



Supporting Information

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Fluorophenoxycarbene inside a hemicarcerand: a bottled singlet carbene

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1. Preparation and Characterization of Hemicarceplexes

1.1. Hemicarceplex 2⊙4: 3-fluoro-3-phenoxydiazirine **4** (90 mg) was added to a suspension of **3** (200 mg, 0.105 mmol), 1,4-butanediol dimesylate (78 mg, 0.32 mmol), and Cs₂CO₃ (1.37 g) in dry HMPA (5 mL). The suspension was stirred for six days under nitrogen in the dark at room temperature. The reaction was quenched by the addition of brine/H₂O (40 mL). The precipitate was filtered off, washed with water (3x10 mL) and methanol (2 mL), and dried at high vacuum. The crude product was dissolved in the minimum amount of CH₂Cl₂ and purified by column chromatography (silica gel, EtOAc/CH₂Cl₂) and repurified by HPLC to give **2⊙4** (51 mg, 23 % yield) as a white powder.

¹H NMR (399.969 MHz, CD₂Cl₂, 25 °C): δ = 6.98 (s, 4 H; aryl-*H*), δ = 6.93 (s, 4 H; aryl-*H*), 6.33 (d, ³*J*(H, H) = 7.6 Hz, 2 H; **4**), 5.67 (d, ²*J*(H, H) = 6.8 Hz, 4 H; OCH_{outer}HO), 5.58 (d, ²*J*(H, H) = 6.0 Hz, 4 H; OCH_{outer}HO), 5.09 (t, ³*J*(H, H) = 7.6 Hz, 2H; **4**), 4.70 (t, ³*J*(H, H) = 7.2 Hz, 8 H; CH_{methine}), 4.23 (d, ²*J*(H, H) = 6.4 Hz, 4 H; OCH_{inner}HO), 4.07 (d, ²*J*(H, H) = 6.8 Hz, 4 H; OCH_{inner}HO), 3.89 (br s, 8 H; OCH₂CH₂), 3.82 (br s, 8 H; OCH₂CH₂), 3.02 (t, ³*J*(H, H) = 7.6 Hz, 1 H; **4**), 2.27-2.25 (m, 16 H; OCH₂CH₂), 1.82 (br s, 16 H), 1.45-1.33 (m, 48 H), 0.93 (t, 24 H);
¹⁹F NMR (282.227 MHz, CD₂Cl₂, 25 °C): δ = -117.3 (s); ¹³C NMR (75.428 MHz, CD₂Cl₂, 25 °C): δ = 151.2 (**4**), 148.4, 148.2, 144.4, 139.4, 138.8, 129.5 (**4**), 124.2 (**4**), 117.5 (**4**), 115.2, 114.3, 98.7, 98.3, 86.9 (d, ¹*J*(C, F) = 270 Hz, **4**), 72.5, 72.3, 37.5, 32.4, 30.3, 28.0, 23.1, 14.3;

FAB-MS (NBA matrix): m/z : 2129 (30) $[M+2]^+$, 1977 (100) $[M-4+1]^+$; C, H, N analysis calcd (%) for $C_{127}H_{157}N_2O_{25}F$: C 71.59, H 7.43, N 1.31, found: C 71.50, H 7.17, N 1.02.

1.2. Hemicarceplex 2⊙1: A solution of 2⊙4 (3-20 mg) and pyridine- d_5 (0 or 30 μ L) in CD_2Cl_2 (450 μ L) was placed in a pyrex NMR tube and was degassed by four freeze-pump-thaw cycles under vacuum. The NMR tube was sealed off under vacuum. The sample was cooled in a partially silvered dewar flask filled with liquid nitrogen. The sample tube was placed in the light beam such that the bottom part of the frozen solution was in the focal point (4-5 mm diameter). It was irradiated with the output of an Oriel Hg Power-Max lamp operating at 200 W. A 10 cm water-filter and a 320 nm cutoff filter (WG 320) were placed between the lamp and the sample. Firstly, the front of the sample was irradiated for 10 minutes, followed by further 10 minutes of irradiation after the sample tube had been turned by 180°. During the irradiation the upper part of the frozen solution was protected from the light beam. After each 2x10 minute irradiation period, the sample was moved downwards in 5 mm steps until all of the frozen solution had been irradiated (typically 6-7 vertical steps). The photolysis yield was determined by the integral of the guest proton H1 ($\delta = 6.28$), using the signal assigned to the host's methyl groups ($\delta = 0.94$) as an internal standard.

1H NMR (399.969 MHz, CD_2Cl_2 , 25 °C): $\delta = 6.96$ (s, 8 H; aryl- H), 6.28 (d, $^3J(H, H) = 7.6$ Hz, 2 H; **1**), 5.62 (d, $^2J(H, H) = 6.8$ Hz, 8 H; $OCH_{outer}HO$), 5.56 (t, $^3J(H, H) = 7.6$ Hz, 2 H; **1**), 4.70 (t, $^3J(H, H) = 7.2$ Hz, 8 H; $CH_{methine}$), 4.06 (d, $^2J(H, H) = 7.2$ Hz, 8 H; $OCH_{inner}HO$), 3.83 (br s, 8 H; OCH_2CH_2), 3.82 (br s, 8 H; OCH_2CH_2), 3.28 (t, (d, $^3J(H, H) = 7.6$ Hz, 1 H; **1**), 2.26-2.23 (m, 16 H; OCH_2CH_2), 1.84 (br s, 16 H), 1.46-1.34 (m, 48 H), 0.94 (t, 24 H); ^{19}F NMR (282.227 MHz, CD_2Cl_2 , 25 °C): $\delta = 149.8$ (s); ^{13}C NMR (75.428 MHz, CD_2Cl_2 , 25 °C): $\delta = 285.7$ (d, $^1J(C,$

F) = 569 Hz, **1**), 148.7, 148.0 (**1**), 144.5, 144.3, 139.2, 138.9, 129.9 (**1**), 124.7 (**1**), 117.4 (**1**), 115.2, 114.4, 114.2, 98.6, 72.6, 72.0, 37.3, 32.3, 30.2, 30.0, 27.9, 27.8, 23.0, 14.1.

1.3. Hemicarceplexes 2⊙5 and 2⊙6: Hemicarceplexes **2⊙5** and **2⊙6** were isolated by semi-preparative HPLC from a photolyzed solution of **2⊙4** after complete hydrolysis of **2⊙1**.

Data for **2⊙5**: ^1H NMR (299.940 MHz, CDCl_3 , 25 °C): δ = 6.88 (s, 8 H; aryl-*H*), 5.95 (d, $^3J(\text{H}, \text{H}) = 8.1$ Hz, 2 H; **5**), 5.61 (d, $^2J(\text{H}, \text{H}) = 6.9$ Hz, 8 H; $\text{OCH}_{\text{outerHO}}$), 5.35 (t, $^3J(\text{H}, \text{H}) = 7.5$ Hz, 2 H; **5**), 4.71 (t, $^3J(\text{H}, \text{H}) = 8.1$ Hz, 8 H; $\text{CH}_{\text{methine}}$), 4.15 (d, $^2J(\text{H}, \text{H}) = 7.2$ Hz, 8 H; $\text{OCH}_{\text{innerHO}}$), 3.84 (br s, 16 H; OCH_2CH_2), 3.36 (s, 1 H; **5**), 3.12 (t, $^3J(\text{H}, \text{H}) = 7.5$ Hz, 1 H; **5**), 2.22-2.17 (m, 16 H; OCH_2CH_2), 1.86 (br s, 16 H), 1.41-1.33 (m, 48 H), 0.93 (t, 24 H); FAB-MS (NBA matrix): *m/z*: 2100 (55) $[M+2]^+$, 1978 (100) $[M-5+2]^+$. Data for **2⊙6**: ^1H NMR (399.968 MHz, CDCl_3 , 25 °C): δ = 6.87 (s, 8 H; aryl-*H*), 6.02 (d, $^3J(\text{H}, \text{H}) = 8.8$ Hz, 2 H; **6**), 5.61 (d, $^2J(\text{H}, \text{H}) = 8.0$ Hz, 8 H; $\text{OCH}_{\text{outerHO}}$), 5.07 (t, $^3J(\text{H}, \text{H}) = 7.6$ Hz, 2 H; **6**), 4.71 (t, $^3J(\text{H}, \text{H}) = 8.4$ Hz, 8 H; $\text{CH}_{\text{methine}}$), 4.22 (m, 8 H; $\text{OCH}_{\text{innerHO}}$), 3.85 (br s, 16 H; OCH_2CH_2), 2.96 (t, $^3J(\text{H}, \text{H}) = 7.6$ Hz, 1 H; **6**), 2.22-2.20 (m, 16 H; OCH_2CH_2), 1.86 (br s, 16 H), 1.44-1.33 (m, 48 H), 0.92 (t, 24 H); ^{19}F NMR (282.227 MHz, CD_2Cl_2 , 25 °C): δ_{F} = -82.9 (d, $^2J_{\text{HF}} = 73.3$ Hz); FAB-MS (NBA matrix): *m/z*: 2122 (30) $[M+2]^+$, 1978 (100) $[M-6+2]^+$.

2. Computations

2.1.1. *cis*-Fluorophenoxycarbene @ RB3LYP/6-31g(d)

1	6	-1.896590	1.098606	.284148
2	6	-.555737	1.289930	-.055060
3	6	.207503	.181128	-.397643
4	6	-.320725	-1.104502	-.427264
5	6	-1.662658	-1.279984	-.086828
6	6	-2.450231	-.182990	.269784
7	1	-2.506844	1.954862	.556617
8	1	-.105377	2.277224	-.058346
9	1	.303667	-1.944182	-.714060
10	1	-2.091273	-2.277927	-.102651
11	8	1.548833	.406025	-.822242
12	6	2.615166	.119746	-.111075
13	9	2.209227	-.406992	1.056420
14	1	-3.494249	-.326851	.532217

Low frequencies --- -3.3946 -0.0009 -0.0006 .0004 6.9749 13.2402

Zero-point correction= .100575(Hartree/Particle)
Thermal correction to Energy= .107875
Thermal correction to Enthalpy= .108819
Thermal correction to Gibbs Free Energy= .067473
Sum of electronic and zero-point Energies= -444.628761
Sum of electronic and thermal Energies= -444.621460
Sum of electronic and thermal Enthalpies= -444.620516
Sum of electronic and thermal Free Energies= -444.661862

2.1.2. PBE1PBE/6-311++G(2D,P) opt NMR \cis-fluorophenoxy

carbene\0,1\C,0,-1.4188147993,0.0640540916,-1.6136811101\C,0
,-1.2977747921,0.1883134548,-0.2369286317\C,0,-0.0411276156,0.38652798
6,0.297754067\C,0,1.0910241018,0.4784270536,-0.4862951175\C,0,0.954976
222,0.3524333094,-1.861313623\C,0,-0.2960479295,0.1444372038,-2.425393
933\H,0,-2.3980572757,-0.0946060643,-2.0512792572\H,0,-2.161248533,0.1
350284441,0.4155457054\H,0,2.0574005392,0.6471155093,-0.0261196686\H,0
,1.8336851215,0.419087616,-2.4929781481\O,0,0.073595246,0.5918342106,1
.6936757733\C,0,0.3501749476,-0.3531195797,2.5374650162\F,0,0.49129150
23,-1.4950760525,1.8706950847\H,0,-0.3966261491,0.0479441657,-3.500470
5881\Version=IBM64-G03RevC.02\State=1-A\HF=-444.3661417.

F Isotropic = -6.8741; C Isotropic = -110.1800

2.2.1. *trans*-Fluorophenoxycarbene: @ RB3LYP/6-31g(d)

1	6	2.151358	-1.098542	.064008
2	6	.769985	-1.279127	-.010379
3	6	-.050468	-.158358	-.080912
4	6	.464459	1.135401	-.092879
5	6	1.848124	1.298346	-.013672
6	6	2.692566	.188579	.064557
7	1	2.802191	-1.966289	.120578
8	1	.322595	-2.267694	-.012139
9	1	-.206456	1.983601	-.155000
10	1	2.265378	2.301288	-.020028
11	8	-1.428089	-.421858	-.186617
12	6	-2.269208	.475728	.290850
13	9	-3.463149	-.041652	.012215
14	1	3.768446	.326657	.120153

Low frequencies --- -11.9773 -6.1403 .0010 .0010 .0011 3.1380

Zero-point correction= .100864 (Hartree/Particle)
Thermal correction to Energy= .108196
Thermal correction to Enthalpy= .109140
Thermal correction to Gibbs Free Energy= .068319
Sum of electronic and zero-point Energies= -444.632265
Sum of electronic and thermal Energies= -444.624933
Sum of electronic and thermal Enthalpies= -444.623989
Sum of electronic and thermal Free Energies= -444.664810

2.2.2. PBE1PBE/6-311++G(2D,P) opt NMR\\trans - fluorophenoxy carbene\\0,1\C,0,-

1.3560619194,0.0743832029,-1.9734634893\C,0,-1
.3544434063,0.0927283721,-0.586809059\C,0,-0.1423766475,0.1041826594,0
.0756230423\C,0,1.0658505991,0.1123035323,-0.5964569965\C,0,1.04675787
44,0.0899936132,-1.9834819038\C,0,-0.1575832029,0.0698503379,-2.673302
241\H,0,-2.2999571909,0.063197201,-2.5067201824\H,0,-2.2756822146,0.09
67448949,-0.0162539889\H,0,1.9947319714,0.1307676155,-0.041109608\H,0,
1.9850973617,0.0944454369,-2.5267697934\O,0,-0.2116153574,0.1598439107
,1.4721346238\C,0,0.6993874394,-0.4799373099,2.1428578119\F,0,0.404587
8961,-0.2336248783,3.4045901716\H,0,-0.1617425549,0.0576910241,-3.7573
379501\\Version=IBM64-G03RevC.02\State=1-A\HF=-444.3716322.

F Isotropic = 12.7800 ; C Isotropic = -122.0287

2.3. Transition State for Cis → Trans Interconversion

C,0,-1.4652969712,0.2862971028,-1.9053036017
C,0,-1.5084355833,0.1236248625,-0.5216907616
C,0,-0.3115378139,-0.0453070941,0.1712741411
C,0,0.9204451003,-0.0584836808,-0.4824484113
C,0,0.9408518799,0.091783725,-1.8703760813
C,0,-0.2445597165,0.2663612401,-2.5851600009
H,0,-2.3931361439,0.4233015502,-2.4534931381
H,0,-2.4456191859,0.124816687,0.0245939028
H,0,1.8400378561,-0.167859707,0.082277387
H,0,1.8951264742,0.0772903584,-2.3894338329
O,0,-0.4011254978,-0.1997983076,1.5516712894
C,0,0.4767399015,-0.7972952464,2.3601050872
F,0,1.2979671842,0.1722723794,2.7764542644
H,0,-0.2183504567,0.3885007041,-3.663805242

Low frequencies --- -309.3541 -0.0011 .0002 .0005 4.5441 6.3964

Zero-point correction= .099365
Thermal correction to Energy= .106344
Thermal correction to Enthalpy= .107288
Thermal correction to Gibbs Free Energy= .066759
Sum of electronic and zero-point Energies= -444.606352
Sum of electronic and thermal Energies= -444.599372
Sum of electronic and thermal Enthalpies= -444.598428
Sum of electronic and thermal Free Energies= -444.638958

2.4. cyclo-[=CHN(CH₃)₂C: @ PBE1PBE/6-311++G(2D,P)

#PBE1PBE/6-311++G(2D,P) opt freq \arduengos carbene
dimethyl analog\0,1\C,0,0.0980510703,-0.9683054937,-0.0000046955\N,
0,0.0121420594,-0.1195418668,1.0563696859\N,0,0.0120528668,-0.11954009
33,-1.0563708963\C,0,-0.1214233257,1.1994029702,-0.6750562307\C,0,-0.1
214575428,1.1993929026,0.6750678731\H,0,-0.2040120777,2.0151636678,1.3
756235061\H,0,-0.2040253101,2.0151757951,-1.3756038788\C,0,0.056965599
9,-0.5661176415,-2.4271377392\H,0,0.1676041445,-1.6484837671,-2.416508
5312\C,0,0.0576630797,-0.5660708722,2.4271323617\H,0,0.1660878581,-1.6
486609765,2.4164918418\H,0,-0.862867231,-0.3009182417,2.9533404968\H,0
,0.9079455329,-0.1236258667,2.9523588534\H,0,0.9057755268,-0.121963858
5,-2.9532911006\H,0,-0.8646662151,-0.3029242235,-2.9524121319\Version
=IBM64-G03RevC.02\State=1-A\HF=-304.5204251

Zero-point correction= .127034
Thermal correction to Energy= .134011
Thermal correction to Enthalpy= .134955
Thermal correction to Gibbs Free Energy= .096101
Sum of electronic and zero-point Energies= -304.393391
Sum of electronic and thermal Energies= -304.386414
Sum of electronic and thermal Enthalpies= -304.385470
Sum of electronic and thermal Free Energies= -304.424324

C2 isotropic = -39.5772
C4 isotropic = 65.9277

2.5. cyclo-[-CH₂N(CH₃)₂C: @ PBE1PBE/6-311++G(2D,P)

C,0,-0.9387023471,-0.1054798916,-0.3554779671
N,0,-0.5571939927,-0.1100704356,0.9279011514
N,0,0.1797399209,0.0676567854,-1.0708395386
C,0,1.4108025362,0.082737164,-0.2795615513
C,0,0.8628901105,0.1727526866,1.1405880549
H,0,0.993105647,1.1720725063,1.5760604664
H,0,1.9854392322,-0.8373799514,-0.4481128995
C,0,0.241912931,-0.0170061046,-2.5005606732
H,0,-0.7761243533,-0.050217115,-2.8848172273
C,0,-1.4649527769,-0.1204242336,2.0374067426
H,0,-2.4663791099,-0.3141359864,1.6569109333
H,0,-1.4652596282,0.8426614027,2.5646040538
H,0,-1.1972120235,-0.9016159807,2.757867969
H,0,0.7743113406,-0.920301774,-2.8262597606
H,0,0.7575267804,0.8522094568,-2.9243727595
H,0,1.3168772599,-0.5518562188,1.822591896
H,0,2.0481906345,0.9299814871,-0.5482715969

Zero-point correction= .149750
Thermal correction to Energy= .157421
Thermal correction to Enthalpy= .158365
Thermal correction to Gibbs Free Energy= .117989
Sum of electronic and zero-point Energies= -305.571277
Sum of electronic and thermal Energies= -305.563606
Sum of electronic and thermal Enthalpies= -305.562662
Sum of electronic and thermal Free Energies= -305.603038

C Isotropic = -63.1001

2.6. Methyl Fluoride

PBE1PBE/6-311++G(2D,P) NMR opt\\methylfluoride
\\0,1\F,0,-0.7491649091,0,-0.0000000818\C,0,0.6317750382,0,0.0000000
69\H,0,0.9839447636,-0.0000002474,-1.0335227806\H,0,0.9839445942,-0.89
50569528,0.5167617657\H,0,0.9839445942,0.8950572002,0.5167613373\\Vers
ion=SGI64-G03RevB.02\State=1-A\HF=-139.6406542.

F Isotropic = 467.4977; C Isotropic = 115.8315

2.7. 1-Fluorocyclopentyl Cation

PBE1PBE/6-311++G(2D,P) opt NMR\\fluorocyclopentyl cation
\\1,1\C,0,-0.501297976,0.4395296691,-0.4311943226\C,0,0.69119467
81,0.9840127722,0.1803572057\C,0,1.154227652,-0.1473694541,1.111273772
3\C,0,0.6311355131,-1.4179784425,0.4244239485\C,0,-0.70408752,-0.97252
04435,-0.1916785373\F,0,-1.2992856665,1.1390457111,-1.1174971586\H,0,0
.5663508252,1.9983929956,0.5710968875\H,0,1.3867335173,1.0873462159,-0
.6812472257\H,0,2.2339813824,-0.1493296539,1.2473211572\H,0,0.69382949
97,-0.0171597688,2.0939827355\H,0,0.50673515,-2.2536206299,1.110446304
7\H,0,1.3074425003,-1.7377191663,-0.3724373053\H,0,-1.1202880833,-1.51
28124598,-1.0473277108\H,0,-1.5082478755,-0.9805535399,0.5765471843\\V
ersion=SGI64-G03RevB.02\State=1-A\HF=-294.6391575.

F Isotropic = 9.6827; C Isotropic = -110.9129

2.8. 1-Fluorocyclopropyl Cation

RPBE1PBE\6-311++G(2d,p) opt nmr \\Fluorocyclopropyl cation \\ 1,1\C,-0.11906565,0.0000000041,-
1.1684702294\C,-0.1075089959,-0.0000000009, 0.1869290895\C,1.0698685184,0.000000004,-0.4846046347\H,-
0.6250922824, 0.0000000065,-2.1274655862\H,2.1532580348,0.0000000065,-0.5293562611\F,-
0.7319921096,0.0000000062,1.2726329439\\Version=SGI64-G03RevB.02\State=1-A\HF=-214.7824567.

F Isotropic = 235.9126; C Isotropic = 12.0442

2.9. Fluorobenzene

PBE1PBE/6-311++G(2D,P) opt NMR\\nmr on fluorobenzene \\0,1\
C\C,1,1.387956\C,2,1.381024,1,118.394482\C,3,1.381009,2,122.444879,1,-
0.001075,0\C,4,1.387973,3,118.391706,2,0.001454,0\C,5,1.388226,4,120.4
76573,3,-0.000327,0\H,1,1.084494,2,119.417006,3,-179.999171,0\H,2,1.08
3524,1,121.944787,6,-179.999508,0\H,4,1.08352,3,119.667912,2,-179.9980
42,0\H,5,1.084495,4,119.416597,3,179.999018,0\H,6,1.083968,5,120.08939
1,4,179.998365,0\F,3,1.343275,2,118.775803,1,-179.995114,0\\Version=SG
I64-G03RevB.02\State=1-A\HF=-331.2085928

F Isotropic = 290.8864; C Isotropic = 18.6426

2.10. 2-Fluoro-2-propyl Cation

PBE1PBE/6-311++G(2D,P) opt NMR\fluoroisopropyl cation
\1,1\C,0,-0.028818632,-0.0000833708,-0.0185794206\C,0,-0.187
2017104,-0.0759235718,1.4137481599\C,0,1.210222081,0.0759151415,-0.754
3796634\F,0,-1.0959575264,0.0000539368,-0.7063750299\H,0,-1.116300753,
-0.5719896431,1.6999522543\H,0,-0.2679341995,0.9795378895,1.7437035741
\H,0,1.0871243379,0.572012246,-1.7187218597\H,0,1.4774388479,-0.979521
7588,-0.9642109288\H,0,2.0199247442,0.4861482965,-0.1494304269\H,0,0.6
981543283,-0.4861216544,1.9013482005\Version=SGI64-G03RevB.02\State=1
-A\HF=-217.2846463.

F Isotropic = -32.9756; C Isotropic = -98.6751

2.11. Trans-Methoxyfluoromethyl Cation

PBE1PBE/6-311++G(2D,P) opt NMR \trans-fluoromethoxy cation\1,1\F,0,-0.5517186302,0.024643362,-
1.6589431985\C,0,-0.54387276,-0.1105539078,-
0.4083756464\O,0,0.50565127,0.124300169,0.186865553\C,0,0.6149128168,-0.0065988779,1.6568120496\H,0,-
1.4785773219,-0.4295286766,0.0624705955\H,0,-0.3415225708,-
0.3252649999,2.0679498972\H,0,1.4028909314,-0.739242245,1.8125068503\H,0,0.9112261325,0.98076102
59,2.0020185996\Version=IBM64-G03RevC.02\State=1-A\HF=-253.1624871

F Isotropic = 104.1226; C Isotropic = 3.5184

2.12. Trichlorofluoromethane

PBE1PBE/6-311++G(2D,P) opt NMR\trichlorofluoromethane
0,1\C,0,0.2361830595,0,-0.0835033411\Cl,0,0.267111898,
-0.0000000108,1.6814286826\F,0,1.4914843658,0,-0.527
3194784\Cl,0,-0.5700400006,-1.4499893084,-0.6863938986\Cl,0,-0.5700399
943,1.4499893192,-0.6863938809\Version=IBM64-G03RevC.02\State=1-A1\HF
=-1518.0206107.

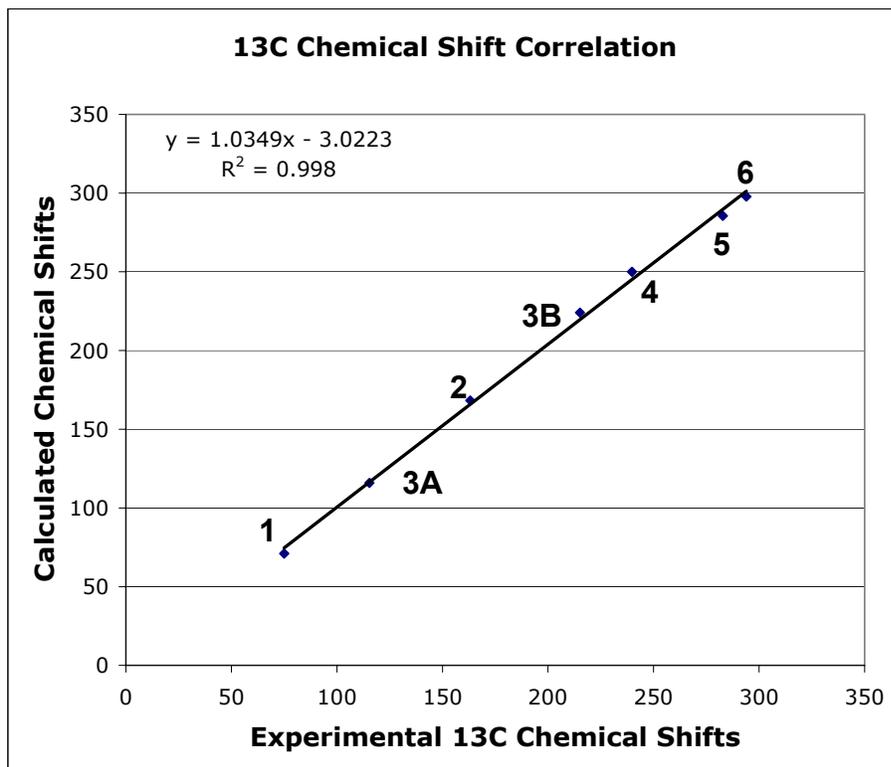
F Isotropic = 172.2044; C Isotropic = 43.7393

2.13. Tetramethyl silane

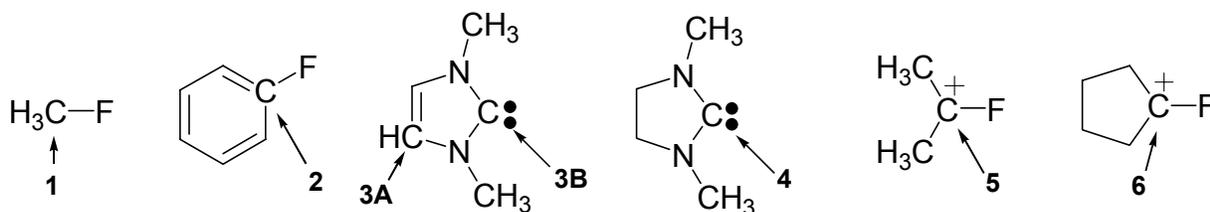
#PBE1PBE/6-311++G(2D,P) NMR\tms at B3LYP/6-311+G(2d,p) geom \0
,1\Si,0,0.0002433436,0.0000198414,0.0003526318\C,0,0.0000197502,-0.000
0606836,1.8966290951\H,0,1.0220747071,-0.000132635,2.2974440176\H,0,-0
.5110115374,0.8852061444,2.2968169022\H,0,-0.5111720299,-0.8852878681,
2.2967978916\C,0,0.8936302645,1.5484505438,-0.6324308856\H,0,0.9118987
957,1.5797609905,-1.7295868008\H,0,0.4004768108,2.4654331751,-0.284483
231\H,0,1.9342049545,1.5810677992,-0.2842348019\C,0,0.89366534,-1.5484
586809,-0.6323284834\H,0,0.4005862746,-2.4654632655,-0.2842495136\H,0,
0.9117697178,-1.5799962226,-1.7295487858\H,0,1.9342160862,-1.580771104
3,-0.2842562015\C,0,-1.7875715885,0.0000454207,-0.6321857413\H,0,-2.33
58145361,0.8851907196,-0.2841285292\H,0,-1.8234280136,0.0000485425,-1.
7293326127\H,0,-2.3356706376,-0.8851936547,-0.284279089\Version=SGI64
-G03RevB.02\State=1-A\HF=-448.9192097

C Isotropic = 186.95; H Isotropic = 31.61

3. Chemical Shift Correlations



All structures fully optimized at PBE1PBE/6-311++G(2D,P).

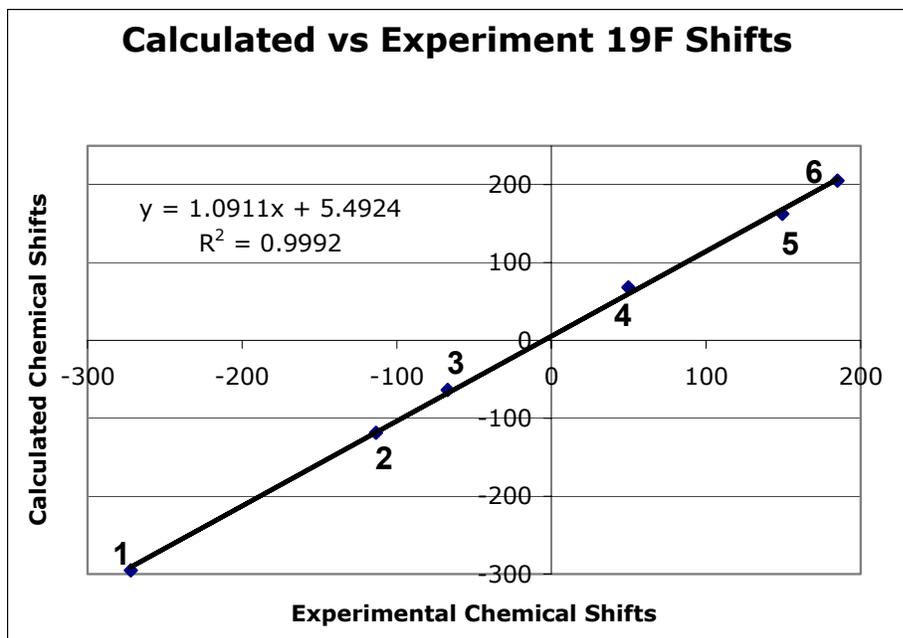


Experimental chemical shifts:

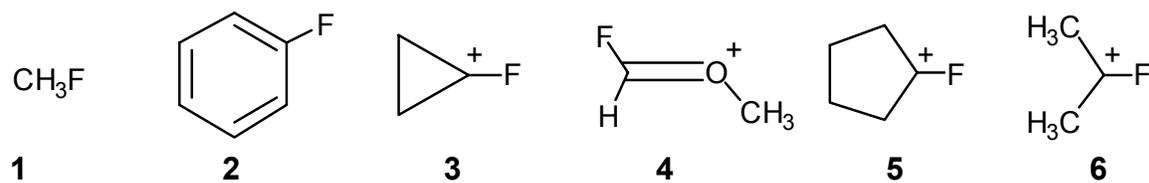
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G. A. Olah, G. Liang, and Y. K. Mo, *J. Org. Chem.* **1974**, *39*, 2394.



All structures fully optimized at PBE1PBE/6-311++G(2D,P).



Experimental chemical shifts:

G. K. S. Prakash, G. Rasul, A. Burrichter, K. K. Laali, and G. A. Olah, *J. Org. Chem.* **1996**, *61*, 9253.

G. A. Olah, G. Liang, and Y. K. Mo, *J. Org. Chem.* **1974**, *39*, 2394.