Computational Information

General Remarks

Calculations were performed with the Gaussian 09 suite of programs[1] using Compute Canada's Shared Hierarchical Academic Research Computing Network (SHARCNET). Model complexes were fully optimized with no symmetry constraints using the M06-2X density functional method,[2] in conjunction with the cc-pVTZ basis set.[3,4] The cc-pVQZ-PP basis set employing a relativistic small-core pseudopotential was used for tin.[327] Geometry optimizations were started using models in which the relevant non-hydrogen atoms were placed in positions found experimentally by X-ray crystallography using Gaussview.[5] Frequency calculations were also performed at the same level of theory in order to confirm that the optimized structures were minima on the potential energy hypersurface and to determine thermochemical and vibrational information. Natural bond orbital (NBO) analyses[6] to determine orbital contributions, Wiberg Bond Indices and orbital energies were obtained using the routine included in the Gaussian distributions.[7] Visualizations of the Kohn-Sham orbitals and optimized geometries were made using VMD.[8]

Parameters for [ClGeBZIMPY]$^+$

1\1\GINC-ORC173\FOpt\RM062X\CC-pVTZ\C11H9Cl1Ge1N5(1+)\BINDERJ\29-Mar-2
018\0\\# M062X/cc-pVTZ scf=tight opt=tight freq pop=(full,nbo6read)\\O
ptimization, frequency test and nbo analysis for GeCl Bzimpy AS660\\1,
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3505474,20.3585851281,13.5748460754\N,7.8909222358,20.3134790894,9.435
2880881\N,8.9241565878,20.7060665323,7.5485898615\C,10.2240572664,20.8
248056413,9.7185542342\C,9.0474409252,20.6194717267,8.8899227938\C,10.
9751130874,20.8486701956,11.9104347609\C,6.9874078207,20.1935794807,8.
4214395016\C,7.6189325242,20.4392158987,7.2348225095\C,11.4810706663,2
1.1689041878,9.2431829029\C,12.5068802606,21.3504625756,10.1553586457\
C,12.2572107646,21.1935643251,11.5082667225\N,11.2798585784,20.7808913
581,14.4234247893\C,9.2182222931,20.2644905388,14.9318436914\C,10.5552
540897,20.6673840311,13.2903155389\C,10.4430915117,20.5289403403,15.47
68052647\H,10.7806872798,20.5622830413,16.4965166526\H,8.2954832087,20
.0262273895,15.4301564135\H,12.2579554677,21.0093805655,14.4968572017\
H,9.6501628701,20.9265804851,6.8863497918\H,7.2600370387,20.4504474667
,6.2219246524\H,5.9545754645,19.9517934229,8.5984397329\H,11.654765097
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.3368035,11.1972899,-2.1544747\PG=C01 [X(C11H9Cl1Ge1N5)]\\@

Zero-point correction= 0.198204 (Hartree/Particle)
Thermal correction to Energy= 0.213304
Thermal correction to Enthalpy= 0.214248
Thermal correction to Gibbs Free Energy= 0.154100
Sum of electronic and zero-point Energies= -3235.279052
Sum of electronic and thermal Energies= -3235.263952
Sum of electronic and thermal Enthalpies= -3235.263008
Sum of electronic and thermal Free Energies= -3235.323156

Parameters for [ClSnBZIMPY]$^{+}$

1\1\GINC-ORC267\FOpt\RM062X\Gen\C11H9Cl1N5Sn1(1+)\BINDERJ\15-Apr-2018\
0\\# M062X/gen pseudo=read scf=tight opt=tight freq pop=(full,nbo6read
)\\Optimization, frequency test and nbo analysis for SnCl Bzimpy AS662
cc-pVTZ (-PP for Sn atom)\\1,1\Sn,-0.0000027768,-1.4963696488,-0.4506
328965\Cl,-0.0000002437,-1.5922305738,1.9475478694\N,0.0000068119,0.94
38292112,-0.1676756477\N,2.2741405313,-0.5402240414,-0.2827710112\N,-2
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.0657470856\C,-1.1548893529,1.607012843,-0.0472340331\C,-2.3437965446,
0.7658610439,-0.1356318544\C,1.1549079109,1.6070039581,-0.0472315051\C
,-3.5562858779,-1.008014514,-0.3110386222\C,-4.4181239432,0.0417898028
,-0.174726611\C,-1.1956535291,2.9785178921,0.1654472659\C,0.0000168826
,3.6682397215,0.2654765866\C,1.1956822923,2.9785083875,0.1654519497\N,
3.6337814217,1.1577084715,-0.0657384272\C,3.5562871616,-1.0080408483,-
0.311037411\C,2.3438100494,0.7658438537,-0.1356275867\C,4.4181313325,0
.041757833,-0.1747205303\H,5.4912527471,0.0897692865,-0.144537672\H,3.
7832502534,-2.0537611297,-0.4188329561\H,3.973549125,2.0989290549,0.04
59836229\H,-3.9735277274,2.098958241,0.0459685368\H,-5.491245418,0.089
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000003,3.2933938,-0.9856054\Quadrupole=32.3723248,1.9242016,-34.296526
4,-0.0001233,0.0000978,5.8333335\PG=C01 [X(C11H9Cl1N5Sn1)]\\@

Zero-point correction= 0.197677 (Hartree/Particle)
Thermal correction to Energy= 0.213051
Thermal correction to Enthalpy= 0.213995
Thermal correction to Gibbs Free Energy= 0.152541
Sum of electronic and zero-point Energies= -1372.502242
Sum of electronic and thermal Energies= -1372.486868
Sum of electronic and thermal Enthalpies= -1372.485924
Sum of electronic and thermal Free Energies= -1372.547378

Parameters for [GeBZIMPY]

1\1\GINC-GRA103\FOpt\RM062X\CC-pVTZ\C11H9Ge1N5\BINDERJ\11-Apr-2019\0\\
M062X/cc-pVTZ scf=tight opt=tight freq pop=(full,nbo6read)\\Optimiza
tion, frequency test and nbo analysis for Ge0Bzimpy\\0,1\Ge,8.19885548
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354\N,9.3707010653,20.408468506,13.5790370782\N,7.7813379302,20.323332
558,9.3442277525\N,8.9710825496,20.704537417,7.5347765815\C,10.1241825
145,20.8204942793,9.7582455691\C,8.9801915557,20.6199045727,8.89451392
29\C,10.9982678396,20.8747849474,11.9703264264\C,6.9706095772,20.21219
33887,8.24550866\C,7.6903797371,20.4452131682,7.1131708342\C,11.354775
8504,21.1267705323,9.2680101663\C,12.4713769239,21.3218212949,10.12255
05388\C,12.2634830093,21.1897800543,11.4646683909\N,11.3533649447,20.7
93842877,14.4842358954\C,9.2602324608,20.2958237078,14.958412026\C,10.
658630744,20.7137667422,13.3051195475\C,10.4673874624,20.5301641258,15
.5141979583\H,10.7773512217,20.5338379835,16.5429204839\H,8.3276372846
,20.0569339851,15.4362249957\H,12.328116942,21.0055255959,14.580833869
5\H,9.7546489735,20.9172566352,6.9445195647\H,7.4194926618,20.45095586

15,6.0733376569\H,5.9255591658,19.9729684999,8.3347519365\H,11.4841855
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95088,0.3045818,-0.2381974\Quadrupole=-3.3747058,-15.0632863,18.437992
2,2.3322659,6.3836899,-0.7455118\PG=C01 [X(C11H9Ge1N5)]\\@

Zero-point correction= 0.193556 (Hartree/Particle)
Thermal correction to Energy= 0.207072
Thermal correction to Enthalpy= 0.208016
Thermal correction to Gibbs Free Energy= 0.152441
Sum of electronic and zero-point Energies= -2775.186967
Sum of electronic and thermal Energies= -2775.173451
Sum of electronic and thermal Enthalpies= -2775.172507
Sum of electronic and thermal Free Energies= -2775.228083

Parameters for [GeDIMPY]

1\1\GINC-GRA103\FOpt\RM062X\CC-pVTZ\C7H7Ge1N3\BINDERJ\10-Apr-2019\0\\#
M062X/cc-pVTZ scf=tight opt=tight freq pop=(full,nbo6read)\\Optimizat
ion, frequency test and nbo analysis for Ge0 Dimpy\\0,1\Ge,8.266917467
2,20.2446136191,11.9986516293\N,9.9271893154,20.6661984806,11.11315937
81\N,9.3959019441,20.3735747207,13.5225120415\N,7.9062750321,20.371892
0747,9.2406213901\C,10.1768040594,20.8201654236,9.7588520538\C,9.07240
98307,20.6526900335,8.8251087329\C,11.0197274332,20.8355192497,11.9878
770737\C,11.4089786884,21.1203429278,9.2728665178\C,12.5193498015,21.2
931800401,10.1517520287\C,12.3103789129,21.1498054215,11.4807941856\C,
10.7024816454,20.6697500977,13.3055463493\H,11.5298498901,21.225551151
7,8.2037710508\H,13.4962149617,21.5317711422,9.7583794167\H,13.1141601
507,21.2690870324,12.1956005014\H,7.2352770106,20.2842824377,8.4824894
961\H,9.1011157641,20.2395537913,14.4771056697\H,9.3311138472,20.78622
63466,7.772500685\H,11.4186892653,20.7637318991,14.1079941695\\Version
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00012,9.3367256,1.0226987,1.9468991,-0.8339767\PG=C01 [X(C7H7Ge1N3)]\\
@

Zero-point correction= 0.135237 (Hartree/Particle)
Thermal correction to Energy= 0.144398
Thermal correction to Enthalpy= 0.145342
Thermal correction to Gibbs Free Energy= 0.100270
Sum of electronic and zero-point Energies= -2512.117277
Sum of electronic and thermal Energies= -2512.108117
Sum of electronic and thermal Enthalpies= -2512.107173
Sum of electronic and thermal Free Energies= -2512.152245

Parameters for [ClGeDIMPY]

1\1\GINC-GRA6\FOpt\RM062X\CC-pVTZ\C7H7Cl1Ge1N3(1+)\CMACD\13-Apr-2019\0
\\# M062X/cc-pVTZ scf=tight opt=tight freq pop=(full,nbo6read) test\\O

ptimization of ClGe(dimpy) cation\\1,1\Ge,-1.7737868444,0.0104286938,0
.2328835907\Cl,-2.1172285766,0.0203294923,-1.9470658443\N,0.3643591032
,0.0002079308,0.1204350289\N,-1.0727951445,-2.1556994756,-0.0035084448
\N,-1.0512494916,2.1711814759,0.0127027484\C,1.0389685781,1.1524703203
,0.1656845799\C,0.1942803941,2.3586318102,0.1183832477\C,1.0274559529,
-1.159024314,0.1570530947\C,2.4223456773,1.1856649528,0.2516700187\C,3
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358265469,0.2828817581\H,4.1964768524,-0.0197240582,0.3466259719\H,2.9
158500346,-2.1620865736,0.2668451243\H,-1.6312763443,3.0063243626,-0.0
112312779\H,-1.6611021166,-2.9848283463,-0.0336475295\H,0.6674512931,3
.3360630472,0.1781604582\H,0.6342089405,-3.3388384198,0.1532614657\\Ve
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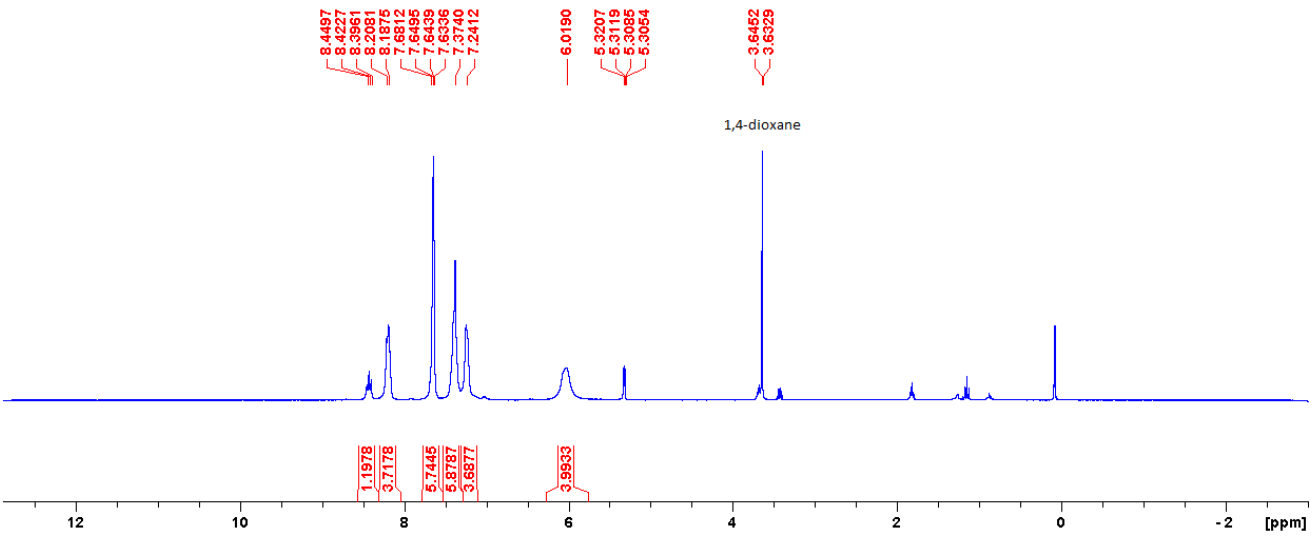
3.728e-06\Dipole=2.6211752,-0.0175488,1.1982929\Quadrupole=5.3399918,1
4.4951636,-19.8351554,0.0435612,0.5491445,0.1255032\PG=C01 [X(C7H7Cl1G
e1N3)]\\@

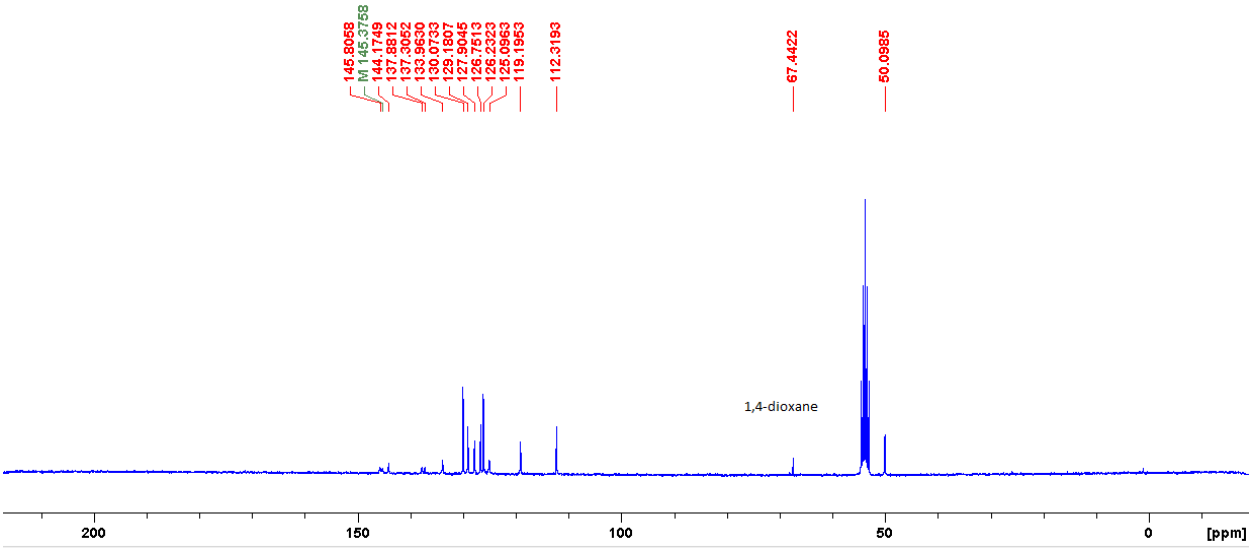
Zero-point correction= 0.138314 (Hartree/Particle)
Thermal correction to Energy= 0.149455
Thermal correction to Enthalpy= 0.150400
Thermal correction to Gibbs Free Energy= 0.100315
Sum of electronic and zero-point Energies= -2972.151938
Sum of electronic and thermal Energies= -2972.140797
Sum of electronic and thermal Enthalpies= -2972.139853
Sum of electronic and thermal Free Energies= -2972.189937

NMR Data:

Compound **1**:

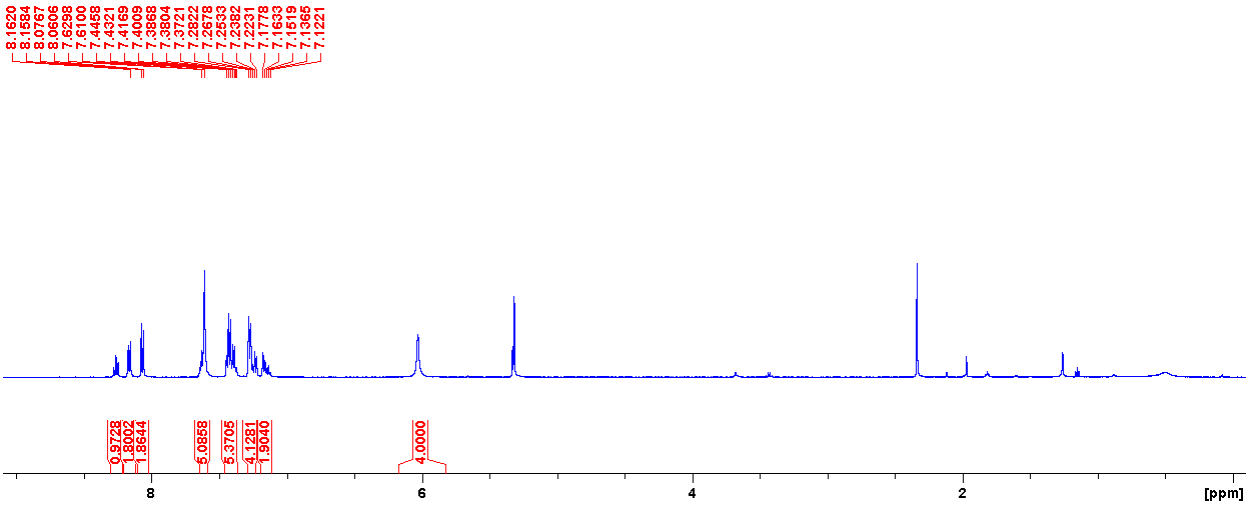


^{1}H NMR of compound **1**.

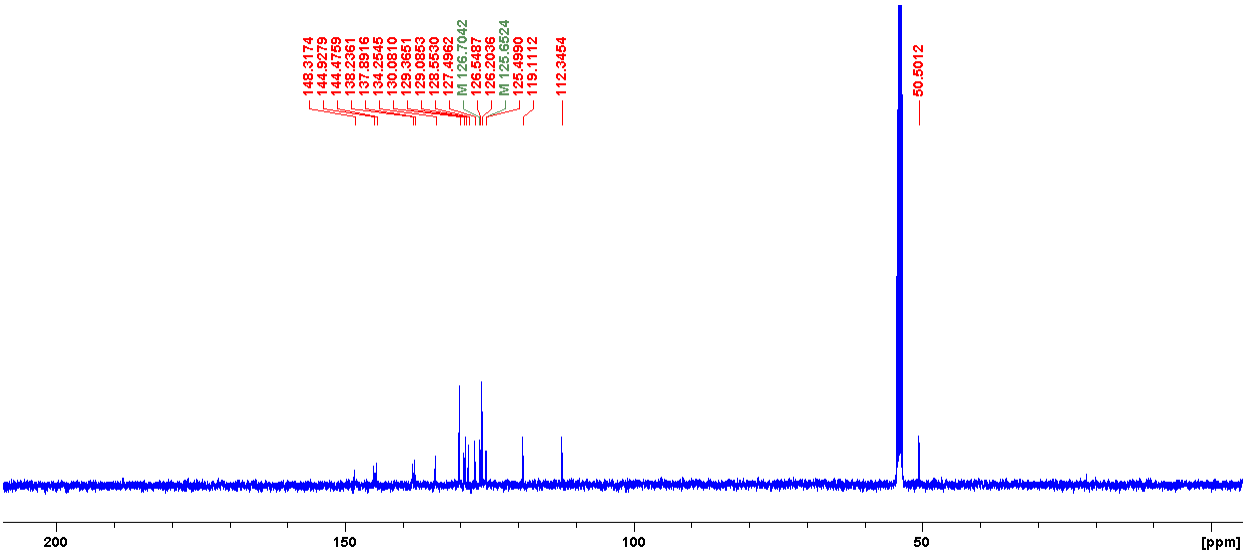


^{13}C NMR of compound **1**.

Compound **2**:

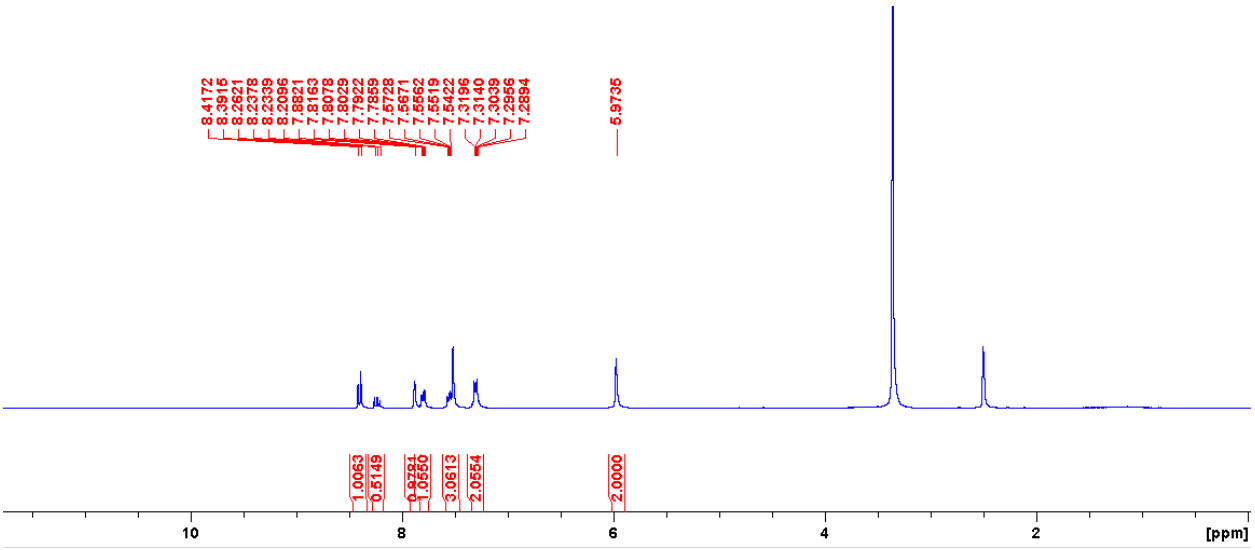


^{1}H NMR of compound **2**.

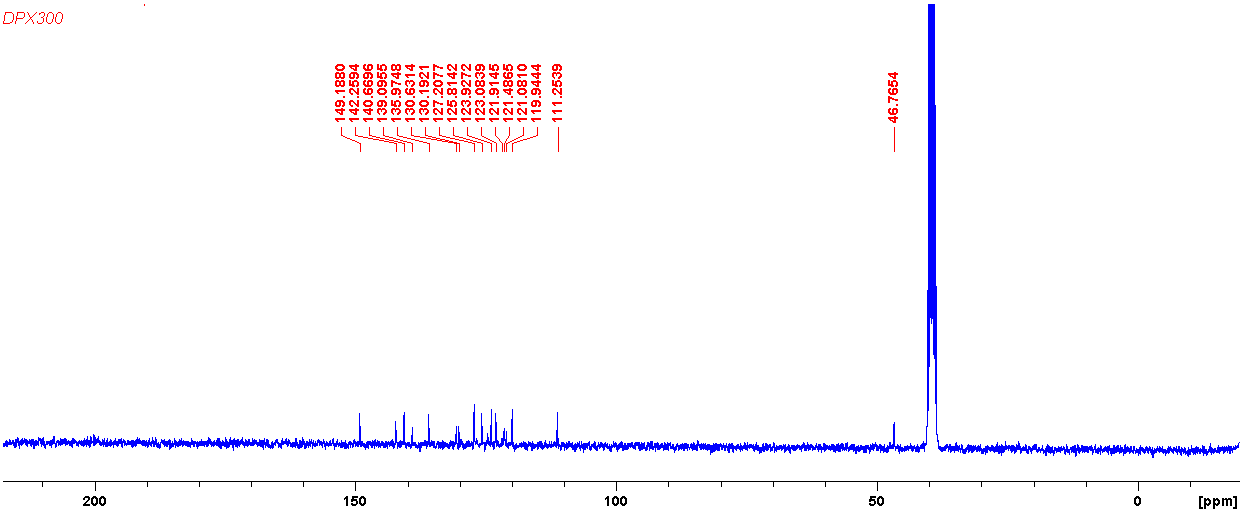


^{13}C NMR of compound **2**.

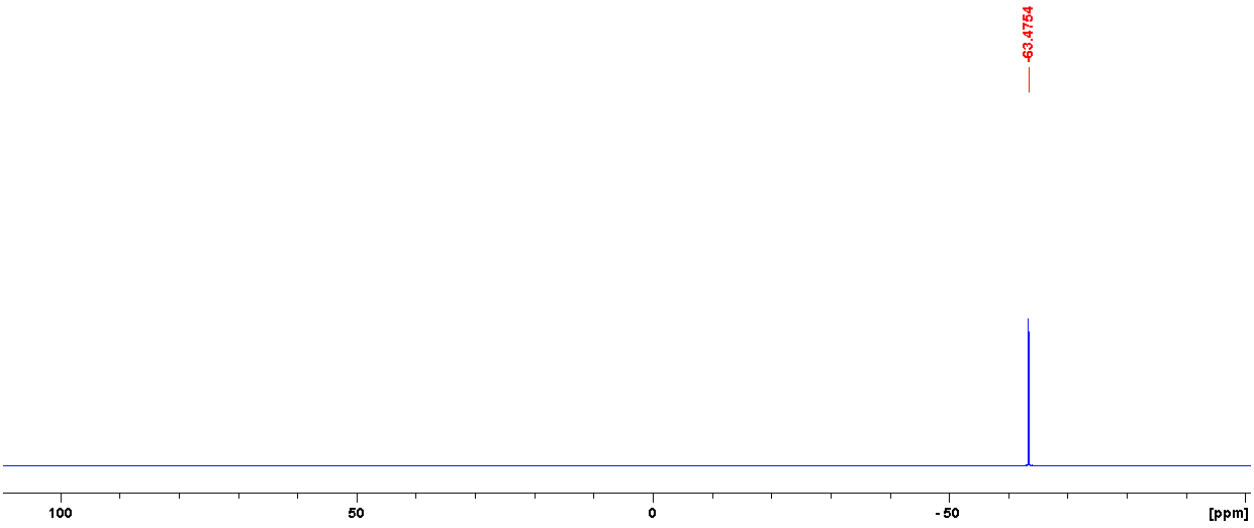
Compound **3**:



^{1}H NMR of compound **3**.

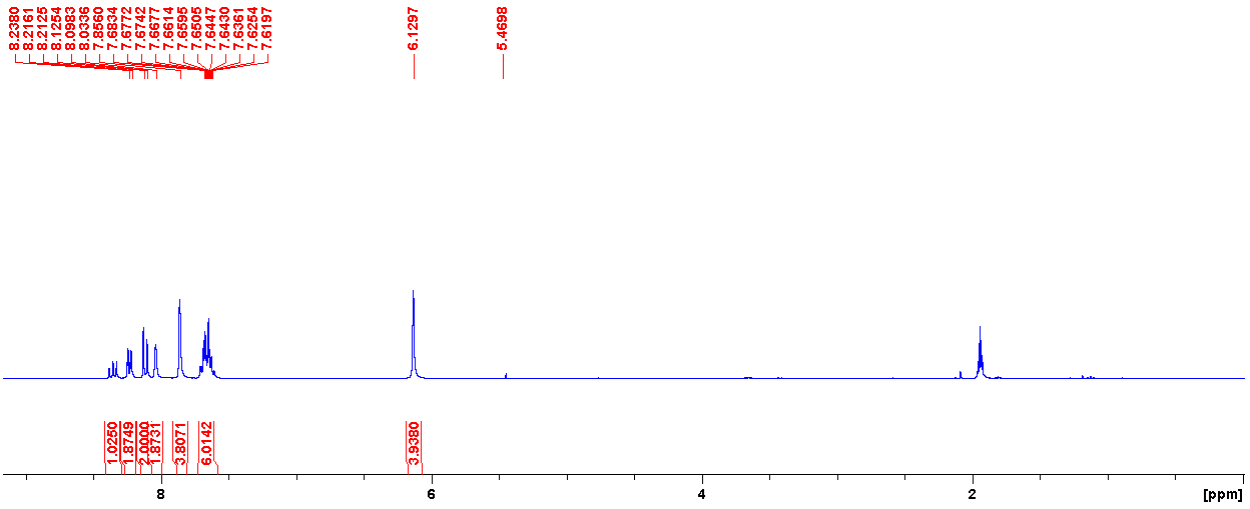


^{13}C NMR of compound **3**.

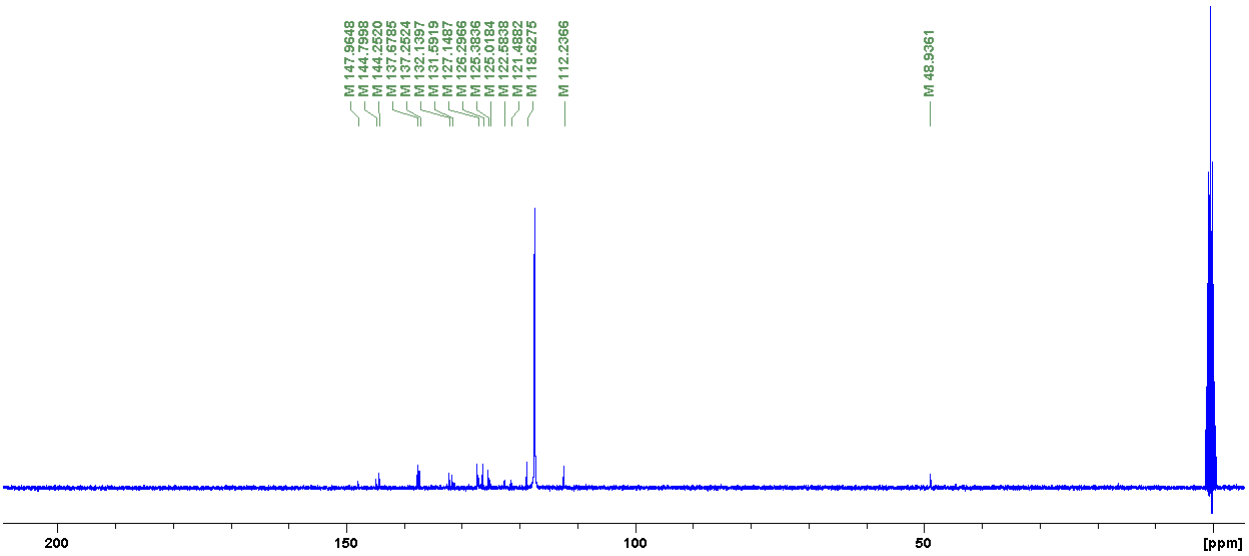


^{19}F NMR of compound **3**.

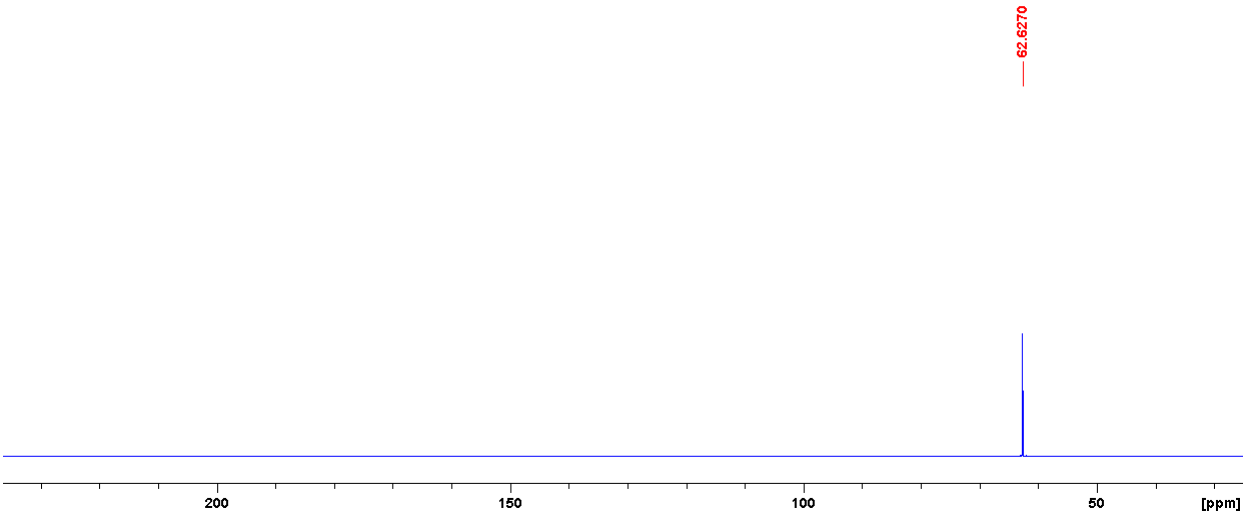
Compound **4**:



^{1}H NMR of compound **4**.

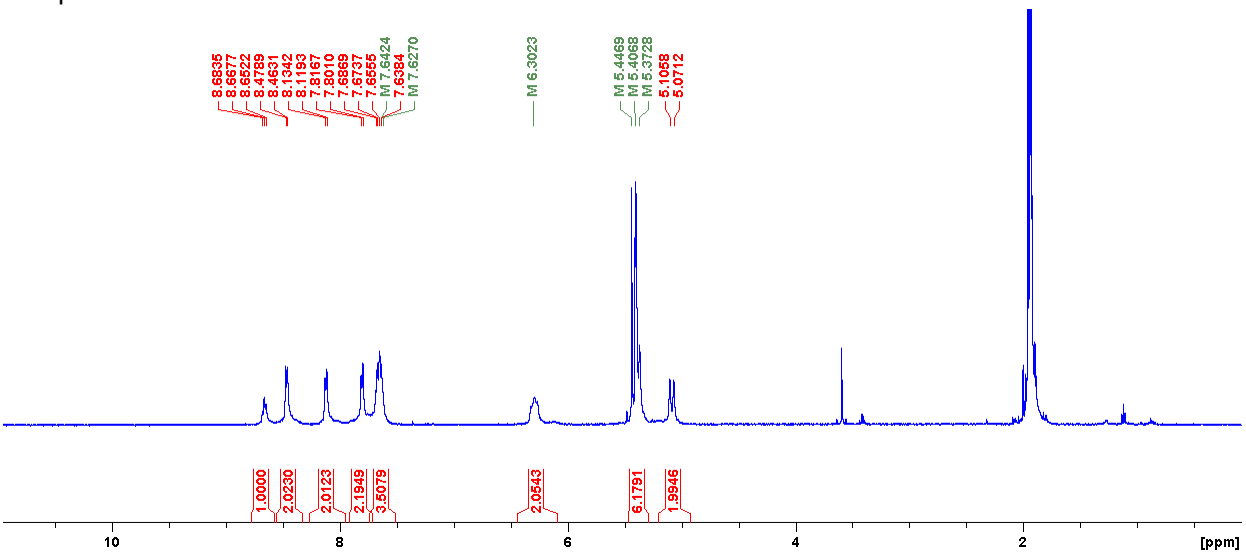


^{13}C NMR of compound **4**.



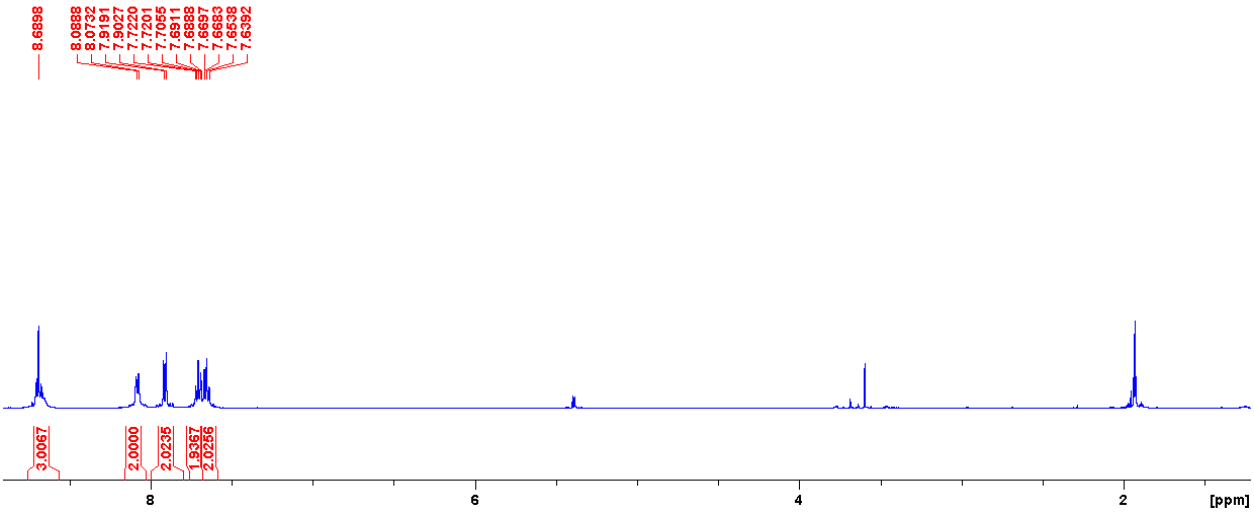
^{19}F NMR of compound **4**.

Compound **5**:

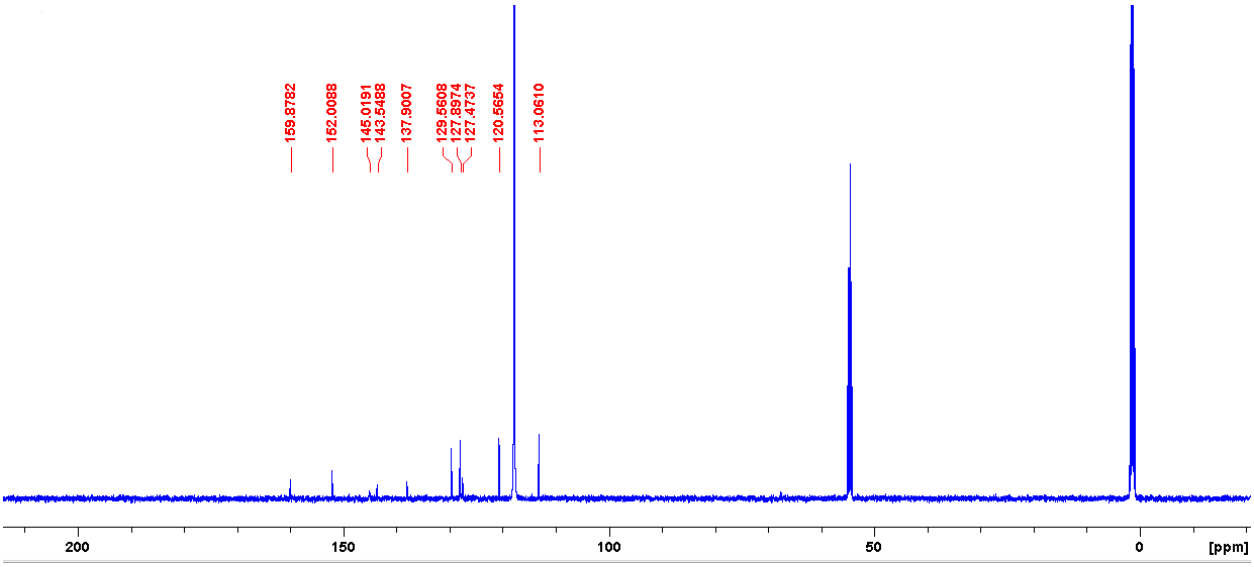


^{1}H NMR of compound **5**.

Compound **6**:

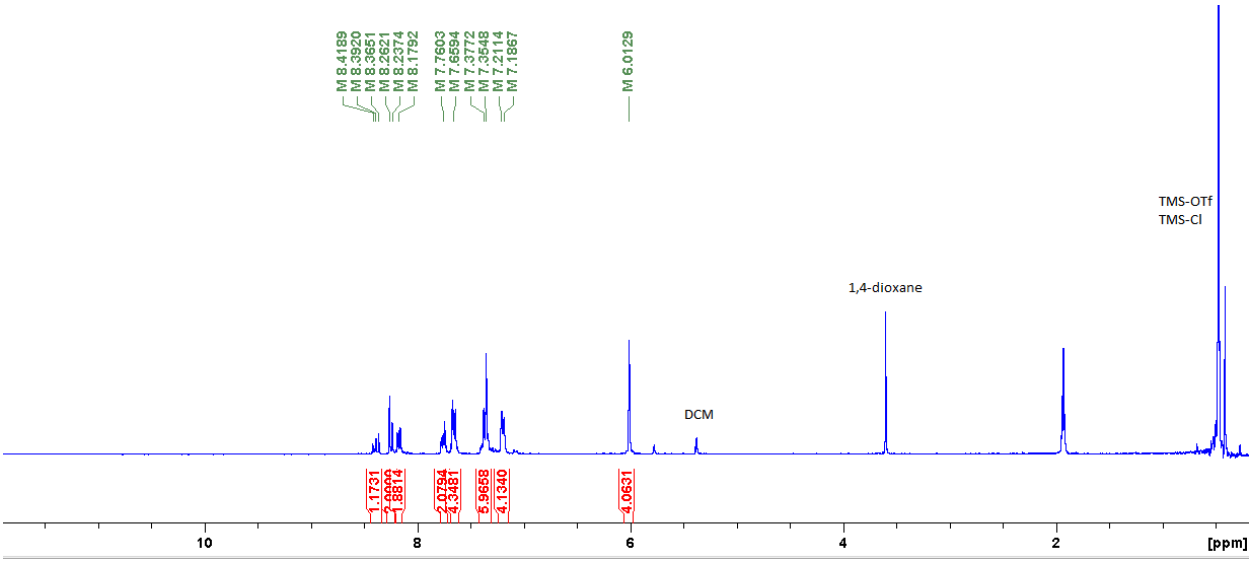


^{1}H NMR of compound **6**.

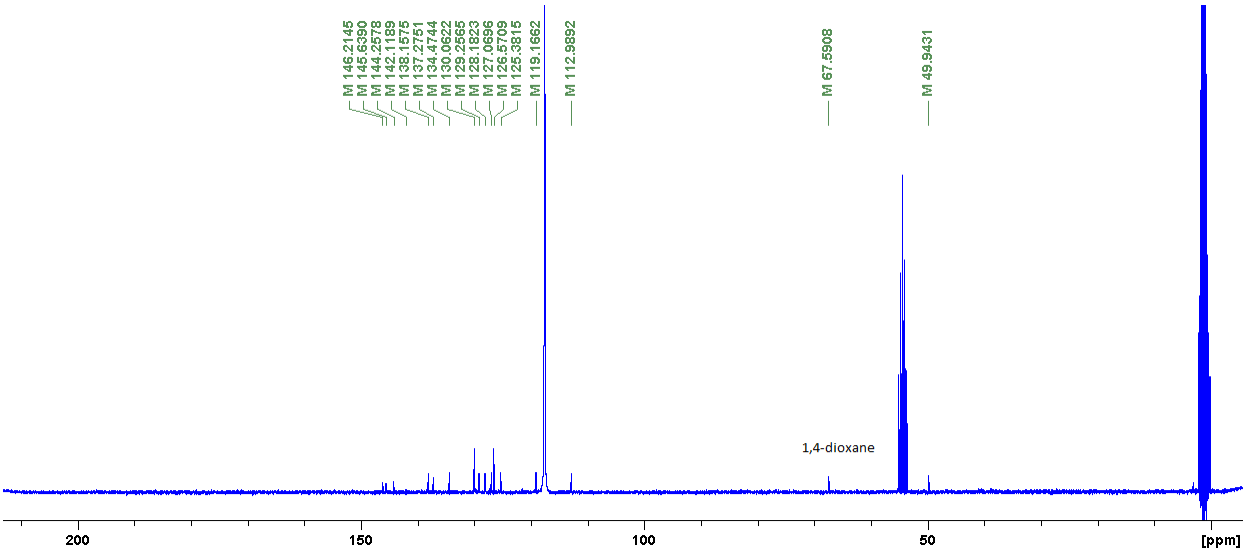


^{13}C NMR of compound **6**.

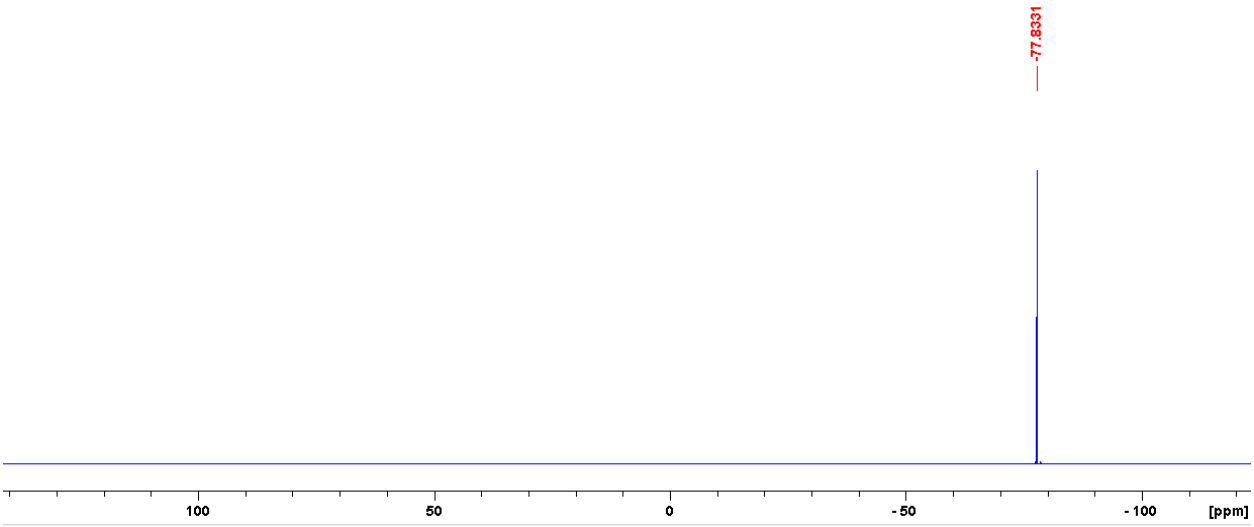
Compound **7**:



^{1}H NMR of compound **7**.

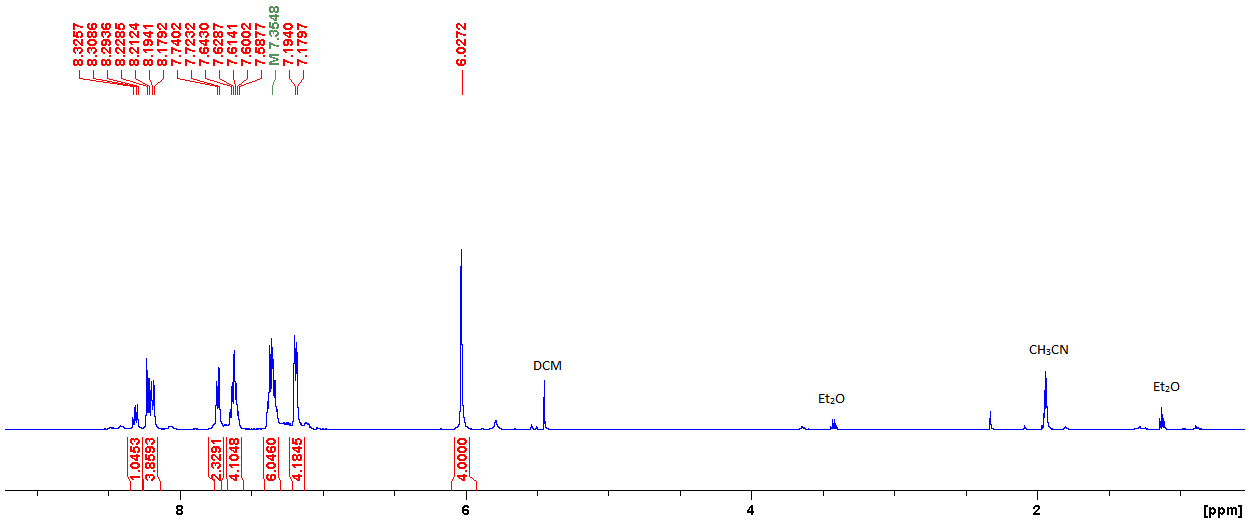


^{13}C NMR of compound **7**.

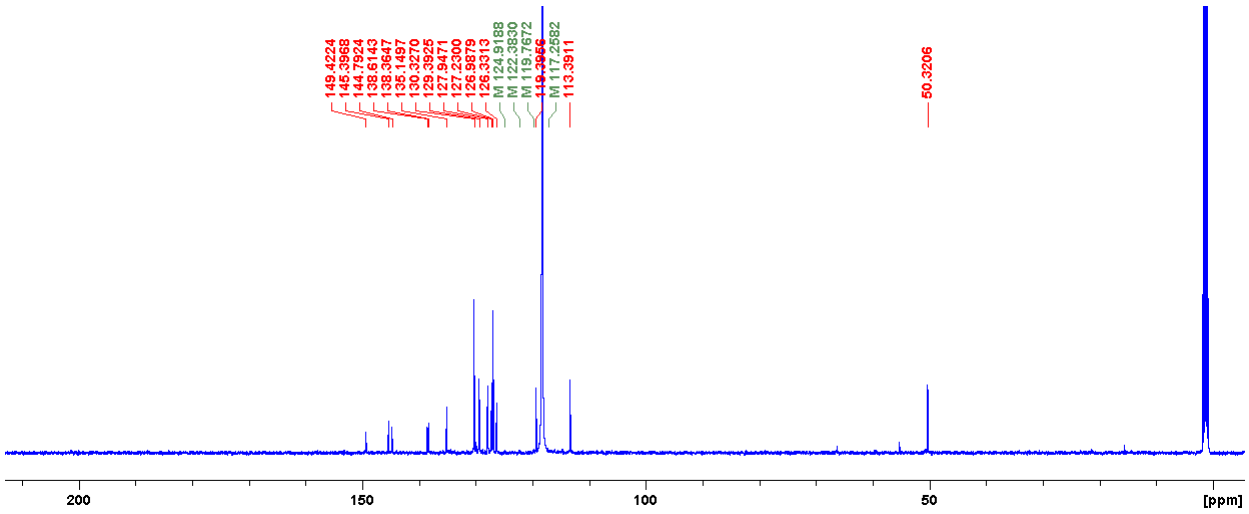


^{19}F NMR of compound **7**.

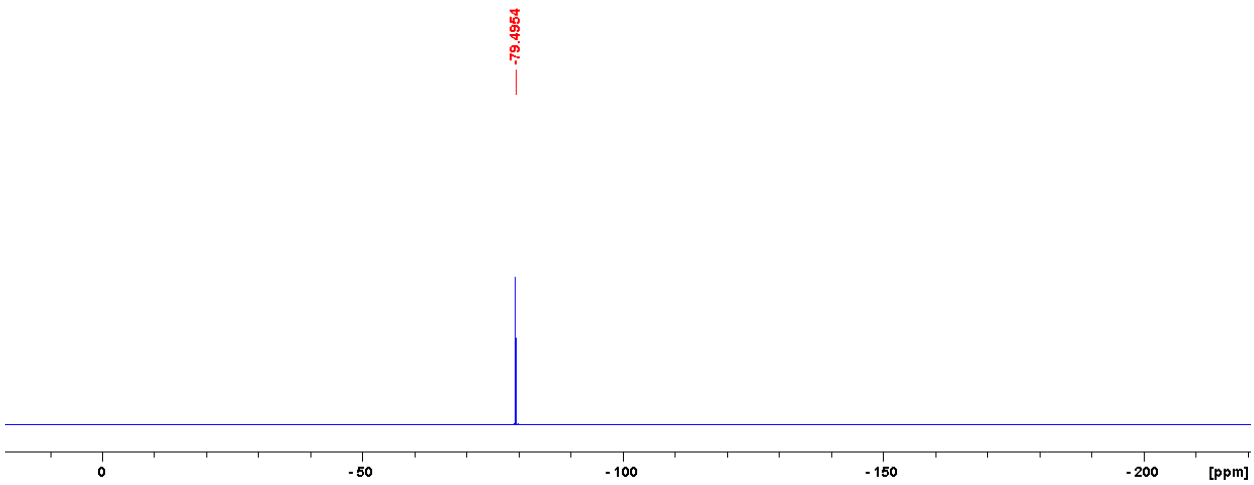
Compound **8**:



^{1}H NMR of compound **8**.



^{13}C NMR of compound **8**.



^{19}F NMR of compound **8**.

References

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