Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information for $ArI(NTf_2)_2$: The boundary of oxidative capacity for $ArIL_2$?

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Contents

General Procedures

All reactions were performed under N_2 atmosphere in either a glovebox or using Schlenk technique. Glovebox solvents were dried using an Innovative Technologies Solvent Purification System. The dried solvents were stored under N_2 atmosphere over 3 Å molecular sieves in the glovebox. Deuterated solvents for NMR spectroscopy were purchased from Cambridge Isotope Laboratories and dried by stirring for three days over CaH_2, distilled prior to use, and stored in the glovebox over 3 Å molecular sieves. NO_2-C_6H_4-IF_2 and NO_2-C_6H_4-$I(OTFA)_2$ were synthesised by following literature procedure.[1-2] All other reagents were purchased from Sigma Aldrich and used as received. Glassware was dried in an oven at 120 °C overnight and transferred to the glovebox port or Schlenk line where it was subjected to three vacuum cycles over 30 minutes prior to use. NMR spectra for all experiments were recorded using Bruker Ultrashield Plus 500 MHz and Ascend 400 MHz spectrometers.

Experimental

Synthesis of NO_2-C_6H_4-$I(NTf_2)_2$ from NO_2-C_6H_4-IF_2 (Procedure 1)

To NO_2-C_6H_4-IF_2 (14 mg, 48 µmol) in $CDCl_3$ (1 ml), $TMSNTf_2$ (34 mg, 96 µmol) was added while stored in cold well filled with metal beads cooled by N_2(l). The predominately insoluble NO_2-C_6H_4-IF_2 rapidly dissolved, turning the solution a slight green. The solvent was removed *in-vacuo* leaving an off-white powder (qualitative conversion as observed by *in-situ* NMR, on attempts at isolation the off-white solid was recovered at 31 mg identified by ^{1}H NMR to be 69:31% NO_2-C_6H_4-$I(NTf_2)_2$:NO_2-C_6H_4-I, yield 54%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.64 (dd, 4H, NO_2-C_6H_4-$I(NTf_2)_2$), ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -72.67, 13C{1H} NMR (126 MHz, CDCl3) δ (ppm): 151.67 (s, NO_2-**C**), 138.77 (s, -**C**H), 127.54 (s, -**C**H), 125.54 (s, **C**-I), 118.65 (q, S-**C**F_3). X-ray quality crystals were grown by vapour diffusion ($CHCl_3$/C_6H_{12}).

Synthesis of NO_2-C_6H_4-$I(NTf_2)_2$ from NO_2-C_6H_4-$I(OTFA)_2$ (Procedure 2)

To a solution of NO_2-C_6H_4-$I(OTFA)_2$ (10 mg, 21.1 µmol) was added $TMSNTf_2$ (15 mg, 42.2 µmol) in CH_2Cl_2. The reaction immediately turned light yellow and was subsequently placed in the freezer for recrystallisation. The solvent was removed in vacuo to provide NO_2-C_6H_4-$I(NTf_2)_2$ as beige coloured crystals. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.64 (dd, 4H, NO_2-C_6H_4-$I(NTf_2)_2$), ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -72.67. X-Ray quality crystals were grown in the NMR tube by leaving the solution undisturbed for 15 minutes.

Reaction of NO_2-C_6H_4-$I(NTf_2)_2$ with 3-methylcyclohexene

To a solution of NO_2-C_6H_4-$I(NTf_2)_2$ generated *in-situ* from synthesis procedure 1 while stored in a cold well filled with metal beads and cooled by N_2(l), 3-methylcyclohexene (1 equivalent, 5 mg, 48 µmol, in 0.5 ml $CDCl_3$) was added dropwise over 5 minutes, turning the reaction mixture a pale brown, the product of toluene and NO_2-C_6H_4-I were identified by ^{1}H NMR. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 2.35 (s, 3H), 7.16 (m, 2H), 7.25 (m, obscured by CDCl3 peak).

X-Ray crystallographic data

Single crystals were selected under n-paratone oil, mounted on a nylon loop, and held under a stream of N_2 (180 K) on a Rigaku SuperNova CCD diffractometer using Cu Ka radiation. Structure solution and refinement were performed using the SHELXTL suite of software. The X-ray data indicated the NO_2-C_6H_4-$I(NTf_2)_2$ crystal included a twin (150° rotation along the 010 direction). The best data set was obtained by removing the twin reflections from the hkl file. From the modified data set a solution was found in the space group $P2_1/n$, R_{int} = 0.0609.

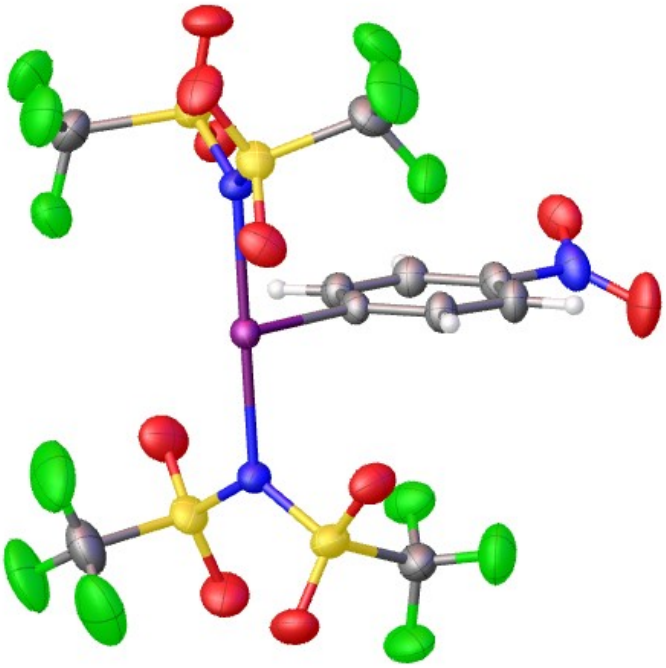

Figure S1 Thermal ellipsoid plot of NO_2-C_6H_4-$I(NTf_2)_2$, thermal ellipsoids are drawn at the 50% probability level. $CDCl_3$ in the lattice has been removed for clarity.

Table S1 Crystallographic information of NO_2-C_6H_4-$I(NTf_2)_2$.

Compound	**NO_2-C_6H_4-$I(NTf_2)_2$**
Empirical Formula	$C_{10}H_4I_1N_3O_{10}F_{12}S_4$
FW (g/mol)	809.28
Crystal System	Monoclinic
Space Group	$P2_1/n$
α (Å)	13.4882(3)
b (Å)	12.8733(3)
c (Å)	15.4391(2)
α (deg)	90
β (deg)	97.786(2)
γ (deg)	90
V (Å^3)	2656.09(10)
Z	2
R1[I>2σI]	0.0338

wR2(F^2)	0.0849
GOF (S)	1.053

NMR Spectra

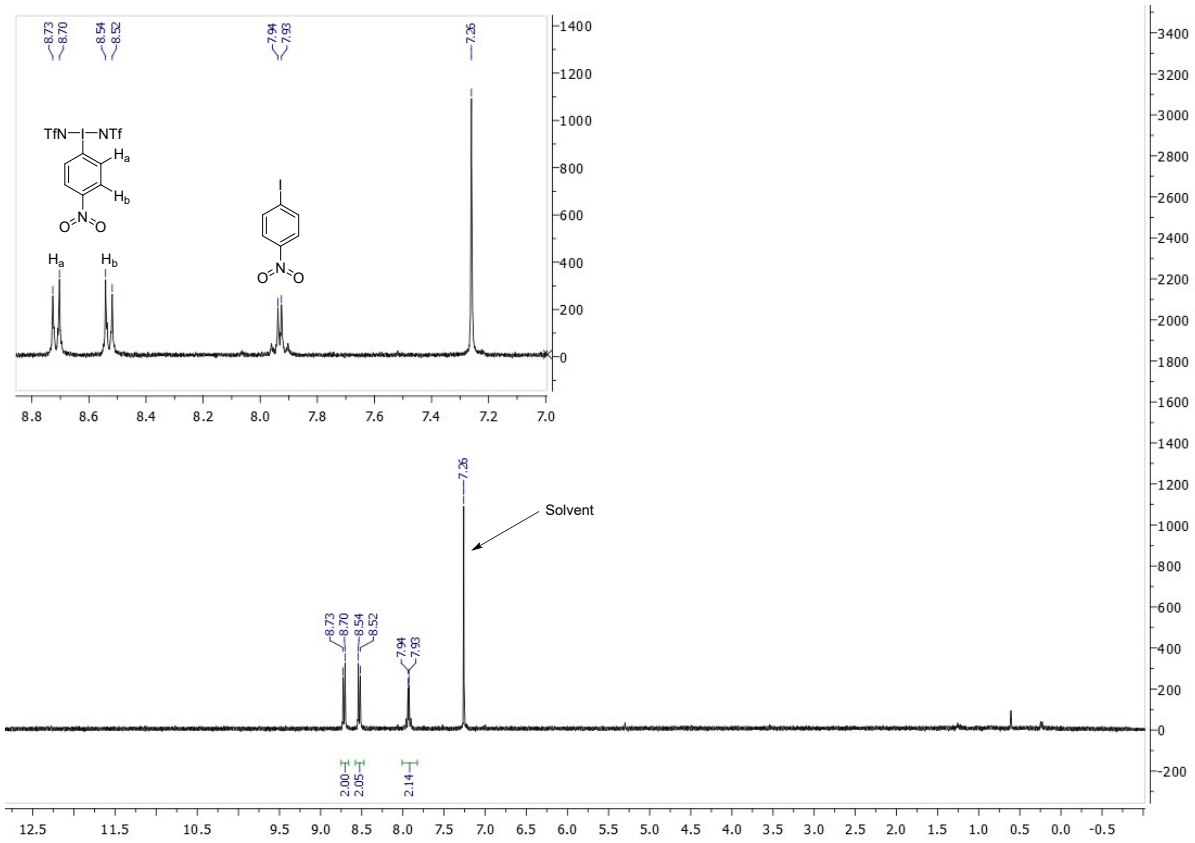

Figure S2 ^{1}H NMR of NO_2-C_6H_4-$I(NTf_2)_2$ isolated by procedure 1.

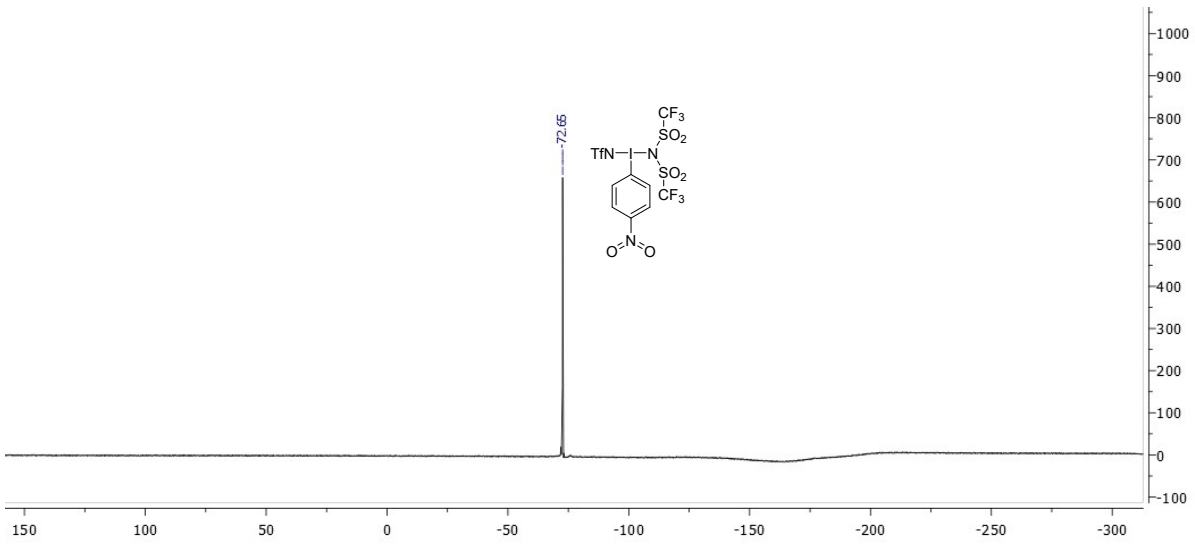

Figure S3 ^{19}F NMR of NO_2-C_6H_4-$I(NTf_2)_2$ isolated by procedure 1.

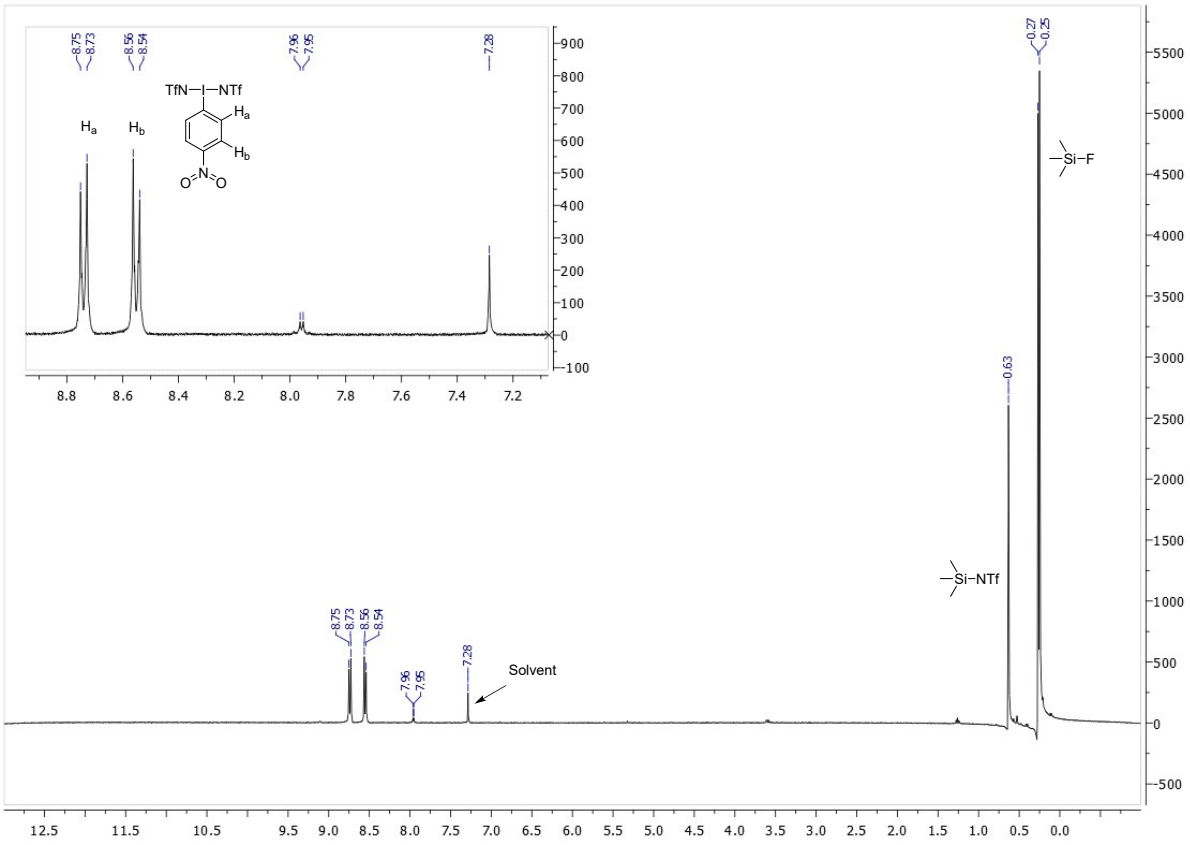

Figure S4 [1]H NMR of in-situ formation of NO_2-C_6H_4-$I(NTf_2)_2$ by procedure 1, TMSF and $TMSNTf_2$ were identified from literature and stock.[3]

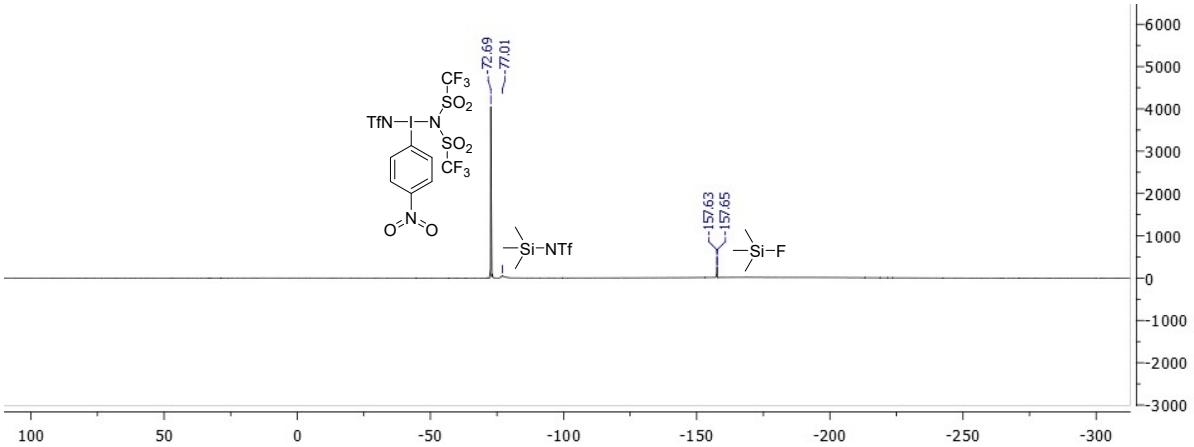

Figure 5 [19]F NMR of in-situ formation of NO_2-C_6H_4-$I(NTf_2)_2$ by procedure 1.

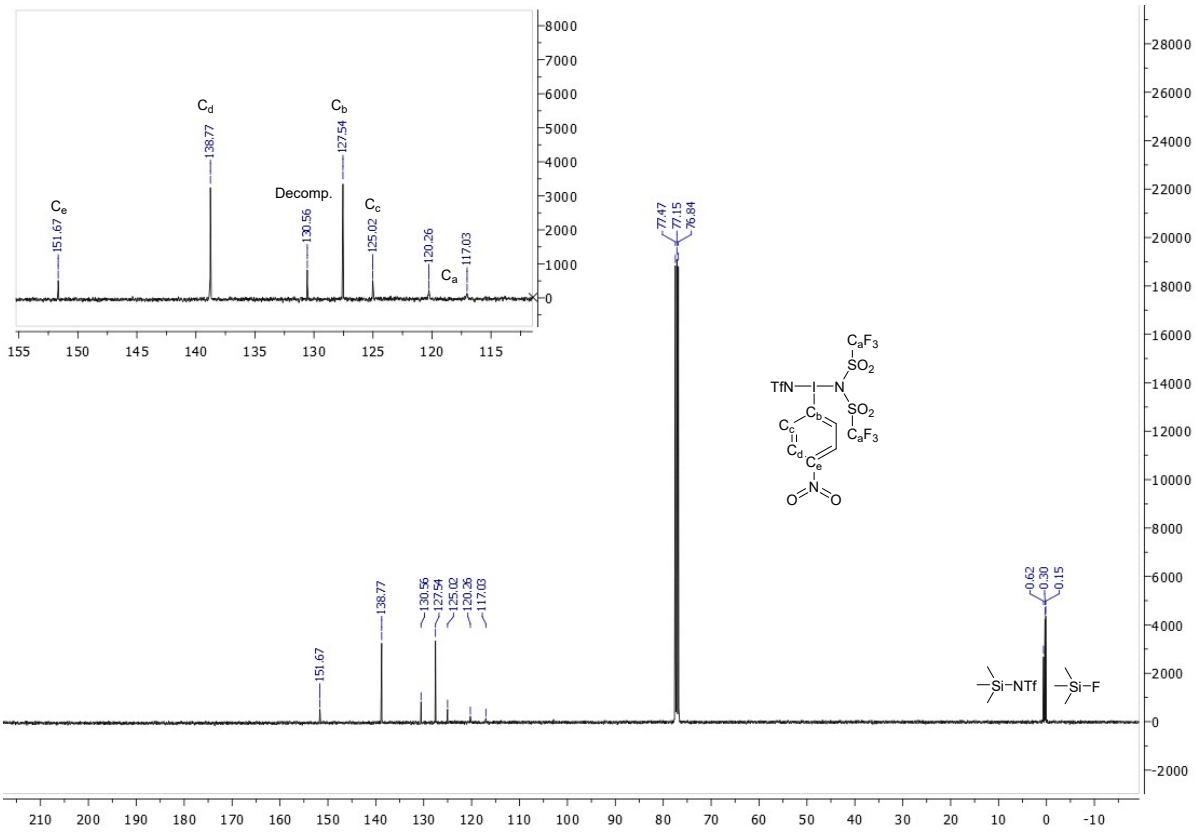

Figure S6 ^{13}C NMR of in-situ formation of NO_2-C_6H_4-$I(NTf_2)_2$ by procedure 1, Instability of the compound lead to decomposition during ^{13}C acquisition.

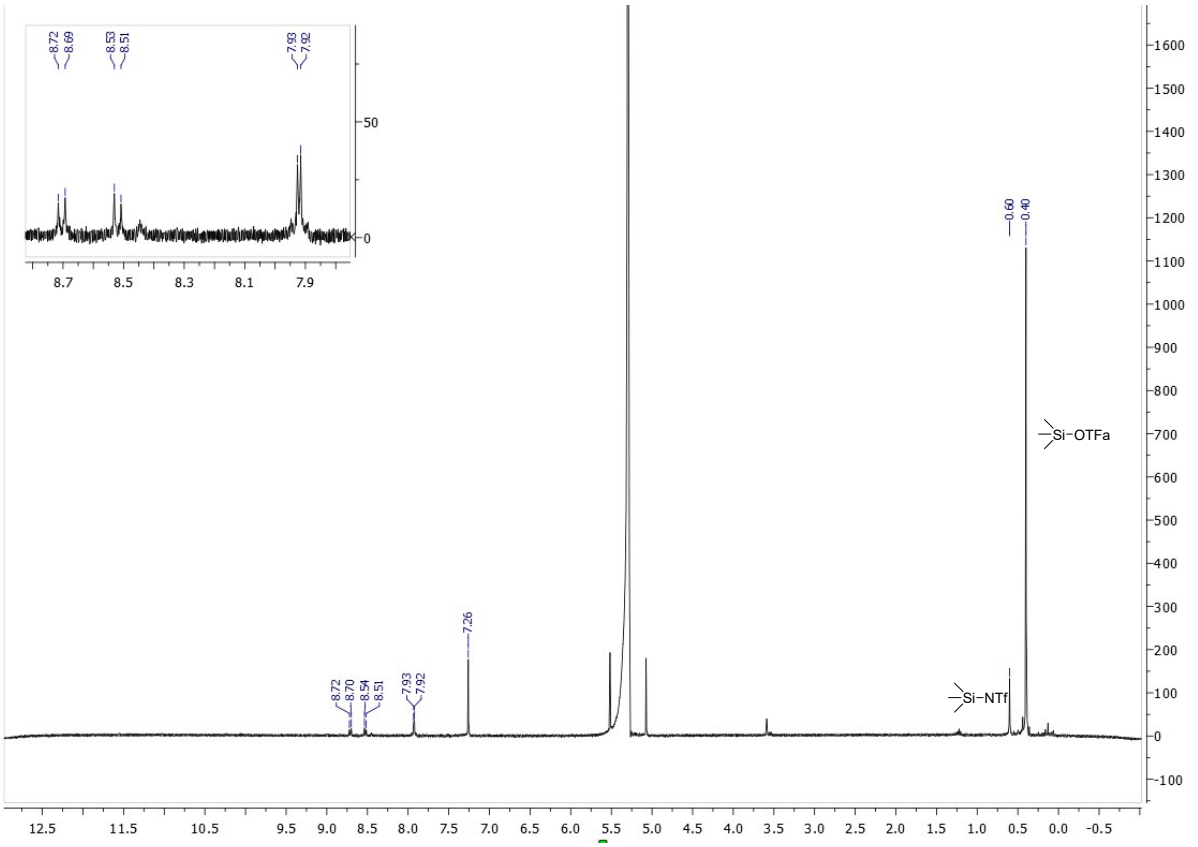

Figure S7 ^{1}H NMR of in-situ formation of NO_2-C_6H_4-$I(NTf_2)_2$ by procedure 2.[4]

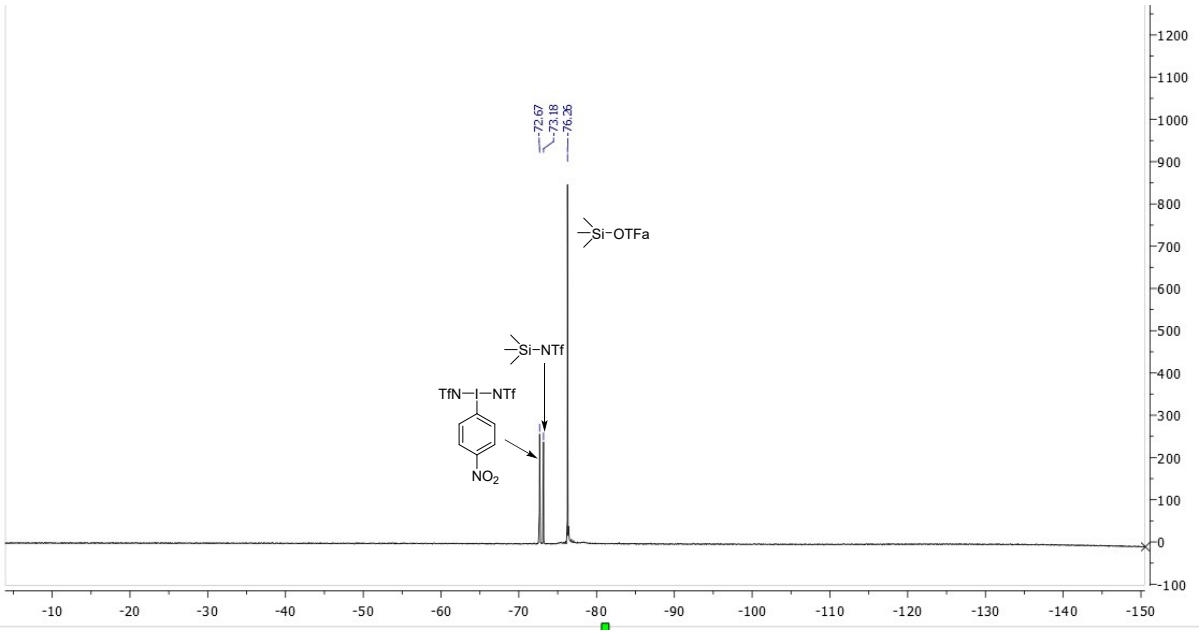

Figure S8 ^{19}F NMR of in-situ formation of NO_2-C_6H_4-$I(NTf_2)_2$ by procedure 2.

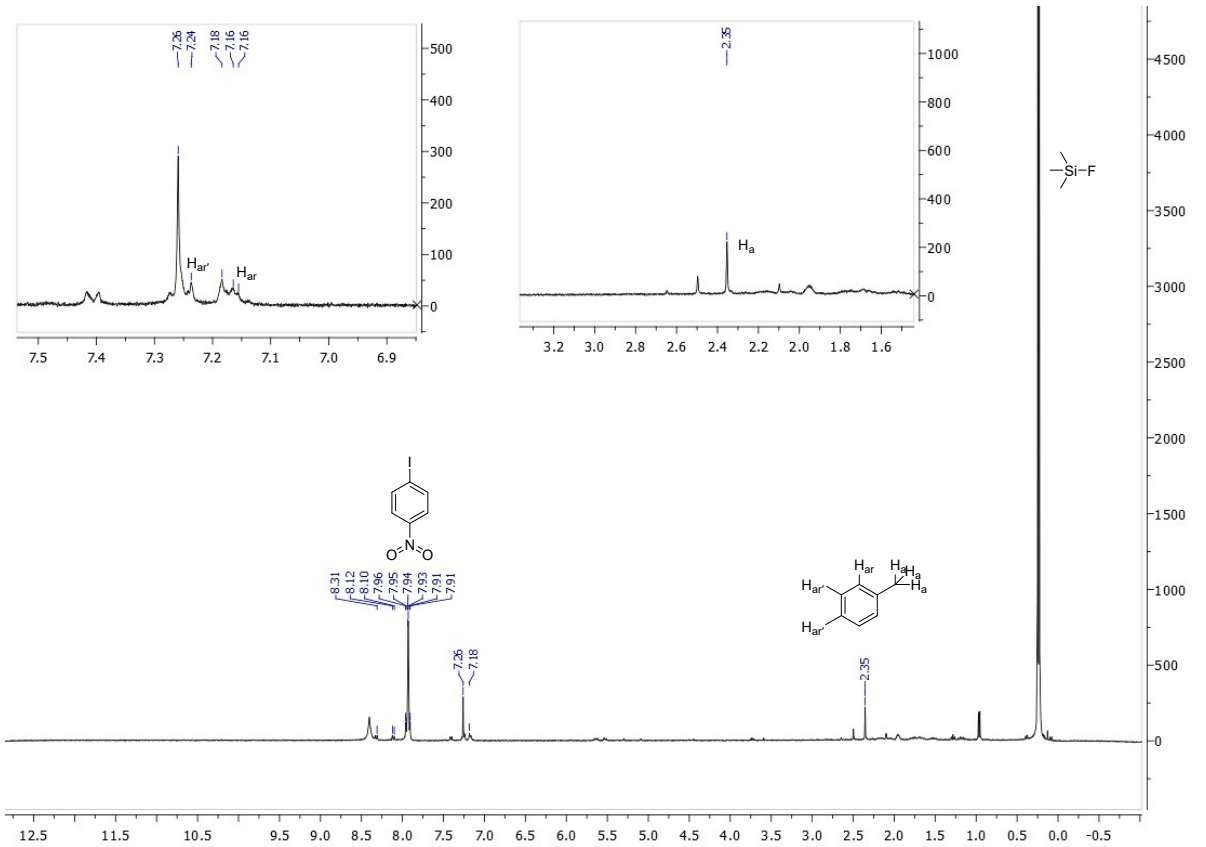

Figure S9 ^{1}H NMR of reaction of NO_2-C_6H_4-$I(NTf_2)_2$ with 3-methycyclohexene.

Computational Details

Cartesian Coordinates for optimised compound geometries:

All geometry optimisation, vibrational frequency were performed using ωPBE/def2-TZVP within Gaussian 16 using the WebMO platform.[5-7] Molecular orbital calculations were performed on the optimized geometries using B3LYP/def2-TZVP.[8, 9]

Coordinates and energies for $PhI(OTf)_2$, NO_2-C_6H_5-$I(OTf)_2$, $PhI(OAc)_2$, PhI(OTf)(OAc) have been previously reported.[1, 10]

Cartesian coordinates are in Å and energies are given in Hartree.

NO_2-C_6H_4-$I(NTf_2)_2$

Electronic Energy: -4387.48746122 Hartree

S	0.00000000	0.00000000	0.00000000
C	-1.15512200	1.11664900	0.90302300
F	-1.67760400	1.95033100	0.01935100
F	-2.11664700	0.42727800	1.48610300
F	-0.48992600	1.81063700	1.82058900
N	0.78591100	-0.79829400	1.20252700
S	0.22987800	-2.19296100	1.87161000
C	0.08233500	-1.71787200	3.64578000
F	-0.73225700	-0.68556800	3.79189400
F	-0.39198900	-2.75659500	4.30715100
F	1.27772300	-1.39564700	4.13668000
O	1.30207900	-3.12621200	1.82785700
O	-1.08003000	-2.50435100	1.44591700
I	3.02554300	-0.61023000	1.29136300
C	2.85395600	1.31869200	2.02257800
C	2.88480500	2.37137900	1.12925500
C	2.80630900	3.65380700	1.63438000
C	2.70201800	3.82233200	2.99650500
C	2.68181200	2.77150900	3.88625400
C	2.76374500	1.48609900	3.39106600
H	2.77420200	0.64060100	4.06433000
H	2.60821300	2.96362300	4.94753100
N	2.61390900	5.19852000	3.53167000
O	2.64871900	6.10182700	2.73585200
O	2.51308700	5.31884800	4.72603500
H	2.82437400	4.51661000	0.98323800
H	2.96415100	2.20275500	0.06510900

N 5.19723100 -0.44195500 1.49889300
S 6.07814900 0.24645100 0.28411500
C 6.76531500 1.82186700 1.01925700
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F 6.68658000 2.75370100 0.08161000
F 6.04380200 2.20301400 2.06729100
O 7.18979800 -0.54997200 -0.07083600
O 5.10228900 0.66573700 -0.66171400
S 5.88707800 -1.06640600 2.84924400
C 6.08846400 -2.85206100 2.43412700
F 6.43748700 -3.48986500 3.53681200
F 7.00507200 -3.02549800 1.50595800
F 4.92309800 -3.32626600 1.99775900
O 7.18249500 -0.52466700 3.02555100
O 4.89273900 -1.03734700 3.86341400
O -0.79821600 -0.85065000 -0.79484100
O 0.98091900 0.85927600 -0.56957700

$C_6F_5I(NTf_2)_2$

Electronic Energy: -4679.12298221 Hartree

S 0.00000000 0.00000000 0.00000000
N 0.76447700 -1.20322300 0.81271200
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C 3.30471100 1.80465500 1.44506100
C 3.24222400 3.00462500 2.11770600
C 2.74187700 3.03460800 3.40778200
C 2.30621100 1.87704800 4.02579300
C 2.37885200 0.67789700 3.34899000
F 1.93582000 -0.41329300 3.93790900
F 1.81941500 1.92529900 5.25310500
F 2.67540000 4.17959700 4.05177100
F 3.64913900 4.12097600 1.54078400
F 3.77589200 1.78277500 0.21563900
N 5.17877000 -1.16253600 1.36406100
S 6.17623700 -0.91175600 0.06259300
O 7.19468700 -1.88977400 0.01426100
C 7.02629500 0.71574000 0.42996100
F 8.26764900 0.50203100 0.80180400
F 7.01308400 1.43022000 -0.68100500
F 6.38413700 1.38166700 1.38387000
O 5.29489600 -0.66778400 -1.02252500
S 5.76665700 -1.58178300 2.84116000
O 7.10724400 -1.14682300 2.96478100

O 4.75423300 -1.24812900 3.77952200
C 5.78382400 -3.42880000 2.81135000
F 5.98869500 -3.84345100 4.04936500
F 6.72792500 -3.89225500 2.02292000
F 4.59935200 -3.86483900 2.38893800
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O -0.99074700 -2.93110300 0.16405400
C -0.00899100 -3.11554900 2.57981900
F -0.84516800 -2.23656500 3.10738900
F -0.52156700 -4.32960200 2.67554100
F 1.14288100 -3.07255200 3.23597900
O -0.72117500 -0.46265600 -1.12176400
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F -2.18816400 -0.30174200 1.40971400
F -0.65818100 0.88571500 2.37005500
O 0.95834100 1.04618900 -0.10229700

PhI(undecafluorocarborane)$_2$

Electronic energy: -3347.32984197 Hartree

C 0.00000000 0.00000000 0.00000000
H -0.05634300 0.67276200 0.86055800
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B -1.48028300 -0.44655300 -0.72246400
B -0.35401800 0.68269500 -1.52381800
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F 0.24608900 -2.81606800 -3.58656900
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B 1.66489500 -1.38509300 -1.69765200
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H -0.65169300 -12.1581000 0.86055800
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B -1.37982100 -11.2652090 -2.66183600
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B -0.88204500 -9.55989800 -2.54472000
B 0.44802800 -9.42026400 -1.34694000
B 0.77224700 -11.0387850 -0.72246400
F 1.93838200 -11.4897750 -0.21059600
B 0.36756400 -10.8339540 -2.44876000
F 1.28469100 -11.0139190 -3.43766000
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B -2.02486200 -11.7210510 -1.06413600
F -2.92104200 -12.6964150 -0.80394400
F 1.37735900 -8.39923000 -1.44016500
F -0.95412500 -8.66927000 -3.58656900
F -3.60481700 -9.67101000 -2.08296200
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F 2.05333200 -1.29320100 1.08840600

$PhI(PF_6)_2$

Electronic Energy: -2410.13571289 Hartree

P 0.00000000 0.00000000 0.00000000
F 1.52154300 -1.31113500 -0.90416900
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C 2.49173700 -4.05465100 -3.49809600

C 2.47696700 -4.05278500 -4.87951800
C 1.52154300 -3.32484000 -5.56479600
C 0.56611900 -2.59689500 -4.87951800
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H -0.19266900 -2.02931900 -2.95225700
H -0.18106300 -2.02918200 -5.41995000
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H 3.22414900 -4.62049800 -5.41995000
H 3.23575500 -4.62036100 -2.95225700
F 1.52154300 -5.33854500 -0.90416900
P 3.04308600 -6.64968000 0.00000000
F 4.01287100 -5.62209700 -0.72409200
F 4.12056100 -7.55260500 0.63736600
F 2.87302500 -7.39240000 -1.37344000
F 1.76144100 -7.37640800 0.53414800
F 2.89687300 -5.59489900 1.17232500
F -1.07747500 0.90292500 0.63736600
F 1.28164500 0.72672800 0.53414800
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$PhI(SbF_6)_2$

Electronic Energy: -2208.07063038 Hartree

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F 3.02836800 -5.25665900 1.33472500

F -1.40500800 0.95730300 0.72383000
F 1.37752800 0.92608700 0.82886300
F 0.23010900 1.00445500 -1.54499400
F -1.06156200 -1.20115500 -0.97975500
F 0.09719200 -1.31467500 1.33472500

$PhI(OTFA)_2$

Electronic Energy: -1581.47924091 Hartree

C 0.00000000 0.00000000 0.00000000
C 1.45865500 0.31253900 -0.41008700
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C 3.93203000 2.55030300 0.12633500
C 3.96172400 3.30423800 1.28335700
C 3.71754500 4.66020100 1.18960000
C 3.45250300 5.23283500 -0.04114200
C 3.42699600 4.45831500 -1.18601700
C 3.66786600 3.09959200 -1.11230300
H 3.63246000 2.48050200 -1.99868400
H 3.21515900 4.91059200 -2.14692500
H 3.26145600 6.29722800 -0.10816900
H 3.73571000 5.27040900 2.08410200
H 4.17184000 2.84741100 2.24205400
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C 7.09956000 0.12273100 0.03090200
O 6.76336400 -1.02446800 0.17814500
C 8.58152000 0.52181400 -0.14931300
F 9.36691000 -0.54359600 -0.12332000
F 8.75448000 1.14799900 -1.31577300
F 8.95842600 1.34999500 0.82873800
O 1.74868900 0.58004500 -1.54263400
F -0.42234100 0.88001100 0.91253700
F -0.08386600 -1.22270400 0.52960700
F -0.81085800 0.06058300 -1.04569900

Undecafluorocarborane anion

Electronic energy: -1409.37849824 Hartree

B 0.00000000 0.00000000 0.00000000
B 0.64930700 -0.68099800 -1.50073900
C 1.39450000 0.63621500 -2.26733300
H 1.39385300 0.63638600 -3.35926800
B -0.08760000 0.93766700 -1.50002600
B 0.35992600 1.76472900 0.00090800

B 2.14933100 1.96865300 0.00129000
F 2.75461200 3.03721300 0.60982100
B 1.39480500 0.63427900 0.92475300
B 1.56798600 -0.88726900 -0.00068700
B 2.41644200 -0.47971700 -1.50104900
F 3.18130300 -1.31365900 -2.26181500
B 2.89617100 0.32932900 0.00002600
F 4.10018500 0.08358200 0.60722100
B 2.77130100 1.26328600 -1.49995000
F 3.80125600 1.73284700 -2.25990200
B 1.22343100 2.13947200 -1.49947800
F 1.09537500 3.26415900 -2.25934700
F 1.70738300 -2.10840800 0.60699100
F 1.39445200 0.63389600 2.29464700
F -0.47010300 2.66901400 0.60930800
F -1.19695400 1.16429800 -2.26004300
F 0.09169300 -1.66522300 -2.26206400
F -1.11745900 -0.50999100 0.60789700

NTf_2^-

Electronic Energy: -1827.03550628 Hartree

S 0.00000000 0.00000000 0.00000000
N 1.13484100 -0.83392000 -0.67747400
S 2.27027800 -1.66709100 -0.00004800
O 2.07973800 -1.99972300 1.37538900
O 2.71824000 -2.68265700 -0.89954200
C 3.66537900 -0.46796100 0.01545400
F 4.74515500 -1.04209500 0.55781600
F 3.37166000 0.61560400 0.73142400
F 3.98793900 -0.07549600 -1.21752700
O 0.19080900 0.33244500 1.37546100
C -1.39581100 -1.19825600 0.01548300
F -1.10303500 -2.28169000 0.73213500
F -2.47546700 -0.62315400 0.55693600
F -1.71792700 -1.59117600 -1.21749200
O -0.44745900 1.01590400 -0.89938400

OTf^-

Electronic Energy

S 0.00000000 0.00000000 0.00000000
O -0.30884800 -1.40822300 -0.00385700
O -0.30866500 0.70083900 1.22159600
C 1.84133700 -0.00008900 0.00000500

F 2.34271500 -0.62028100 -1.08022400
F 2.34266600 1.24580400 0.00298600
F 2.34272500 -0.62548200 1.07722500
O -0.30869800 0.70751600 -1.21771000

OAc^-

Electronic Energy: -228.473727979 Hartree

C 0.00000000 0.00000000 0.00000000
C -1.54664500 0.05106200 -0.00037000
O -2.03467500 1.19974700 0.00049900
O -2.13634100 -1.04764400 0.00050200
H 0.38094000 0.54823900 -0.86479100
H 0.36605300 -1.02718900 -0.02292300
H 0.37656300 0.50464400 0.89299300

$OTFA^-$

Electronic Energy: -526.201174403 Hartree

C 0.00000000 0.00000000 0.00000000
C 1.57222400 -0.00226600 -0.00027300
O 2.03715500 -1.14663300 -0.00008500
O 2.09572600 1.11460600 -0.00004400
F -0.55919300 1.22468800 -0.00576800
F -0.50802400 -0.64233500 -1.07724100
F -0.50665500 -0.63164000 1.08438700

PhI

Electronic Energy: -529.28930457 Hartree

C 0.00000000 0.00000000 0.00000000
C 0.68444400 -1.20169300 0.00003400
C 2.06692200 -1.19584900 0.00005400
C 2.76043200 -0.00015400 0.00014400
C 2.06708500 1.19553000 0.00010000
C 0.68448500 1.20147900 -0.00001900
H 0.14232700 2.13868000 -0.00012300
H 2.60410600 2.13679000 0.00027100
H 3.84385600 -0.00025500 0.00020000
H 2.60395900 -2.13710900 0.00008800
H 0.14204400 -2.13873900 0.00003600
I -2.07167500 -0.00011600 0.00009000

NO_2-C_6H_4-I

Electronic Energy: -733.753165608 Hartree

C	0.00000000	0.00000000	0.00000000
C	0.68403600	-1.20383500	-0.00019100
C	2.06385400	-1.20621000	-0.00017400
C	2.72866100	0.00000000	0.00000300
C	2.06385400	1.20621000	0.00017800
C	0.68403700	1.20383500	0.00019200
H	0.14266500	2.14085700	0.00036300
H	2.62675300	2.12937200	0.00028300
N	4.20009300	0.00000000	0.00000600
O	4.75717800	-1.07037700	0.00046100
O	4.75717800	1.07037700	-0.00048000
H	2.62675300	-2.12937200	-0.00027800
H	0.14266500	-2.14085700	-0.00036300
I	-2.06702800	0.00000000	-0.00000300

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