

Supporting Information

Activation of SF₅CF₃ by the *N*-heterocyclic Carbene SIMes

Domenique Herbstritt¹, Pooja Tomar¹, and Thomas Braun^{1*}

Humboldt-Universität zu Berlin, Department of Chemistry, Brook-Taylor-Straße 2, D-12489 Berlin, Germany. E-mail: thomas.braun@chemie.hu-berlin.de

NMR Spectra

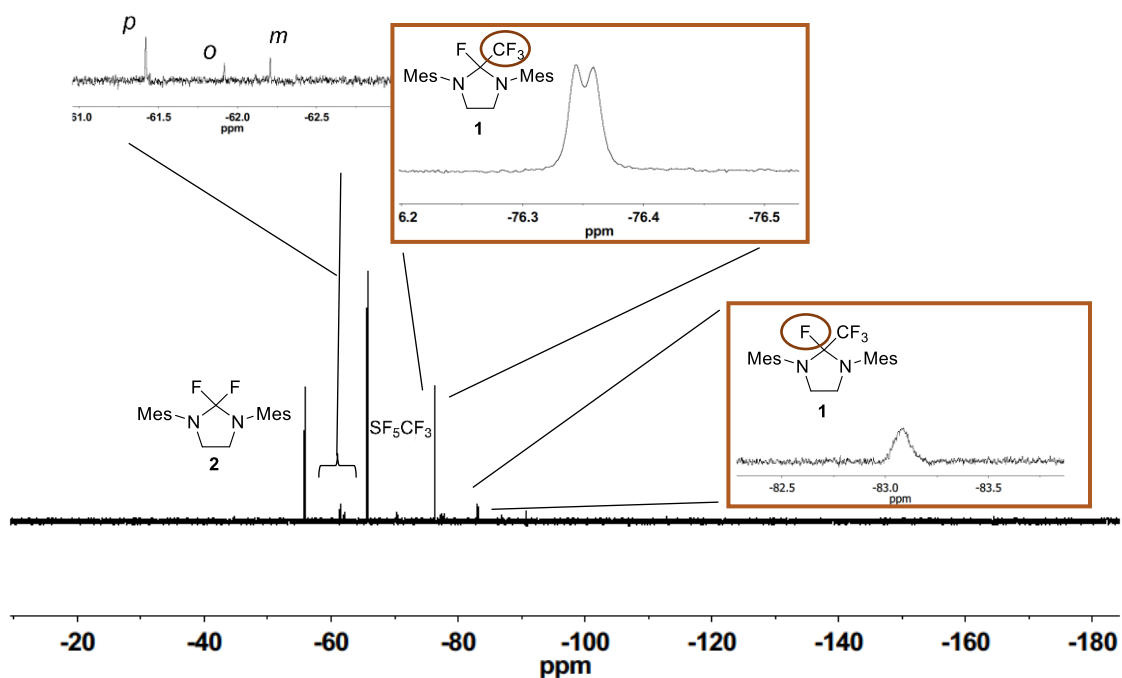


Figure S1: ^{19}F NMR spectra for 1,3-dimesityl-2-fluoro-2-trifluoromethylimidazolidine (**1**) and 1,3-dimesityl-2,2-difluoroimidazolidine (**2**) in toluene-d_8 after heating of SIMes and SF_5CF_3 at 90°C .

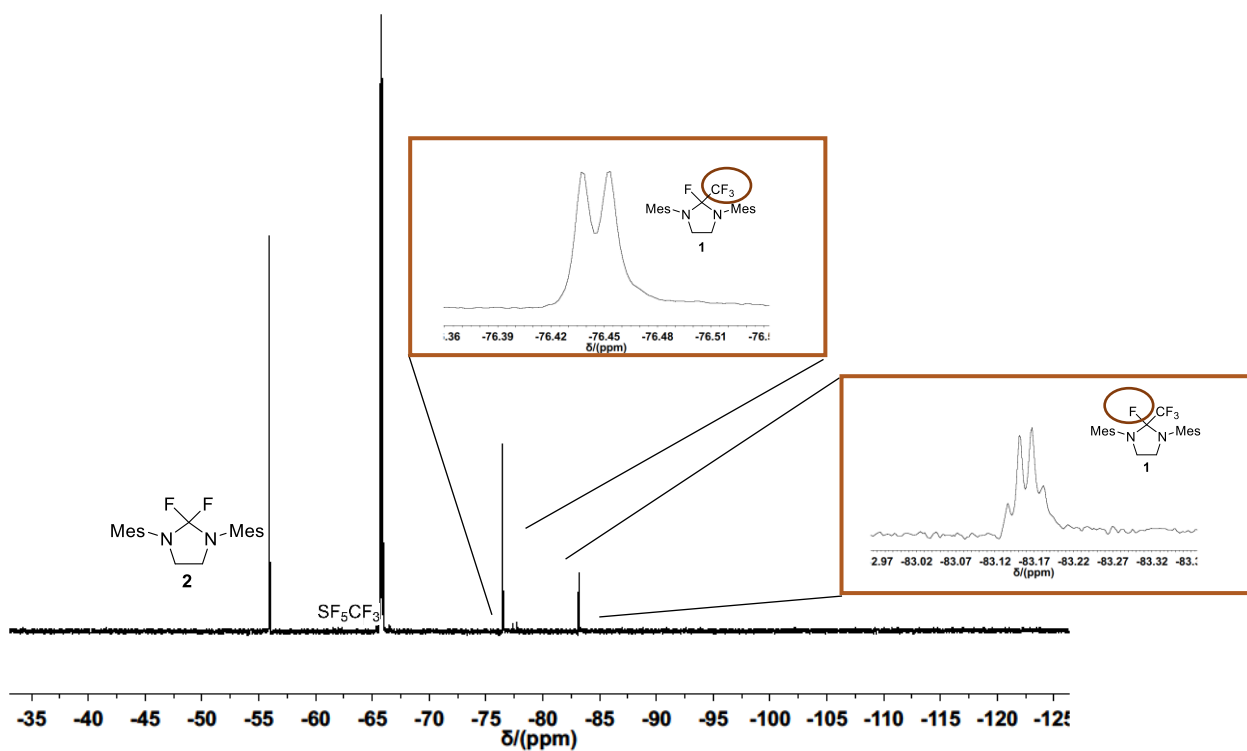


Figure S2: $^{19}\text{F}\{^1\text{H}\}$ NMR spectra for 1,3-dimesityl-2-fluoro-2-trifluoromethylimidazolidine (**1**) and 1,3-dimesityl-2,2-difluoroimidazolidine (**2**) in toluene- d_8 after heating of SIMes and SF_5CF_3 at 90 °C.

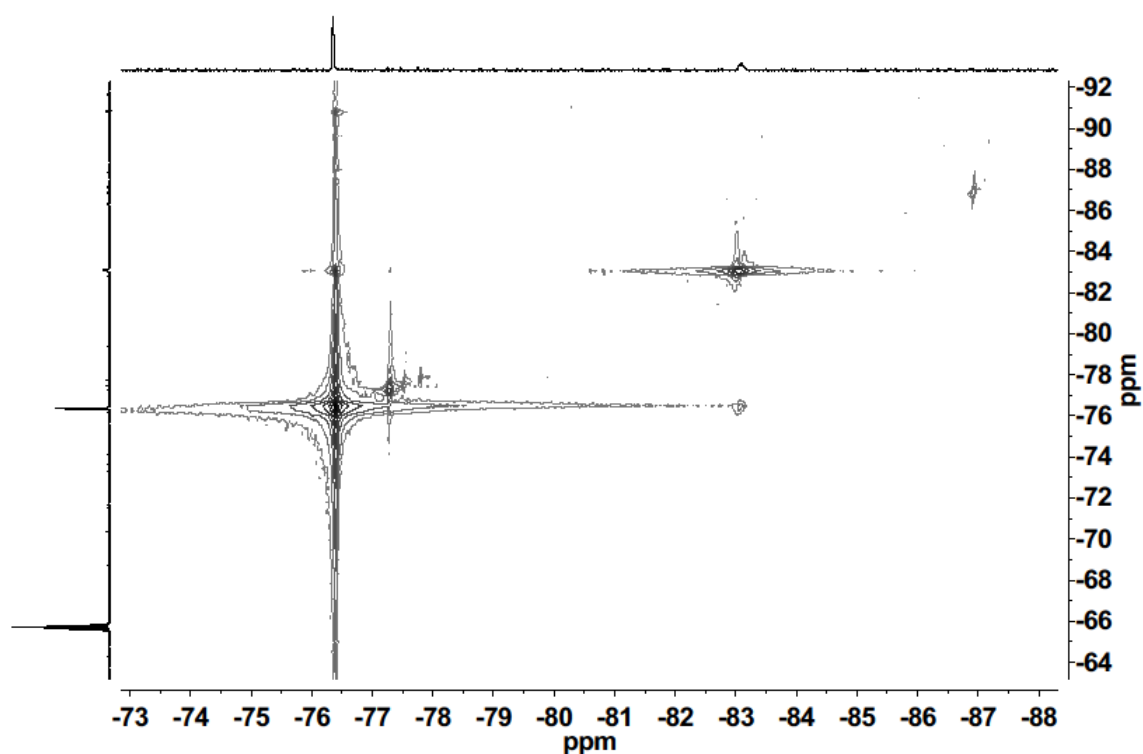


Figure S3: $^{19}\text{F}^{19}\text{F}$ COSY NMR spectrum for 1,3-dimesityl-2-fluoro-2-trifluoromethylimidazolidine (**1**) in toluene- d_8 after heating of SIMes and SF_5CF_3 at 90 °C.

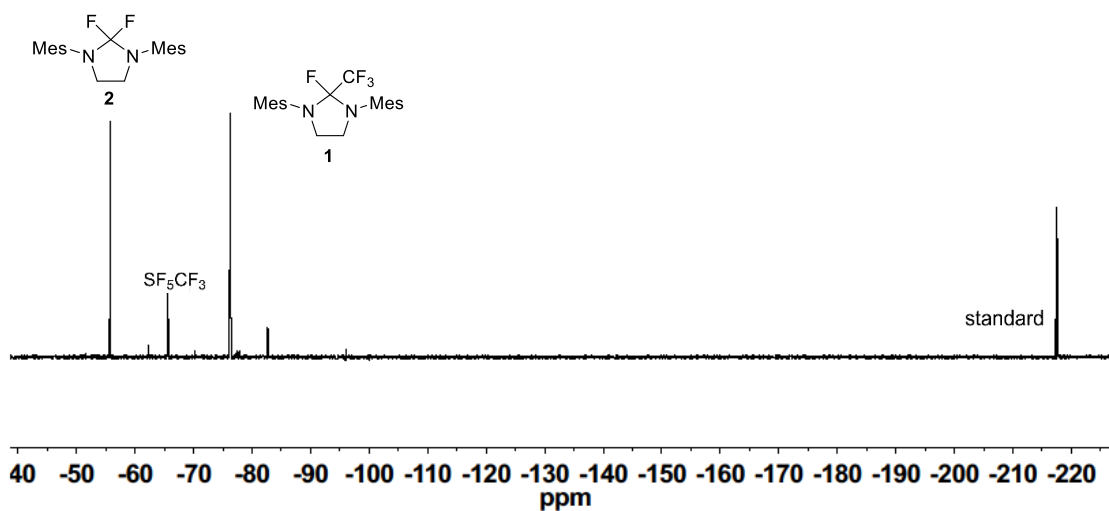


Figure S4: ^{19}F NMR spectrum for 1,3-dimesityl-2-fluoro-2-trifluoromethylimidazolidine (**1**) and SiMesF_2 (**2**) in C_6D_6 after irradiation of SiMes and SF_5CF_3 at 311 nm after 3 h.

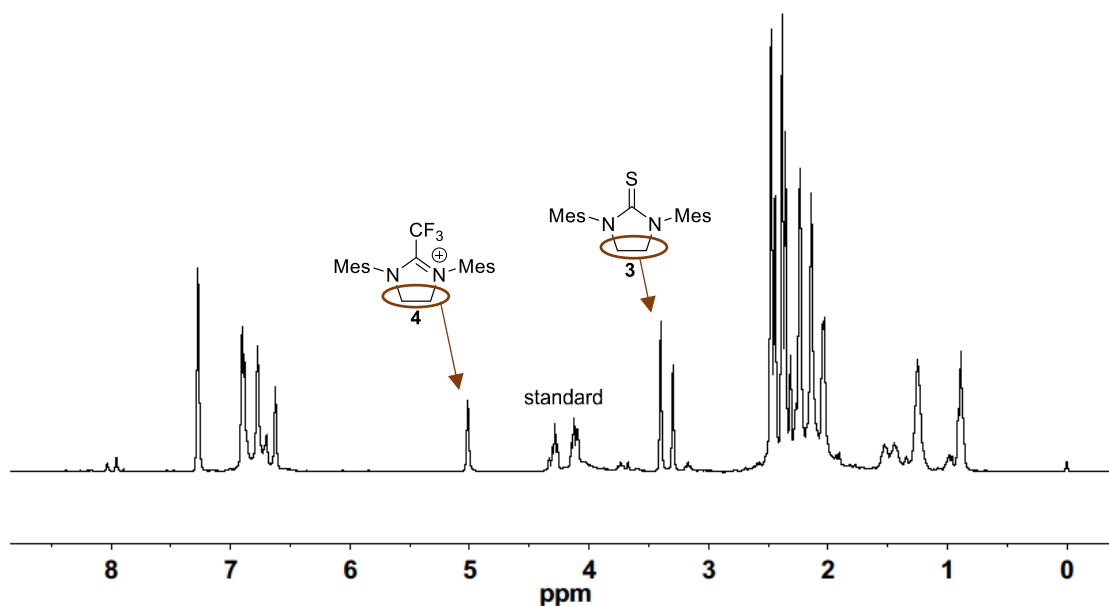


Figure S5: ^1H NMR spectrum for compounds **3** and **4** in C_6D_6 after irradiation of SiMes and SF_5CF_3 at 311 nm after 16 h.

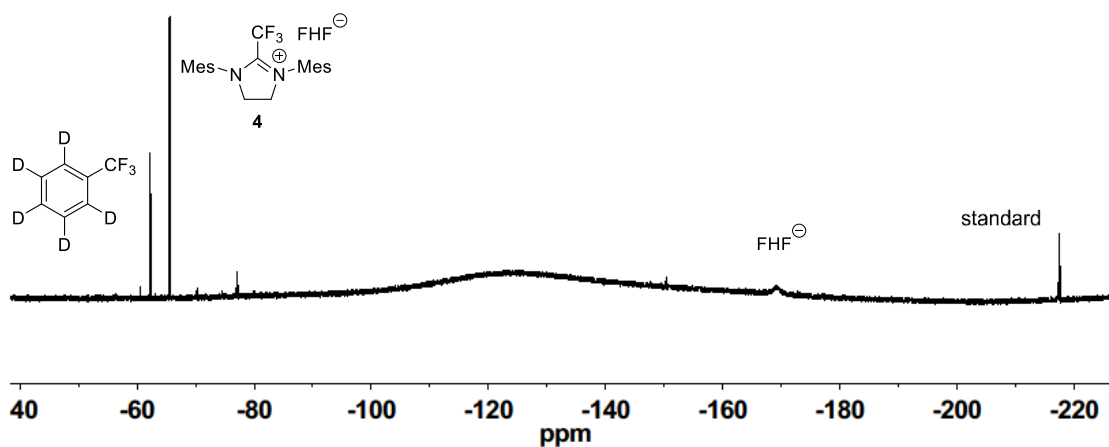


Figure S6: ^{19}F NMR spectrum for compound **4** in C_6D_6 after irradiation of SIMes and SF_5CF_3 at 311 nm after 16 h.

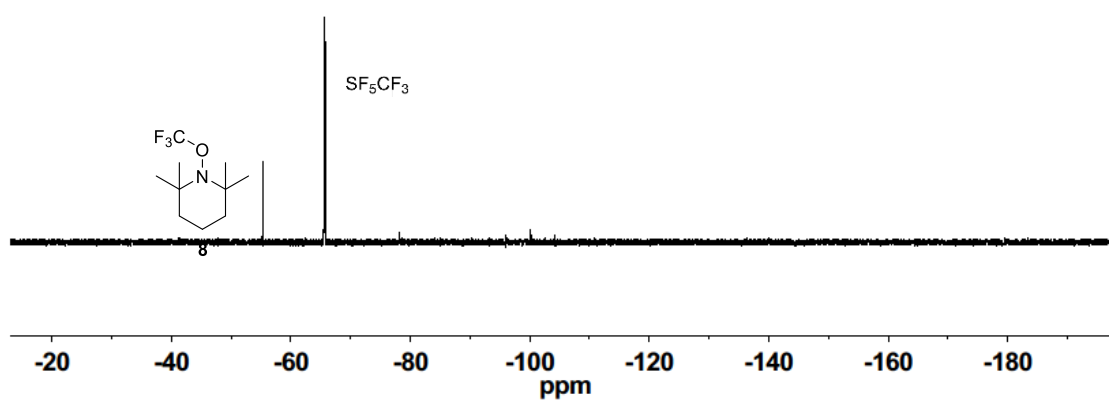


Figure S7: ^{19}F NMR spectrum for compound **8** in C_6D_6 .

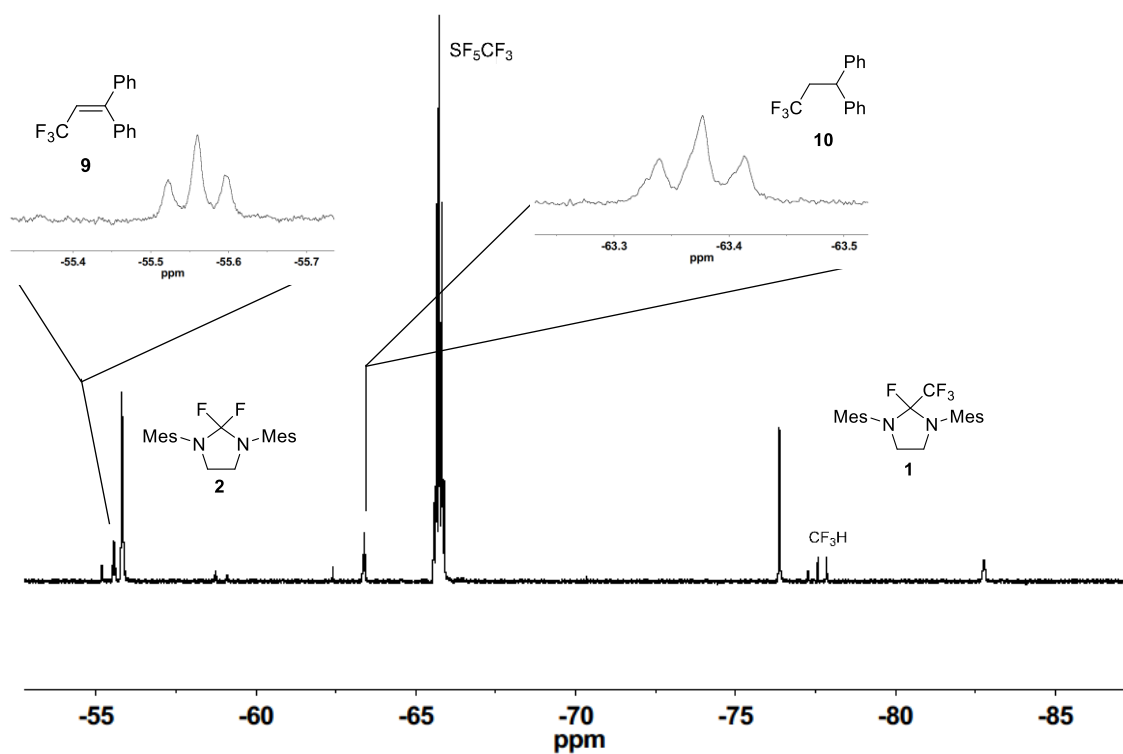


Figure S8: ^{19}F NMR spectrum for compounds **1**, **2**, **9** and **10** in C_6D_6 after irradiation of SIMes, SF_5CF_3 and 1,1-diphenylethylene at 311 nm for 3 h.

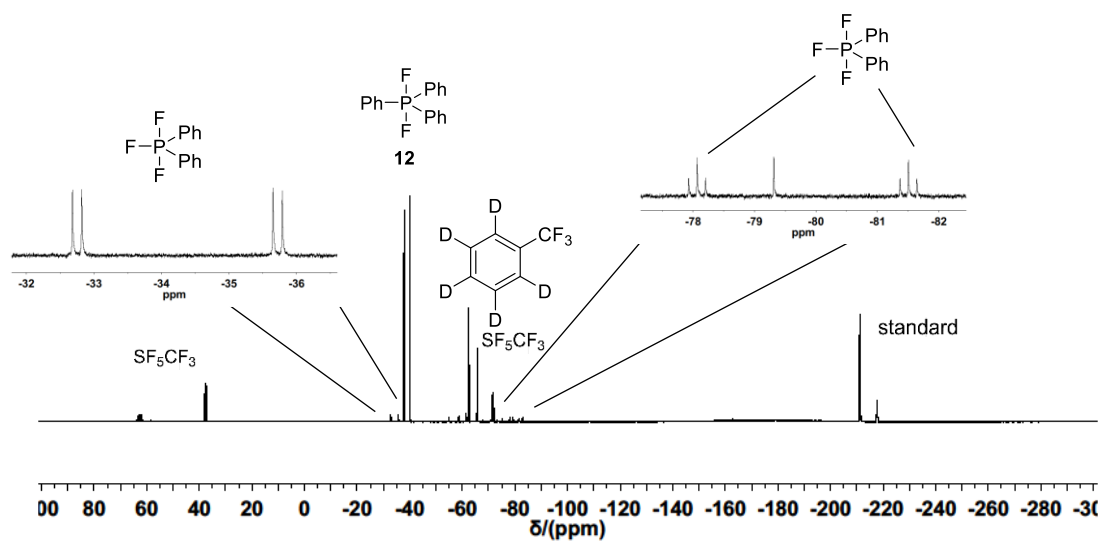


Figure S9: ^{19}F NMR spectrum for compound **12** and α,α,α -trifluorotoluene- d_5 in C_6D_6 .

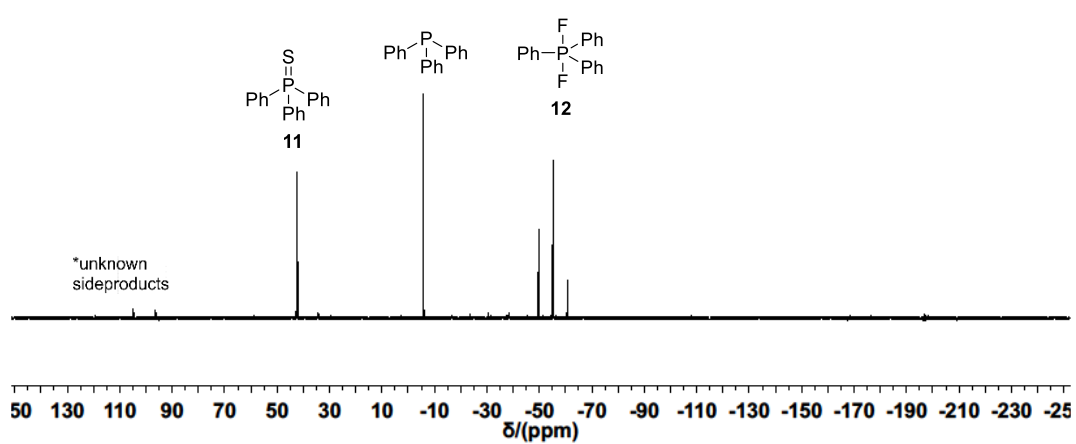


Figure S10: ^{31}P NMR spectrum for compounds **11** and **12** in C_6D_6 .