Supporting Information

Contents:

I) Synthesis and experimental data

I.A) General Information

I.A.1) Chemicals

Chemicals were obtained from *ABCR*, *Alfa Aesar*, *Carbolutions*, *Merck*, *Sigma-Aldrich* or *VWR*. Commercially available reagents and starting materials were, unless mentioned otherwise, used without further purification. Solvents which were to be used in moisture-sensitive experiments were taken from a solvent drying system by *M. Braun* (type: *MB SPS-800*) and stored under an argon atmosphere. Other solvents were used after single distillation.

For reactions including oxygen- or moisture-sensitive reagents, glassware was baked out under high-vacuum conditions and procedures carried out under an argon atmosphere. Reagents were injected via a septum or added under argon counterflow.

I.A.2) Appliances and materials

Thin layer chromatography (TLC) was performed on plates from *Merck* (silica gel 60, F254). Detection of the substances was obtained by fluorescence detection under UV light (wavelength λ = 254 nm). The corresponding R_f values and solvents used as eluents are listed in the experimental part. Column chromatographies were performed with silica gel (grain size 0.04-0.063 cm, *Merck, Si60*) at approximately 1.5 atm (hand pump).

Nuclear magnetic resonance spectra (NMR-spectra) were obtained on instruments of the type *AV-250* (for ^{1}H-, ^{13}C- and ^{19}F-spectra) or *AV-400* (for ^{13}C-spectra) from *Bruker*. Chemical shifts (δ) are given as parts per million (ppm) and refer to the shift of the hydrogen or carbon atoms in the solvent used. Chemical shifts in ^{13}C titration experiments are referred to tetraethylsilane as internal standard (δ = 3.33 ppm). In ^{19}F-spectra, hexafluorobenzene was used as internal standard (δ = -161.99 ppm).

The following abbreviations were used for the assignment of the signals and their multiplicities: s (singlet), bs (broad singlet), d (doublet), t (triplet), q (quartet), p (pentett), m (multiplet), dd (doublet of doublet), dddd (doublet of doublet of doublet of doublet). The given coupling constants *J* are listed as the average of the experimental findings.

Mass spectrometry spectra (MS-spectra) were obtained by using electron spray ionization (ESI). Assigned m/z-relations are listed in ascending order. ESI-spectra were measured on a *Thermo Scientific* LTQ Orbitrap XL.

I.B) Syntheses

I.B. 1) Starting materials and precursors

Sodium tetrakis(3,5-bis(trifluoromethyl)phenyl)borate (Na–BArF),[S1] tetramethylammonium-tetrakis(3,5-bis(trifluoromethyl)phenyl)borate (TMA–BArF),[S2] *N*,*N'*-bis[3,5-bis(trifluoromethyl)phenyl]thiourea,[S3] octyl trifluoromethane sulfonate (Oct–OTf),[S4] 1,3-Bis(2-iodo-3-octyl-imidazolium)phenyl-bis(trifluoromethanesulfonate) [S5] (**2/OTf**) and 1-methyl-2-iodo-imidazole[S6] were synthesized according to literature-known procedures.

I.B. 2.1) General Methods

General Procedure A - Octylation:

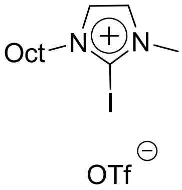
Under an argon atmosphere, the respective imidazolium-derivative was dissolved in CH_2Cl_2 (50 mM), 1.50 equivalents of octyl trifluoromethanesulfonate were added and the solution was stirred at room temperature over night. Removal of the solvent and repeated precipitation from acetonitrile *via* addition of diethyl ether yielded the desired products.

General Procedure B - Anion Exchange:

The respective triflate salt was dissolved in CH_2Cl_2/MeOH = 3:1 (12 mM) and 1.10 eq (for imidazolium compound) or 2.20 eq (for bis-imidazolium compound) of tetramethylammonium tetrakis(3,5-bis(trifluoromethyl)phenyl)borate were added and the reaction mixture stirred at room temperature over night. After removal of the solvent, the resulting mixture was suspended in Et_2O (40 mL per mmol of employed triflate salt), cooled to -25 °C and the resulting precipitate filtered and washed with cold Et_2O. The solvent is removed and the resulting mixture suspended in $CHCl_3$ (40 mL per mmol of employed triflate salt), cooled to 0 °C and the resulting precipitate filtered *via* syringe filter (25 µm) and washed with cold $CHCl_3$. Removal of the solvent yields to the corresponding product.

I.C) Experimental Data

I.C.1) 2-Iod-1-methyl-3-octyl-imidazoliumtrifluoromethanesulfonate



The compound was synthesized by general procedure A.

Yield: 89% (white solid)

^{1}H-NMR (400 MHz, CD_2Cl_2): $\delta = 0.88$ (t, 3H, $^3J = 6.70$ Hz), 1.22-1.41 (m, 10H), 1.85 (p, 2H, $^3J = 7.20$ Hz), 3.93 (s, 3H), 4.17 (t, 2H, $^3J = 7.50$ Hz), 7.63 (d, 1H, $^3J = 2.10$ Hz), 7.75 (d, 1H, $^3J = 2.10$ Hz) ppm.

^{13}C-NMR (100 MHz, CD_2Cl_2): $\delta = 14.2$, 22.9, 26.5, 29.3, 29.3, 30.1, 32.0, 40.3, 53.7, 97.6, 121.1 (d),[S7] 125.8, 127.4 ppm.

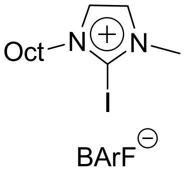
^{19}F-NMR (235 MHz, CD_2Cl_2): -78.14 ppm.

Elemental analysis: *calc.*: C: 33.20 H: 4.72 N: 5.96 S: 6.82

found: C: 32.94 H: 4.61 N: 5.94 S: 6.66

ESI-MS: m/z = 791 [$(2M+OTf)^+$] (2), 321 [M^+] (100), 209 [$(M-C_8H_{13})^+$] (3)

I.C.2) 2-Iod-1-methyl-3-octyl-imidazolium-bis(tetrakis(3,5-bis-(trifluoromethyl)phenyl)-borate **(3/BAr^{F}$_4$)**



The compound was synthesized by general procedure B.

Yield: 82% (beige solid)

^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 0.88 (t, 3H, ^3J = 6.40 Hz), 1.21-1.44 (m, 10H), 1.80-1.89 (m, 2H), 3.84 (s, 3H), 4.11 (t, 2H, ^3J = 7.50 Hz), 7.46 (s, 2H), 7.58 (s, 4H), 7.73 (bs, 8H) ppm.

^{13}C-NMR (100 MHz, CD_2Cl_2): δ = 14.3, 23.1, 26.7, 29.4, 29.5, 30.2, 32.2, 40.7, 54.5, 95.4, 117.7-118.5 (m), 125.2 (q, ^1J = 270 Hz), 126.3, 127.5, 129.6 (dddd, ^2J = 31.5 Hz), 135.5 (bs), 162.4 (dd, ^1J = 50.0 Hz) ppm.

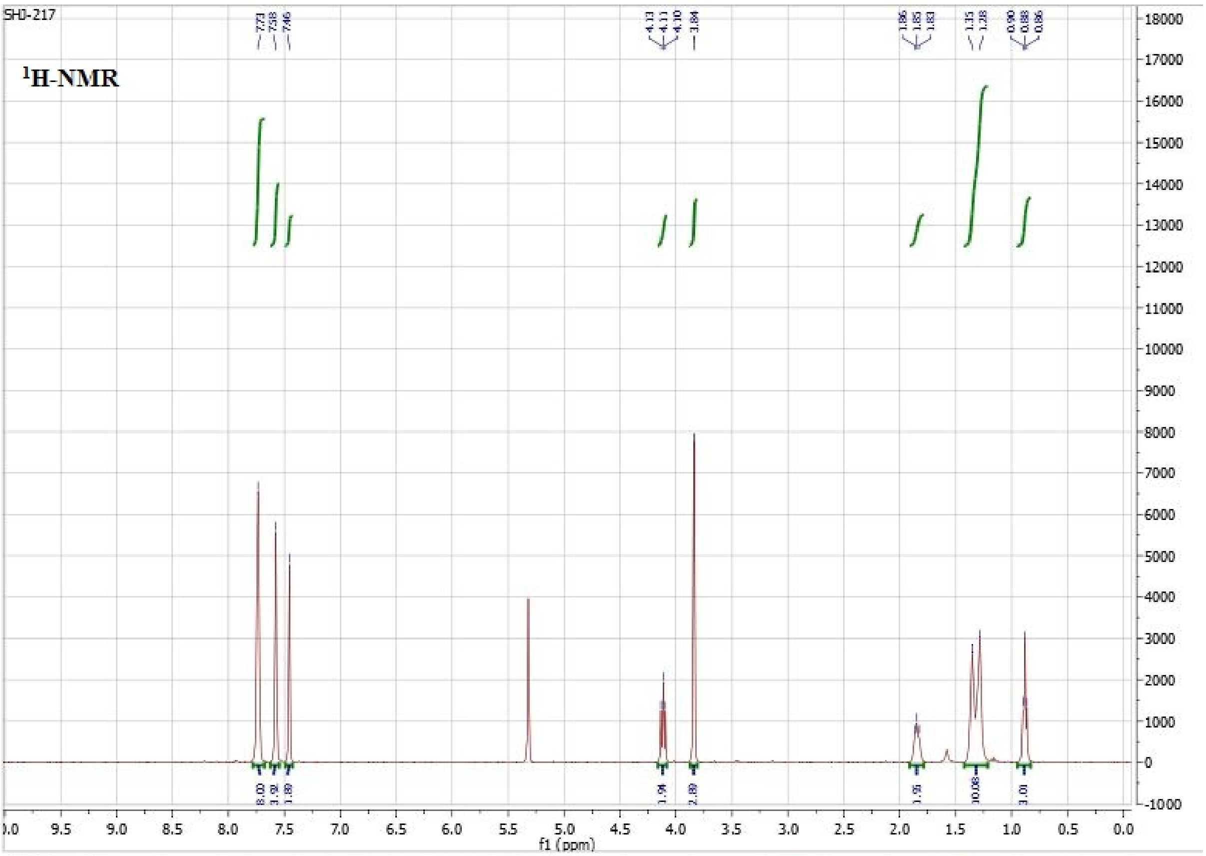
^{19}F-NMR {^{1}H} (235 MHz, CD_2Cl_2): -62.15 ppm.

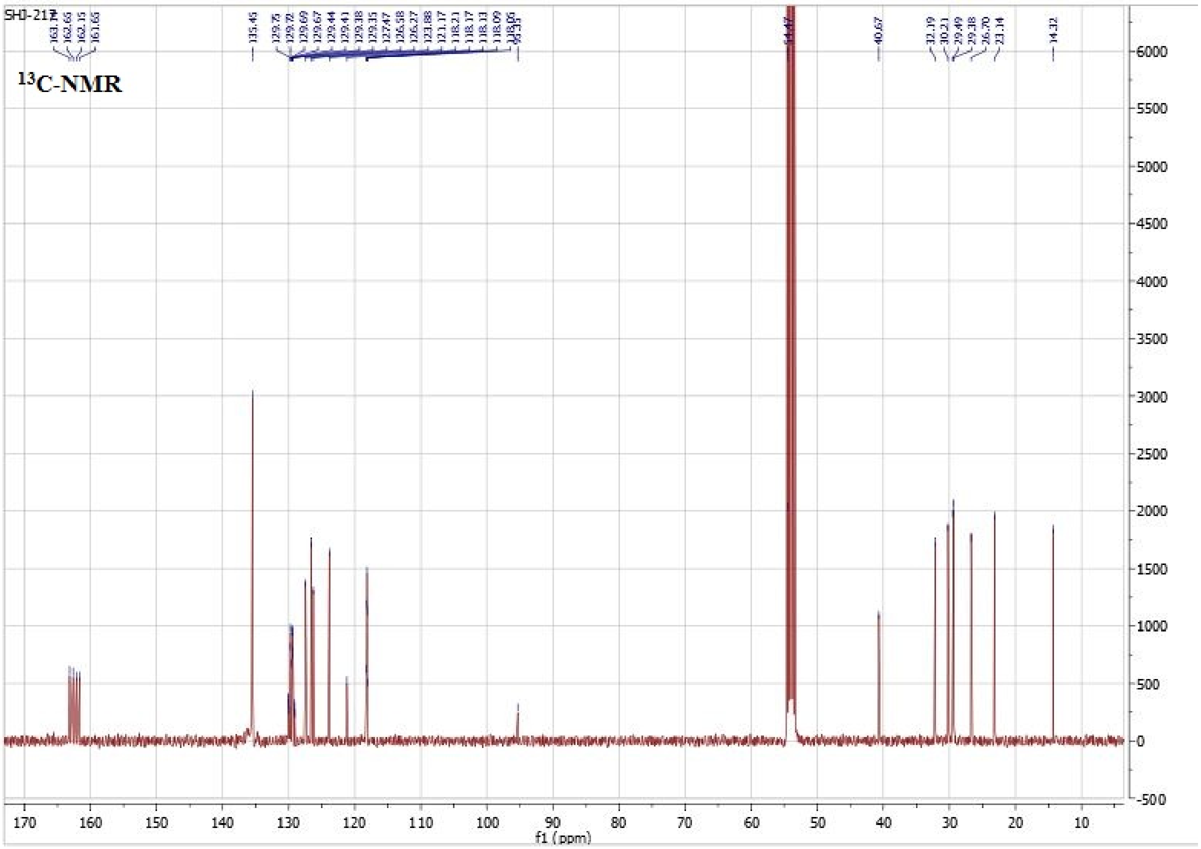
Elemental analysis: *calc.*: C: 44.62 H: 2.89 N: 2.37

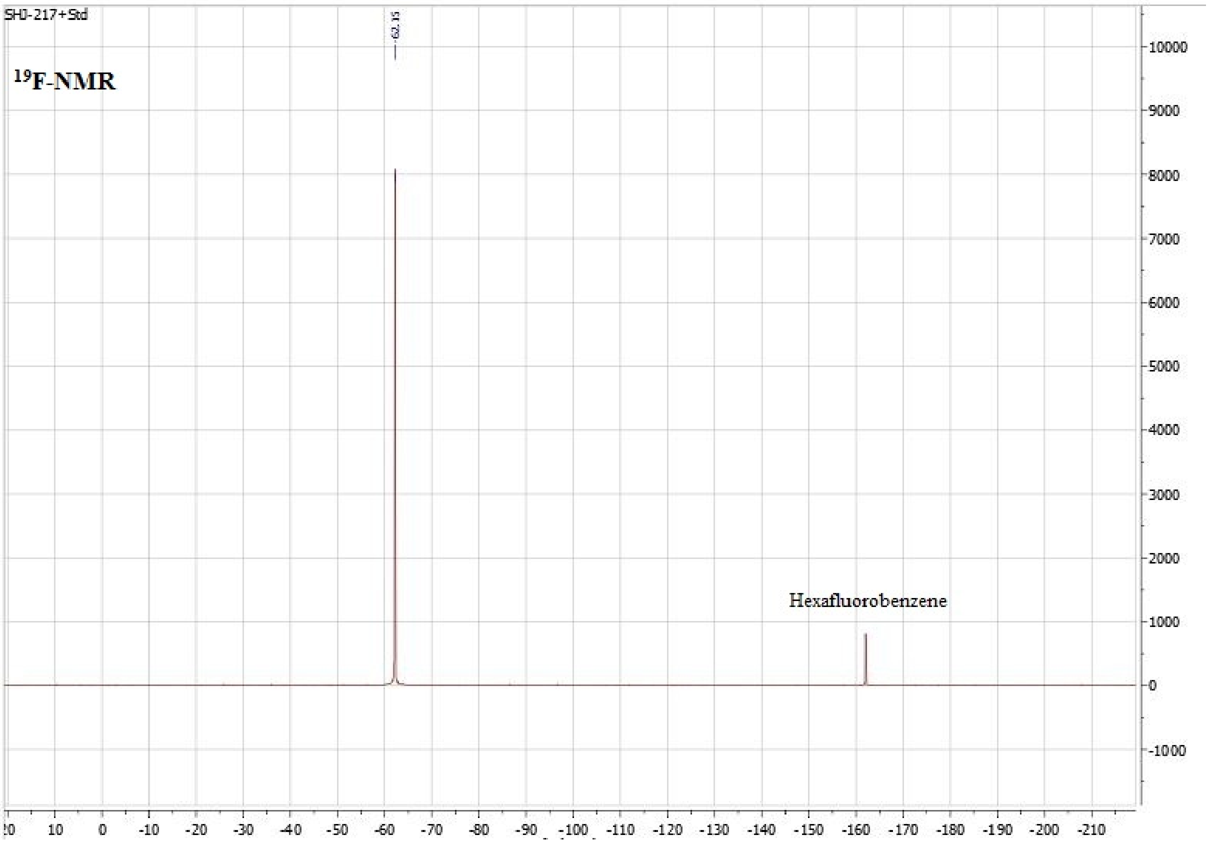
found: C: 44.82 H: 2.51 N: 2.33

ESI-MS: m/z = 321 [M^+] (100), 209 [$(M-C_8H_{17})]^+$ (26)

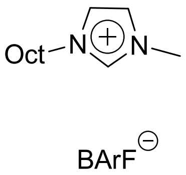
I.C. 2.1) ^{1}H-, ^{13}C- and ^{19}F-spectra of (**3/BAr^{F}$_{4}$**)






SHJ-217+Std
^{19}F-NMR
62.15
Hexafluorobenzene
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210

I.C.3) 1-methyl-3-octyl-imidazolium-bis(tetrakis(3,5-bis-(trifluoromethyl)phenyl) borate (**4/$\mathbf{BAr^F_4}$**)



The compound was synthesized by general procedure B.

Yield: 87% (yellow solid)

^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 0.88 (t, 3H, ^3J = 6.80 Hz), 1.11-1.46 (m, 10H), 1.87 (p, 2H, ^3J = 7.40 Hz), 3.87 (s, 3H), 4.11 (t, 2H, ^3J = 7.40 Hz), 7.20-7.23 (m, 1H), 7.24-7.28 (m, 1H), 7.57 (s, 4H), 7.73 (bs, 8H), 8.07 (s, 1H) ppm.

^{13}C-NMR (100 MHz, CD_2Cl_2): δ = 14.3, 23.1, 26.7, 29.3, 29.5, 30.5, 32.2, 37.4, 51.5, 117.9-118.4 (m), 123.6, 124.7, 125.2 (q, ^1J = 271 Hz), 129.5 (dddd, ^2J = 31.5 Hz), 134.4 (bs), 135.4 (bs), 162.4 (dd, ^1J = 49.7 Hz) ppm.

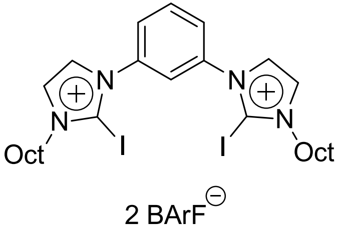
^{19}F-NMR {^{1}H} (235 MHz, CD_2Cl_2): -62.16 ppm.

Elemental analysis: *calc.*: C: 49.92 H: 3.33 N: 2.65

found: C: 50.05 H: 2.31 N: 2.52

ESI-MS: m/z = 195 [M^+] (100)

I.C.4) 1,3-bis(2-iodo-3-octyl-imidazol-1yl)benzene-bis(tetrakis(3,5-bis-(trifluoromethyl)phenyl)borate) (**2/BAr$^F_4$**)



The compound was synthesized by general procedure B.

Yield: 68% (yellow foam)

^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 0.88 (t, 6H, ^{3}J = 6.20 Hz), 1.17-1.53 (m, 20H), 1.93 (p, 4H, ^{3}J = 15.3, 7.60 Hz), 4.23 (t, 4H, ^{3}J = 7.50 Hz), 7.42-7.50 (m, 1H), 7.57 (bs, 8H), 7.62-7.68 (m, 4H), 7.74 (bs, 18H), 7.92 (t, 1H, ^{3}J = 8.10 Hz) ppm.

^{13}C-NMR (100 MHz, CD_2Cl_2): δ = 14.3, 23.1, 26.8, 29.4, 29.4, 29.5, 30.2, 32.2, 55.4, 97.5, 118.1-118.4 (m), 125.1 (q, $^1J_{CF}$ = 270 Hz), 127.3, 127.8, 129.6 (dddd, $^2J_{CF}$ = 31.6 Hz), 131.1, 134.4, 135.5 (bs), 137.7 162.4 (dd, ^{1}J = 49.9 Hz) ppm.

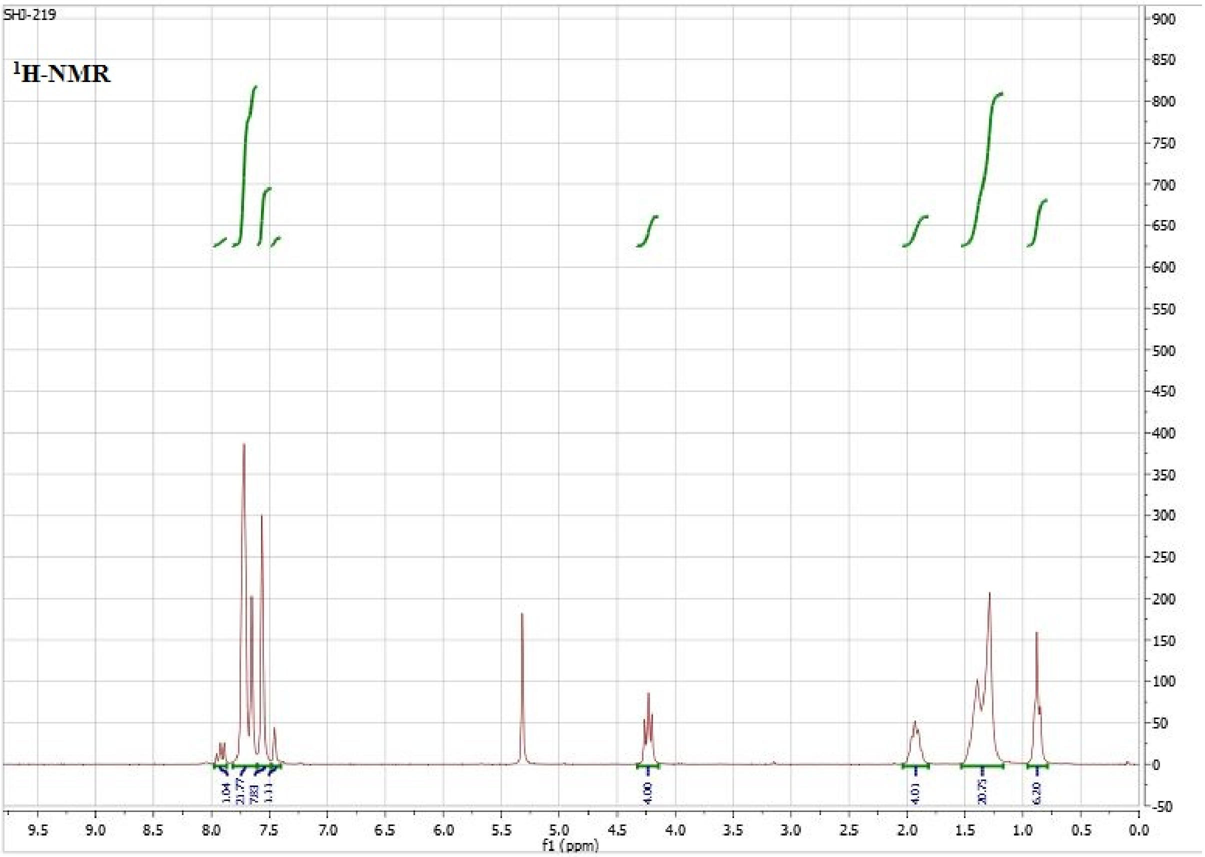
^{19}F-NMR {^{1}H} (235 MHz, CD_2Cl_2): -62.03 ppm.

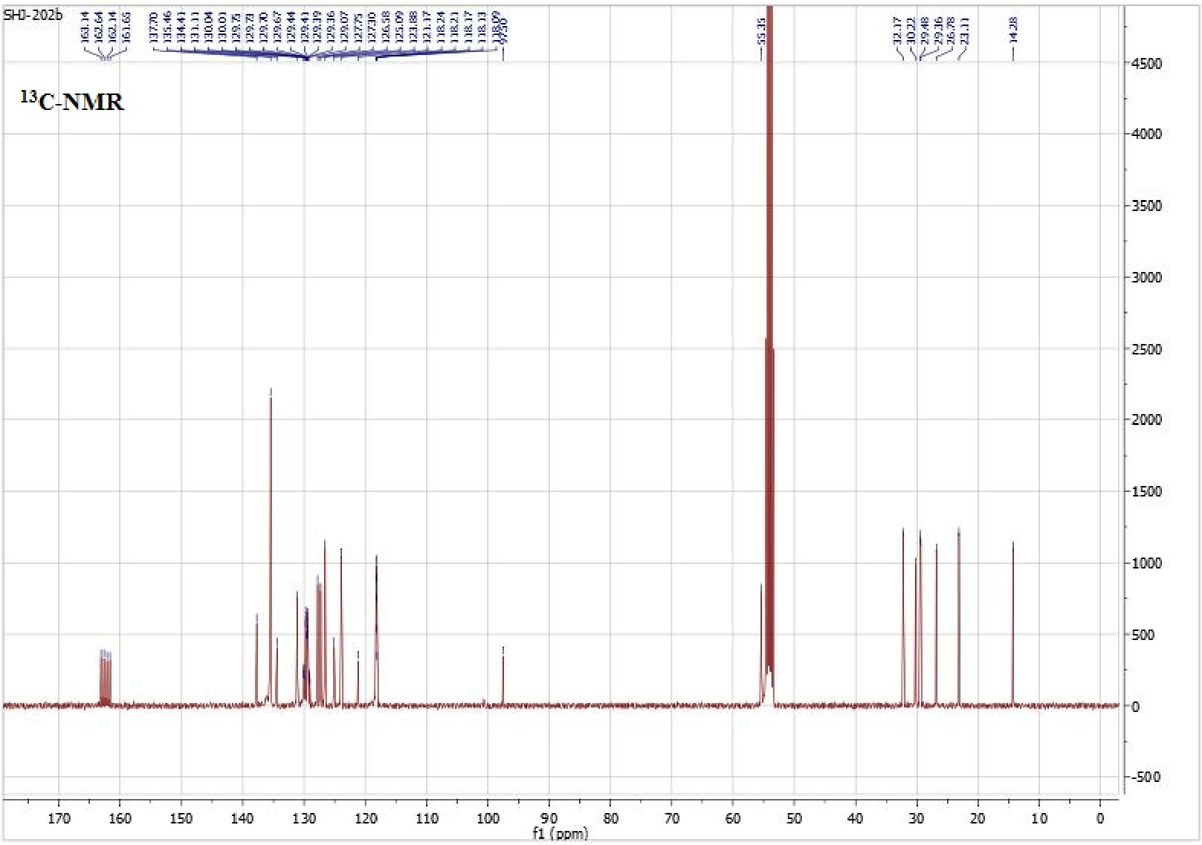
Elemental analysis: *calc.*: C: 45.76 H: 2.75 N: 2.32

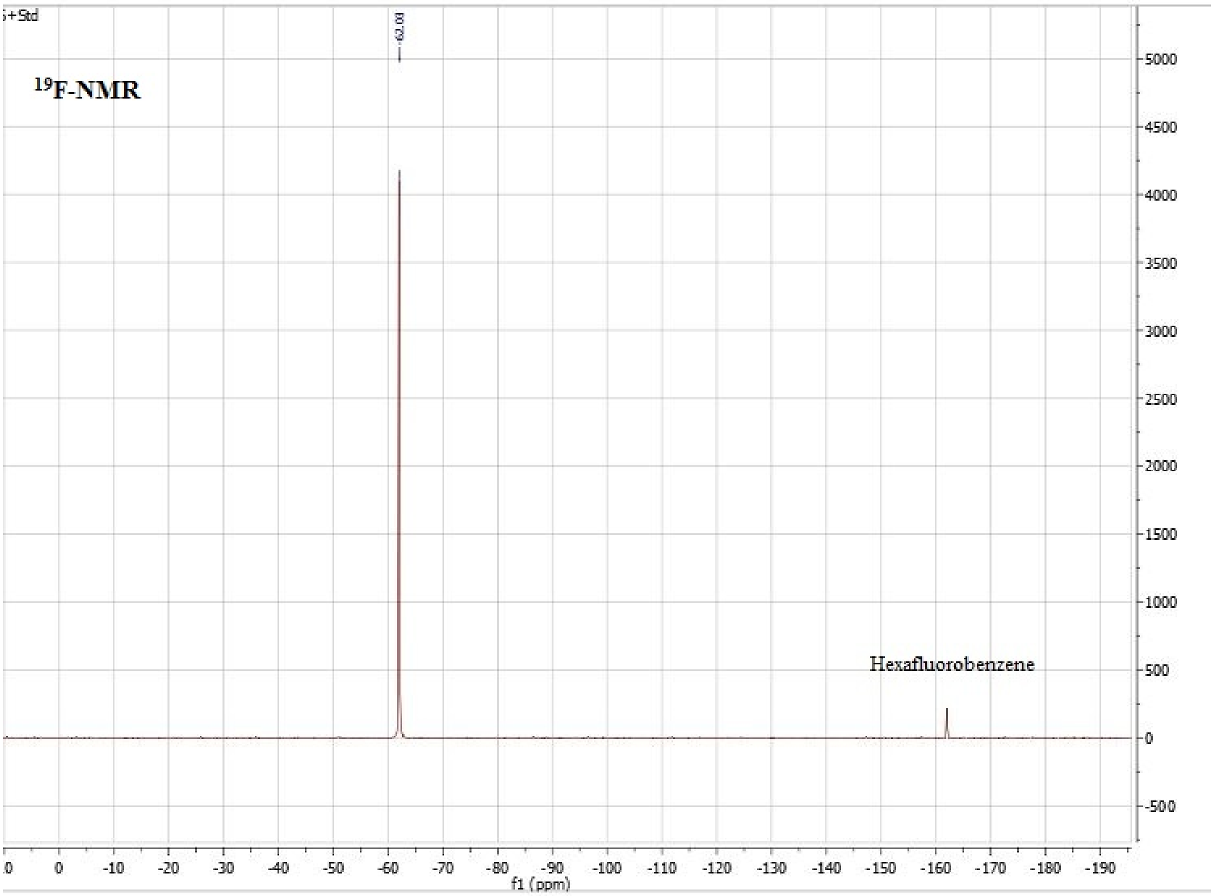
found: C: 45.74 H: 2.73 N: 2.31

ESI-MS: m/z = 1151 [(M+BArF)$^+$] (100), 575 [(M-C_8H_{17})$^+$] (38), 463 [(M-$C_{16}H_{34}$)$^+$] (18), 344 [(M-$C_{14}H_{21}IN_2$)$^+$] (24)

I.C. 4.1) ^{1}H-, ^{13}C- and ^{19}F-spectra of (**4/BAr$^{F}_{4}$**)







+Std
-62.03
^{19}F-NMR
Hexafluorobenzene
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

I.D) NMR-Experiments

I.D. 1) General setup for halogen- and hydrogen-bond catalyzed reactions and determination of the yield

CD_2Cl_2 was dried over 3Å molecular sieves and stored under argon-atmosphere. H_2O-content was measured *via Karl-Fischer*-Titration and kept below 10 ppm in all measurements.
To an NMR tube, 300 µL of CD_2Cl_2 and 100 µL out of a stock solution of activators and/or suppressor (see Table 1) were added. Stock solutions of freshly distilled methyl vinyl ketone (MVK, 6.30 mM) and freshly distilled cyclopentadiene (CPD, 63.0 mM, including 1 µL tetraethylsilane (TES) per 100 µL solvent) were prepared and 100 µL, respectively, added to the NMR tube. The reaction progress was monitored *via* ^{1}H-NMR spectroscopy. An error margin of 5% is assumed. Important measurements were reproduced several times.

The yields were determined *via* the following procedure. The ethyl peak of TES (0.52 ppm, q, *J* = 8.00 Hz) was calibrated as 1. The peaks of the methyl group of the *exo* product (s, 2.18 ppm), the methyl peak of the *endo* product (s, 2.09 ppm), and the methyl peak of methyl vinyl ketone (s, 2.25 ppm) were integrated.

I.D. 2) Acid catalyzed reaction

To an NMR-tube filled with 400 µL of CD_2Cl_2, 2.00 µL of a 0.0378 mM stock-solution of HOTf (1.2 Mol-%) in CD_2Cl_2 were added. A second NMR-tube was charged with 200 µL CD_2Cl_2 and 2.00 µL of the same HOTf stock-solution. Additionally 200 µL of a 3.15 mM stock-solution of Tetrabutylammonium methanesulfonate (50 Mol-% = 2.50 eq based on **2/BAr^F$_4$** were placed in this NMR-tube.
Each tube was then charged with 100 µL cyclopentadiene and 100 µL methyl vinyl ketone out of the corresponding stock-solutions mentioned above.

I.D. 3) Titration experiments for binding constant

To an NMR tube, filled with 15.0 µmol of **2/BAr$^{F}_{4}$** (added via a 52.0 mM stock solution in CD_2Cl_2) and 0.90 µL tetraethylsilane as internal standard, varying amounts of cyclohexanone were added (either from a 188 mM stock solution in CD_2Cl_2 or directly). Varying amounts of CD_2Cl_2 were added in order to reach a total volume of 600 µL. The existing ratio of **2/BAr$^{F}_{4}$** and cyclohexanone was calculated from ^{1}H-spectra. The adjusted ratios and detected ^{13}C shifts of *C*-I are shown in SI IV).

I.D. 4) Acid titrations of cyclohexanone

To three NMR tubes, each filled with 600 µmol of cyclohexanone and 0.90 µL tetraethylsilane as internal standard, 6.00 µmol, 12.0 µmol and 18.0 µmol HOTf (corresponding to 1, 2, and 3 mol%) were added respectively (from a 58.0 mM stock solution in CD_2Cl_2). Varying amounts of CD_2Cl_2 were added in order to reach a total volume of 600 µL.

II) Kinetics of *Diels-Alder* Reaction (Graphical Representations)

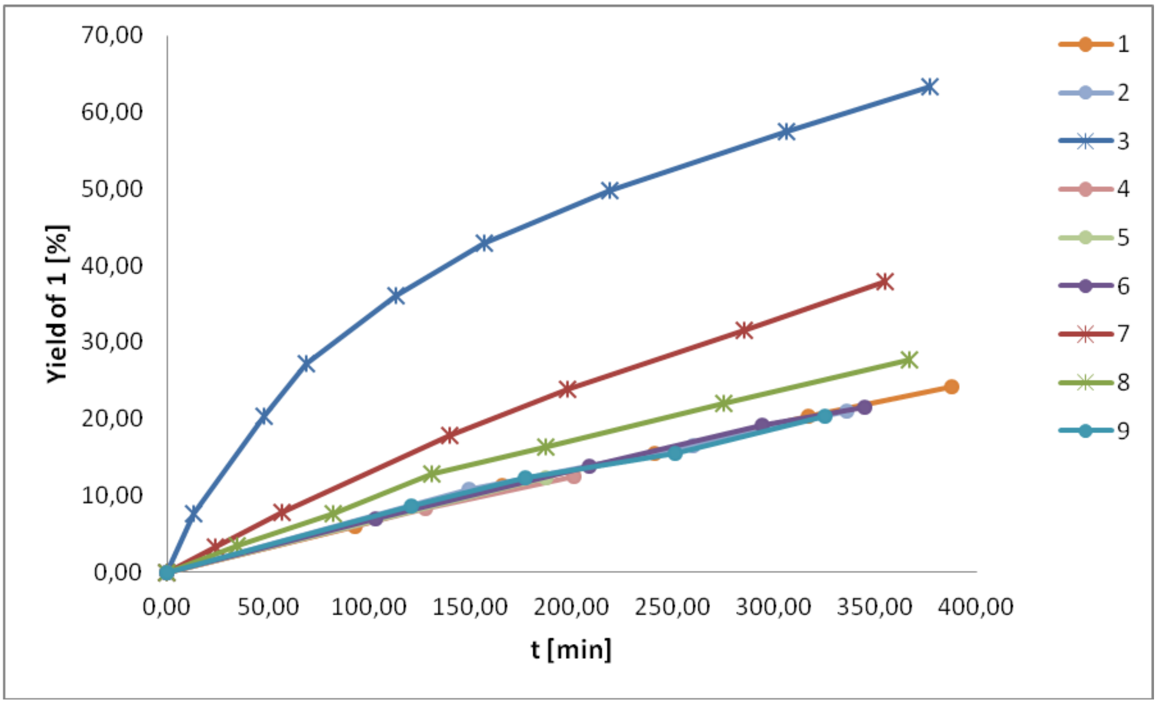


Figure SI-1: Graphic representation of NMR-experiments #1 to 9 (see Table 1 and Figure 2)

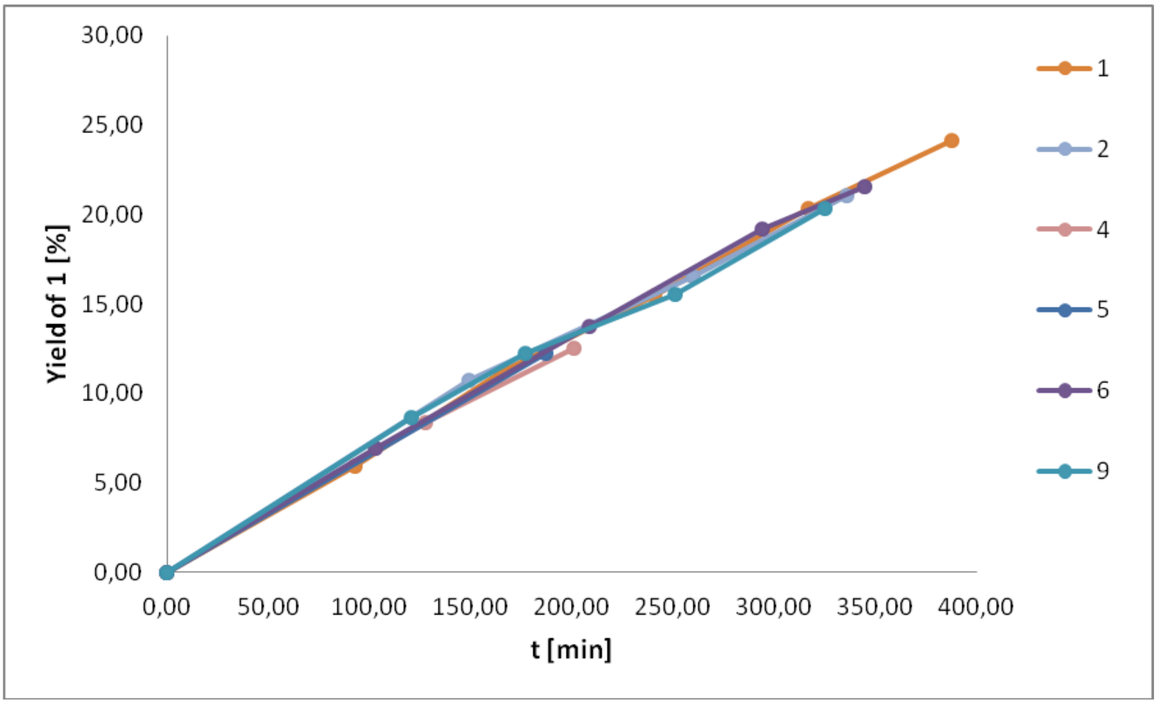


Figure SI-2: Graphic representation of NMR-experiments #1,2,4,5,6 and 9 (see Table 1 and Figure 2)

III) Tabulated results of *Diels-Alder* Reaction (Graphical Representations)

Activating reagent/Additive	Equiv.	t [min]	Yield [%][a]	Endo/Exo Ratio[a]
2/BAr^F_4	0.20	13	7.60	8.00
		48	20.3	9.30
		69	27.3	8.60
		113	36.2	10.3
		157	42.9	10.3
		219	49.7	11.4
		306	57.6	10.0
		377	63.3	10.1
3/BAr^F_4	0.20	35	3.50	3.00
		82	7.60	5.30
		131	12.8	4.30
		187	16.4	4.50
		275	22.0	5.70
		367	27.8	6.70
7	0.20	24	3.30	10.0
		57	7.70	7.70
		140	17.9	6.40
		198	23.9	6.90
		285	31.5	7.00
		355	38.0	7.40
2/OTf	0.20	149	10.8	5.00
		260	16.6	5.20
		336	21.1	5.40
2/$BAr^F_4{}^+$ 2.50 eq TBA-OTf	0.20+0.50	103	6.90	6.70
		209	13.8	4.60
		294	19.2	4.30
		345	21.6	5.50
TMA-BAr^F	0.20	128	8.30	6.00
		201	12.50	6.00
MeOH	0.02	187	12.30	5.30
4/BAr^F_4	0.20	121	8.70	3.80
		177	12.2	4.30
		251	15.5	5.50
		325	20.4	5.30
Blank	-	93	6.00	5.70
		166	11.2	4.40
		241	15.4	5.50
		317	20.3	5.70
		388	24.1	5.30

[a] Determined *via* ^{1}H-NMR

IV) Titration data

The results of the titration of **2/BAr$^F_4$** with cyclohexanone are depicted below.

Concentration of **2/BAr$^F_4$**	Equivalents of cyclohexanone	δ (*C*-I) [ppm]
0.025	0	97.21
0.025	0.68	97.55
0.025	1.39	97.81
0.025	2.19	98.03
0.025	2.77	98.22
0.025	4.28	98.49
0.025	6.00	98.69
0.025	8.41	99.02
0.024	33.3	100.25
0.022	97.8	100.95
0.021	224	101.21

Graphical depiction:

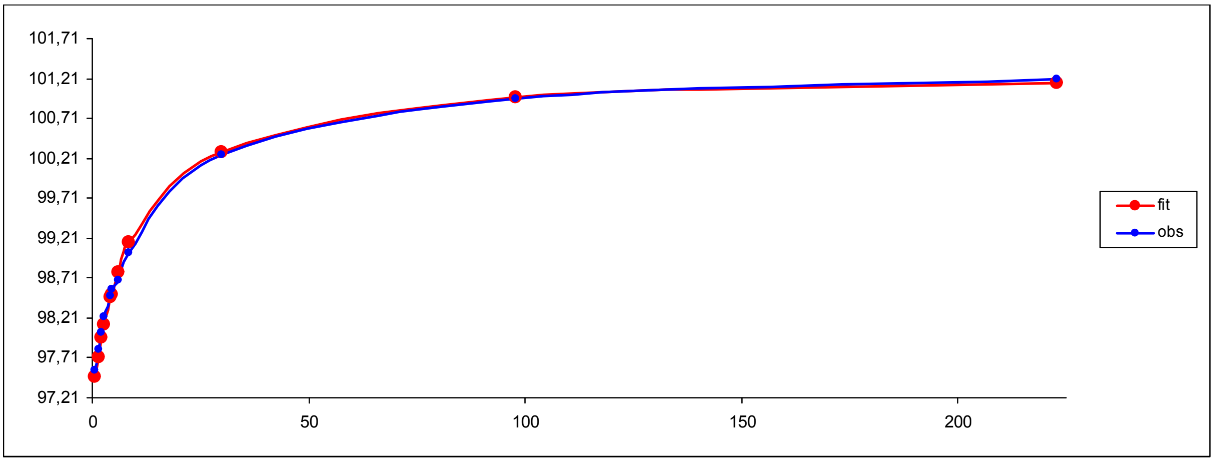


Figure SI-3: Experimental (blue) and fitted (red) titration curve; y-axis: C-I NMR shift in ppm; x-axis: equivalents of cyclohexanone.

Fitting of the titration curve (1:1 stoichiometry) resulted in K = 4 M^{-1}.

V) Data for Exclusion of Acid Traces

The results of the titration of cyclohexanone with HOTf are depicted below.

Equivalents of HOTf	δ (*C*=O) [ppm]
0	211.49
1 mol%	211.67
2 mol%	211.88
3 mol%	212.17

A solution containing one equivalent of cyclohexanone and 0.5 equivalents of **2/BAr$^F{}_4$** gave a shift of the carbonyl carbon atom of cyclohexanone of δ (*C*=O) = 212.23 ppm. Since the shift corresponding to 2 mol-% of acid (211.88) is lower than the one corresponding to 0.5 equivalents of **2/BAr$^F{}_4$** (212.23), it can be concluded that 0.5 equivalents of **2/BAr$^F{}_4$** would need to contain more than 2% of acid traces to induce a similar shift. This corresponds to more than 4% of alleged acid impurities for one equivalent of **2/BAr$^F{}_4$**.

The activity of **2/BAr$^F{}_4$** can be quenched by 2.5 equivalents (based on the amount of **2/BAr$^F{}_4$**) of NBu_4OTf (see paper). However, even 1.2% of acid* - far less than the 4% derived above - are still active in the Diels-Alder reaction in the presence of the same 2.5 equivalents of NBu_4OTf, see below:

* based on the amount of **2/BAr$^F{}_4$** used in the comparison experiment mentioned in the previous sentence

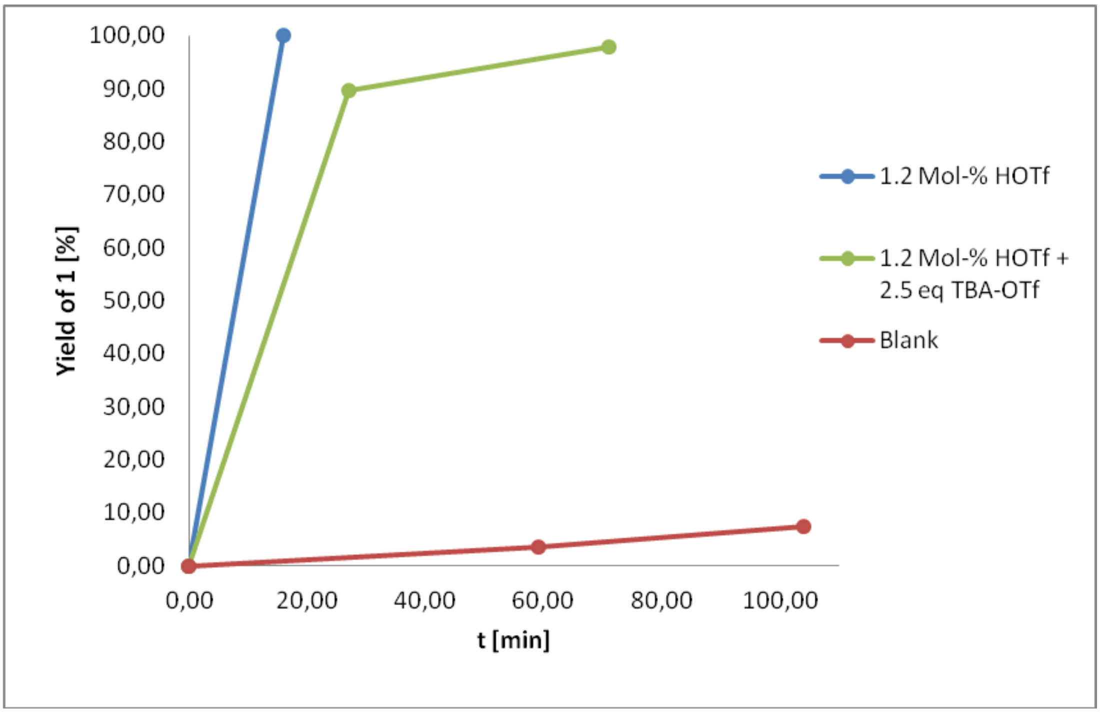
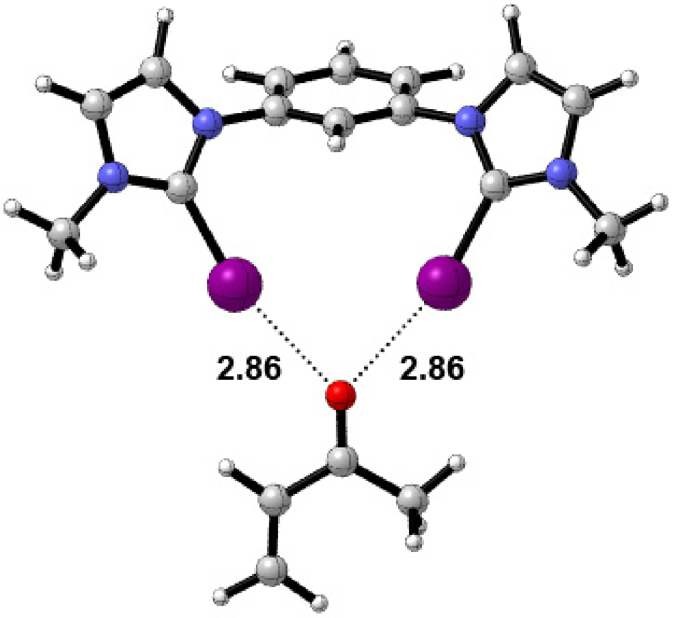


Figure SI-4: Acid catalyzed reaction

VI) DFT calculations

Orientating density functional (DFT) calculations were performed with the Gaussian09 suite of programs (Revision D.01).[S8] The M06-2X density functional was used, which is recommended for weak non-covalent interactions.[S9] The basis set (def2-TZVPP)[S10] was of triple-zeta quality, and the corresponding pseudopotential for iodine was employed.[S11] The nature of the obtained minimum and transition state structures was confirmed by the expected number of imaginary frequencies ($N_{imag}=0$ for minima, $N_{imag}=1$ for transition states). For transition states, the imaginary frequency was followed in both directions (starting materials and product) to ensure that the correct transition state was found. Subsequently, single-point calculations on these structures were performed which additionally included the D3 dispersion correction by Grimme[S12] and the SMD solvation model[S13] with the predefined parameters for dichloromethane. The free energies of the respective compounds were obtained by adding the thermodynamic corrections at the lower level (M06-2X TZVPP) to the energy obtained at the higher level (M06-2X-D3 TZVPP SMD). In all computations, the non-coordinating counterions were omitted and the octyl side chains were substituted with methyl groups, in order to allow an efficient use of computational resources.

For the adduct of methyl vinyl ketone with halogen-bond donor **2**, a stable minimum was found (distances in Ångstrom; C-I-O angles: 165° for both halogen bonds):



For the corresponding transition state in the reaction with cyclopentadiene, see Figure 4 in the manuscript.

Coordinates of minima and transition states:

Cyclopentadiene

C	1.17369900	-0.27878200	-0.00018700
H	2.20295200	-0.60321400	-0.00048200
C	0.73289200	0.98596900	0.00012600
H	1.34627800	1.87493900	0.00019900
C	-0.73445200	0.98481000	-0.00011600
H	-1.34934400	1.87272900	0.00018700
C	-1.17319800	-0.28061200	-0.00008200
H	-2.20194100	-0.60657800	-0.00002000
C	0.00094900	-1.21162800	0.00005500
H	0.00097200	-1.86898900	-0.87532000
H	0.00174000	-1.86742800	0.87666100

Methyl vinyl ketone

C	-1.91865000	0.16768100	-0.00012500
C	-0.87093000	-0.64547300	0.00020200
H	-1.80602400	1.24438000	-0.00071600
H	-0.98860400	-1.72242100	0.00062900
C	0.54560700	-0.18849200	0.00003800
O	1.43518800	-1.00523800	-0.00019200
C	0.83394200	1.29339900	0.00011300
H	0.39653600	1.76622400	-0.87983500
H	0.39706200	1.76602300	0.88041200
H	1.90933100	1.44165900	-0.00024300
H	-2.92962000	-0.21665900	-0.00008100

Transition state (uncatalyzed reaction)

C	-0.79475100	-0.92543800	-0.92516200
H	-0.34038600	-1.78103700	-1.40260500
C	-0.79807200	0.36393500	-1.43675300
H	-0.21987000	0.69775000	-2.28577300
C	-1.52969400	1.18848900	-0.57691900
H	-1.62011100	2.26162600	-0.66512700
C	-1.97925100	0.43180300	0.50538000
H	-2.69000400	0.79237800	1.23530800
C	-0.18918400	0.23573200	1.62625100
C	0.58816900	-0.62032900	0.86050000
H	0.07263200	1.28073800	1.70594600
H	0.56935900	-1.68552400	1.05098900
C	1.76752300	-0.18993700	0.08510700
C	-1.90980400	-1.00929300	0.07337100

H	-2.83311300	-1.23717600	-0.47452500
H	-1.78791000	-1.74193000	0.86516100
O	2.51722200	-1.00125600	-0.41449400
C	2.03170500	1.29345700	-0.04593700
H	1.12102900	1.84424900	-0.28257200
H	2.40654400	1.67454100	0.90615900
H	2.78185700	1.45397600	-0.81492700
H	-0.71764900	-0.16006000	2.48287500

Methyl vinyl ketone complexed by analogue of halogen-bond donor 2

H	0.38149900	-1.71695500	-1.03847300
C	0.46504600	-2.15927100	-0.05487600
C	0.69717200	-3.37979100	2.44792400
C	-0.64184500	-2.69542900	0.58576100
C	1.68641900	-2.22634000	0.59857400
C	1.81597300	-2.83163800	1.83945600
C	-0.54004500	-3.30645400	1.82643900
H	2.78122000	-2.86424500	2.32685500
H	-1.42244200	-3.71158900	2.30346800
C	-2.63388800	-1.55934300	-0.38239800
N	-3.78911800	-1.96838700	-0.90762400
C	3.09258100	-0.40674700	-0.35487300
N	4.32231800	-0.33559700	-0.86514400
I	-2.03623800	0.39275000	-0.10217700
I	1.77960500	1.15937200	-0.09241900
C	-4.85913000	-1.09416700	-1.39252900
H	-5.64977200	-1.72035700	-1.79236900
H	-4.47242200	-0.44639100	-2.17498300
H	-5.24358500	-0.49778400	-0.56892500
C	4.97483100	0.88504600	-1.34336700
H	5.95020200	0.61417200	-1.73367200
H	5.09001800	1.58367100	-0.51849300
H	4.37504500	1.33239200	-2.13171600
C	-2.15342900	4.44946100	0.58556100
H	-2.90767900	3.67727900	0.49335700
C	-2.48954000	5.71439800	0.81581700
H	-1.75056900	6.49932500	0.91151800
C	-0.76372800	3.99219100	0.43983800
O	-0.53940100	2.80309900	0.22577500
H	0.78679600	-3.85116600	3.41599400
C	-2.66763000	-3.77933200	-0.37116900
C	-3.82864600	-3.34499300	-0.90775600
C	3.98553000	-2.43927800	-0.33023800
C	4.89325600	-1.58876900	-0.85672400

N	-1.92744400	-2.65673400	-0.05282600
N	2.86364600	-1.69192100	-0.02644500
C	0.36321000	4.97366800	0.55337900
H	0.25871100	5.75442700	-0.20039600
H	0.34310500	5.45721000	1.53034900
H	1.31399000	4.46623200	0.41997100
H	-3.52500100	6.00894700	0.91720500
H	-4.67260700	-3.88891000	-1.29296200
H	-2.29068400	-4.77168100	-0.20039100
H	4.02143900	-3.49995200	-0.15795200
H	5.88684100	-1.76265800	-1.22964400

Transition state (reaction catalyzed by analogue of halogen-bond donor 2)

C	5.20458100	-0.20807800	-1.24587300
H	4.50301900	0.06833300	-2.02047600
C	5.56884300	-1.49202100	-0.91386300
H	5.16390700	-2.39568800	-1.34567600
C	6.49056100	-1.43805800	0.14285900
H	6.93202900	-2.29495900	0.63411400
C	6.66391600	-0.10992000	0.54546600
H	7.48747100	0.20000000	1.17442900
C	5.10164300	0.12705100	1.76042700
C	3.95579400	0.27378400	0.97163400
H	5.20274100	-0.74276900	2.39453600
H	3.67487100	1.25803900	0.61680200
C	2.99572900	-0.74967100	0.74089600
C	6.15035000	0.74041700	-0.59077700
H	6.98996500	0.89438200	-1.28265300
H	5.75277800	1.71640800	-0.32830800
H	-2.46300500	0.38220400	-1.05231200
C	-2.93157100	0.48264700	-0.08177800
C	-4.21344700	0.75597300	2.38533000
C	-3.00032500	1.71206800	0.55609700
C	-3.49498500	-0.61179700	0.55730100
C	-4.13693000	-0.48898200	1.78035800
C	-3.63699700	1.86149700	1.77916400
H	-4.56237500	-1.36275600	2.25735600
H	-3.67091900	2.83303400	2.25574200
C	-1.14204500	3.08525100	-0.37275300
N	-1.04755900	4.31748900	-0.87443200
C	-2.35346200	-2.62005700	-0.37159000
N	-2.76488000	-3.78179900	-0.88133300
I	0.39952100	1.72323700	-0.11559400
I	-0.39871300	-2.00059100	-0.09892400

C	0.18866100	4.95036700	-1.33496100
H	-0.05435900	5.94824000	-1.68721100
H	0.61618500	4.36741900	-2.14790400
H	0.89453800	5.01396000	-0.50972300
C	-1.88990500	-4.85908600	-1.34588700
H	-2.51570600	-5.67522900	-1.69399600
H	-1.26516700	-5.20071200	-0.52352800
H	-1.26814400	-4.49816200	-2.16245300
O	1.89598100	-0.50665100	0.18672200
H	-4.70760800	0.86204700	3.34125000
H	-4.22568400	4.06554100	-0.21308200
H	-5.56914600	-2.26213600	-0.22444000
C	-3.16285900	4.01342400	-0.37139400
C	-2.29141300	4.90982300	-0.88102100
C	-4.57628600	-2.64663300	-0.37939800
C	-4.14190100	-3.81715000	-0.89364300
N	-2.43677700	2.87805400	-0.06381700
N	-3.45321500	-1.90574600	-0.06346500
H	-2.44435500	5.90832500	-1.25184300
H	-4.68605300	-4.66590500	-1.26993900
H	5.51035000	1.02581000	2.20626700
C	3.24438000	-2.15643000	1.20953200
H	4.30016200	-2.39317200	1.31557500
H	2.76975200	-2.28479900	2.18611700
H	2.78710600	-2.85696900	0.51161200

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