Abstract

The pentafluorosulfanyl (SF₅) group displays remarkable and unique properties, including large dipole moment, high electronegativity, high thermal and chemical stability, as well as high lipophilicity. However, only a few synthetic methods for the preparation of aromatic pentafluorosulfanyl building blocks have been developed to date. This work aims at improving availability and accessibility of aryl sulfurpentafluoride building blocks.

In the first part of the work, the synthesis of aryl sulfurpentafluorides by the direct fluorination of diaryl disulfides with elemental fluorine is described. Nowadays, this synthetic strategy is used by industry on a multi-kilogram scale. However, the scope of the reaction is only limited to 3- and 4-nitro-1-(pentafluorosulfanyl)benzenes. In this work, the synthesis of various *para*-, *meta*- and *ortho*-substituted-(pentafluorosulfanyl)benzenes following the same approach was carried out.

In the second part, the derivatization of aryl sulfurpentafluoride building blocks was investigated. Direct fluorination of 3-nitro-1-(pentafluorosulfanyl)benzene afforded 3-fluoro-5-nitro-1-(pentafluorosulfanyl)benzene. The titled compound was derivatized by two different processes: nucleophilic aromatic substitution (S_NAr) of fluorine and vicarious nucleophilic substitution of hydrogen (VNS).