compounds by reaction of XeF_2 with metal alkynylides (Na, Zn, Hg) didn't lead to success.

The preparation of (alkynyl)xenon(II) fluorides, which were containing a NMR active nucleus (for example ^{31}P) as bonding partner at the carbon-carbon triple bond didn't succed in the case of phosphorus, because the (trimethylsilylethynyl)phosphanes, which were used as educts, weren't stable against oxidation by XeF_2 even at low temperatures.

The preparation of (perfluoralkyl)- and (alkyl)xenon(II) compounds by reaction of XeF_2 with (trimethyl)(perfluoralkyl)- respectively (trimethyl)(alkyl)silanes didn't succeed.

The reaction of (trimethyl)(phenylethinyl)silane with XeF_2 in presence of CsF in dichloromethane/propionitrile gave NMR spectroscopic reference to the formation of a compound with a F-Xe-N moiety.

Primary transfer reactions with the isolated (phenylethynyl)xenon(II) compounds and organic molecules took an unspecific course.

The calculation of optimized structures and vibrational spectra of (alkynyl)xenon(II) compounds with several hundred basis functions on PC-based systems by the use of DFT methods with the cc-pVTZ-PP basis set could be carried out in an acceptable time frame. A comprehensive comparison of calculated data with experimental data could yet not be achieved because of the poor data basis of experimental results.