

Electronic supplementary information

Half-sandwich complexes of osmium containing guanidine-derived ligands

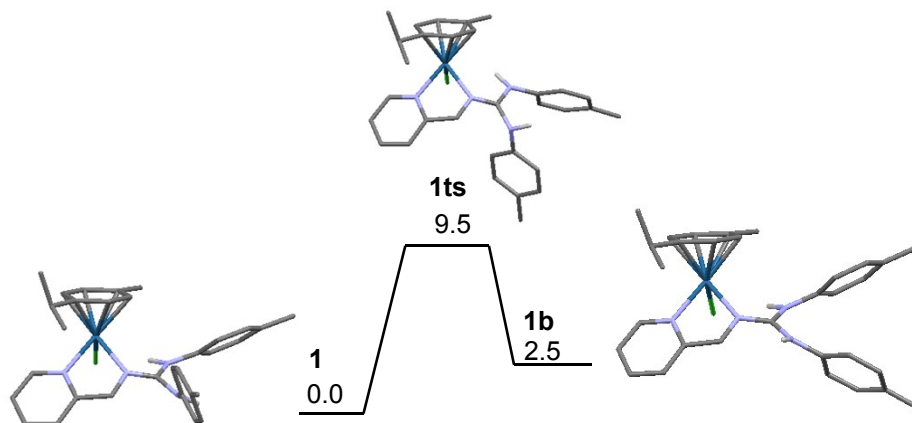
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Table of Contents	page
1- DFT calculations on the complexes 1, 2 and 5	S2
2- H-bond interactions of complex 4	S5
3- H-bond interactions of complexes 6 and 8	S5
4- NMR spectra of the complexes 1-11	S7
5- Atomic coordinates of calculated structures	S23

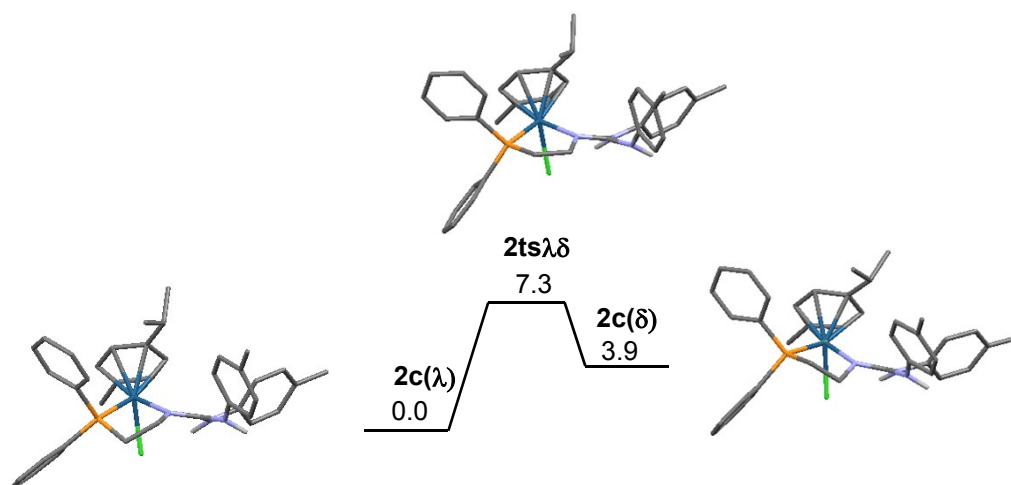
1-DFT calculations on the complexes 1, 2 and 5

Free energy of the rotamers of 1



Gibbs free energy profile of the equilibrium between rotamers **1** and **1b**. For clarity, except the NH protons, hydrogen atoms have been omitted. Free energies are in kcal·mol⁻¹.

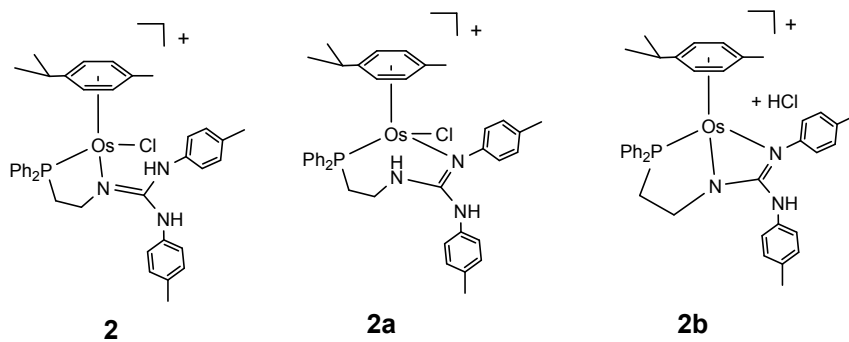
Free energy of the conformers of 2



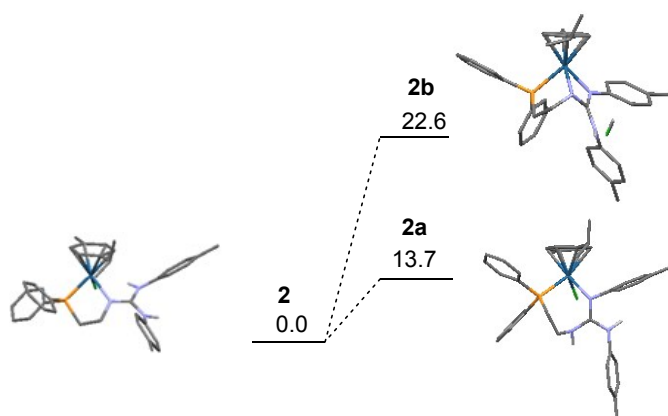
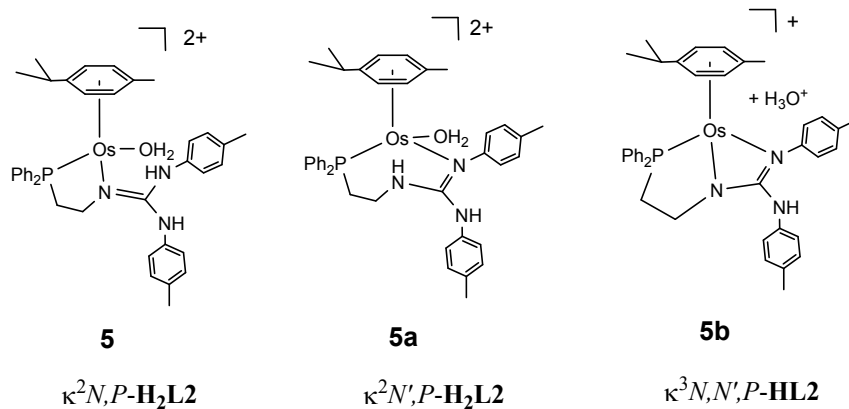
Gibbs free energy profile of the equilibrium between conformers **2c(λ)** and **2c(δ)**. For clarity, except the NH protons, hydrogen atoms have been omitted. Free energies are in kcal·mol⁻¹.

Free energy of the isomers of 2 and 5

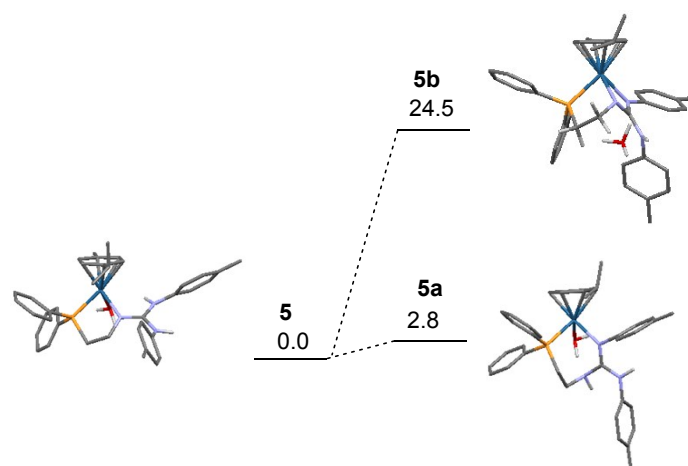
Compound 2



Compound 5



The values are free energies (kcal mol⁻¹), relatives to the complex 2



The values are free energies (kcal mol⁻¹), relatives to the complex **5**

Complete reference 33:

Gaussian 09 (Revision D.01): M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2011.

2- H-bond interactions of complex 4

Table S1. Geometrical parameters (Å, °) of H-bond interactions of complex **4**

D-H...A	D-H	D...A	H...A	D-H...A
N(4)-H(4N)...F(4')	0.87(7)	3.037(9)	2.29(7)	144(7)

Symmetry operation: $x, y+1, z+1$

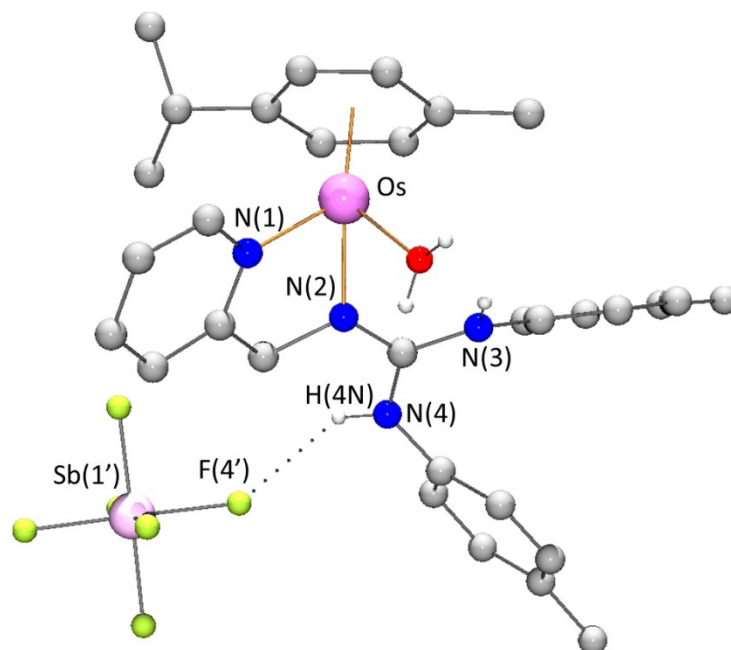


Figure S1. H-bond interactions in complex **4**. For clarity, only hydrogen atoms of N-H fragments have been depicted. Symmetry operations: i) $x, 1+y, 1+z$.

3- H-bond interactions of complexes 6 and 8

Table S2. Geometrical parameters (Å, °) of H-bond interactions of complexes **6** and **8**

D-H...A	D-H	D...A	H...A	D-H...A
N(4)-H(4N)...F(8)	0.87(9)	3.068(12)	2.29(9)	148(8)
N(3)-H(3N)...F(1')	0.87(12)	3.083(11)	2.58(10)	117(9)
N(4)-H(4N)...F(22'')	0.87(4)	2.934(9)	2.15(7)	150(8)
N(54)-H(54N)...F(7')	0.94(10)	2.911(10)	1.98(11)	168(10)

Symmetry operation: $x, y+1, z$

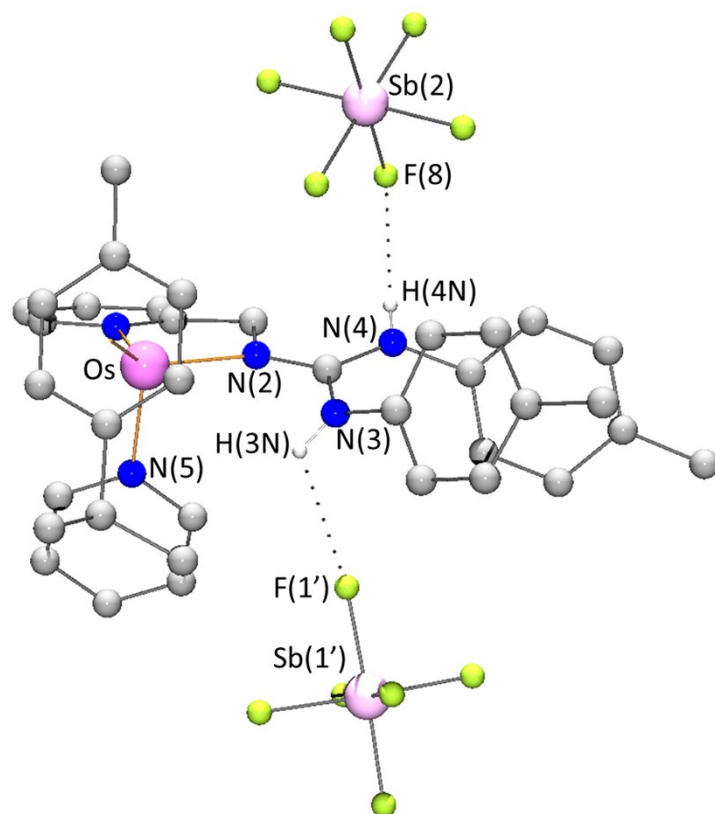


Figure S2. H-bond interactions in complex **6**. For clarity, only hydrogen atoms of N-H fragments have been depicted. Symmetry operations: i) $x, 1+y, z$.

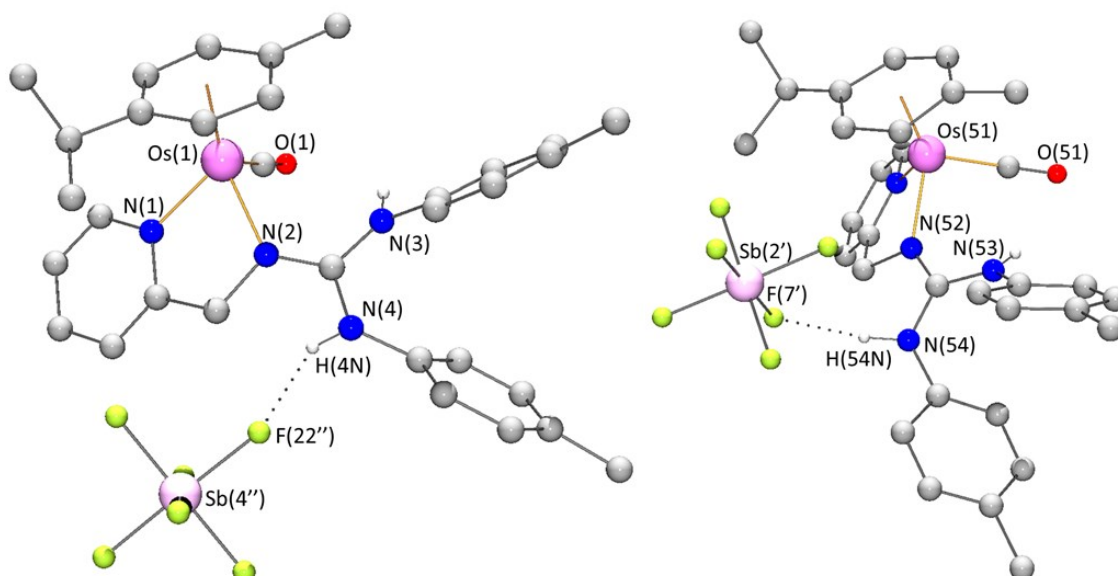
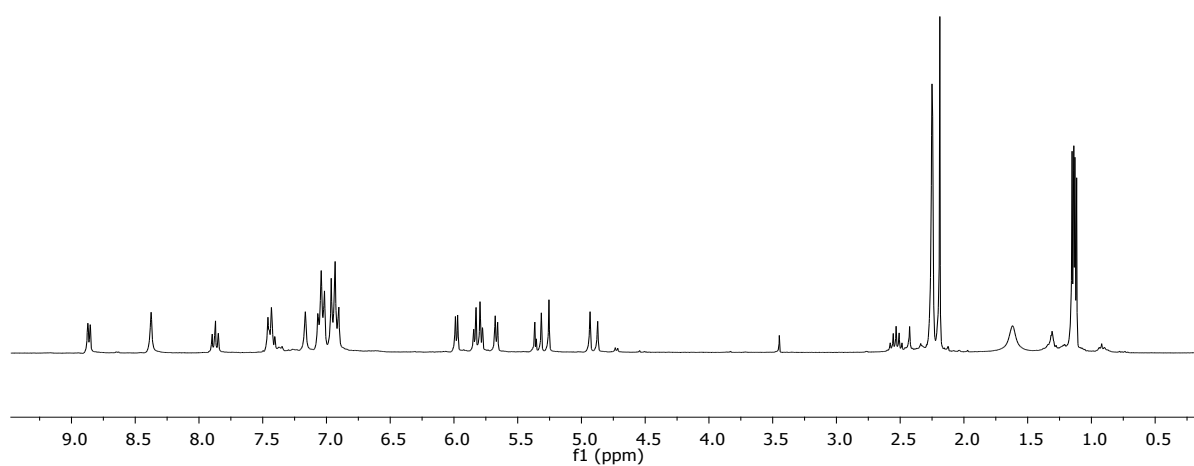


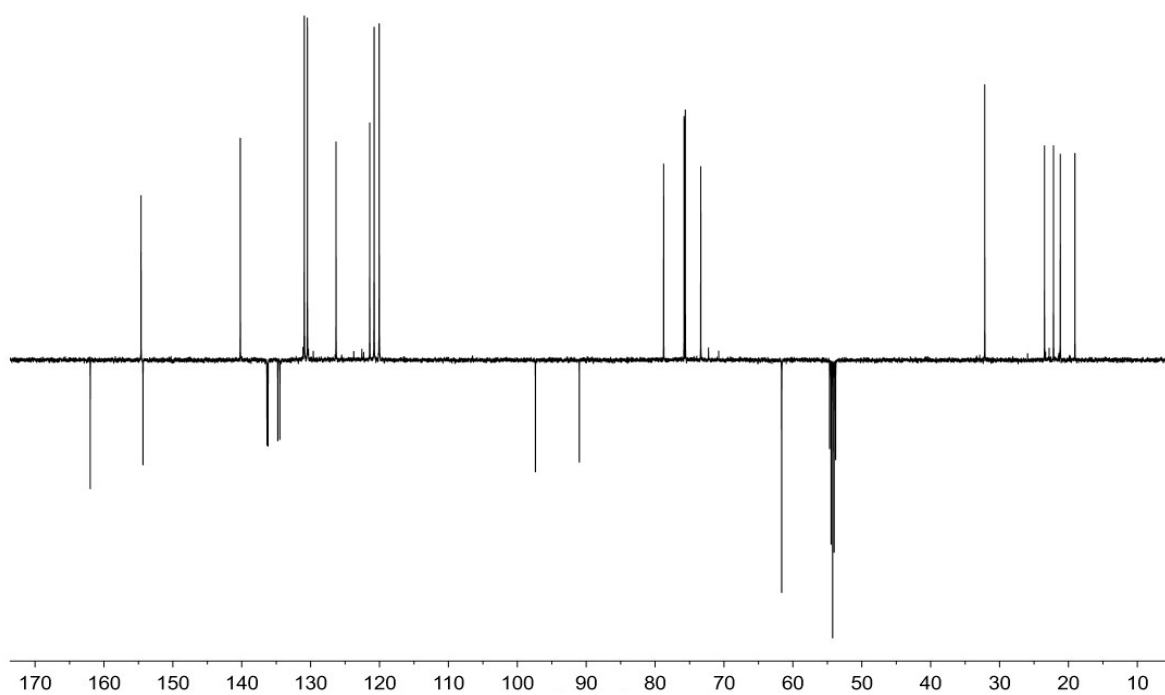
Figure S3. H-bond interactions in complex **8**. For clarity, only hydrogen atoms of N-H fragments have been depicted. Symmetry operations: i) $x, 1+y, z$; ii) $1-x, 1-y, 1-z$.

4- NMR spectra of the complexes 1-11

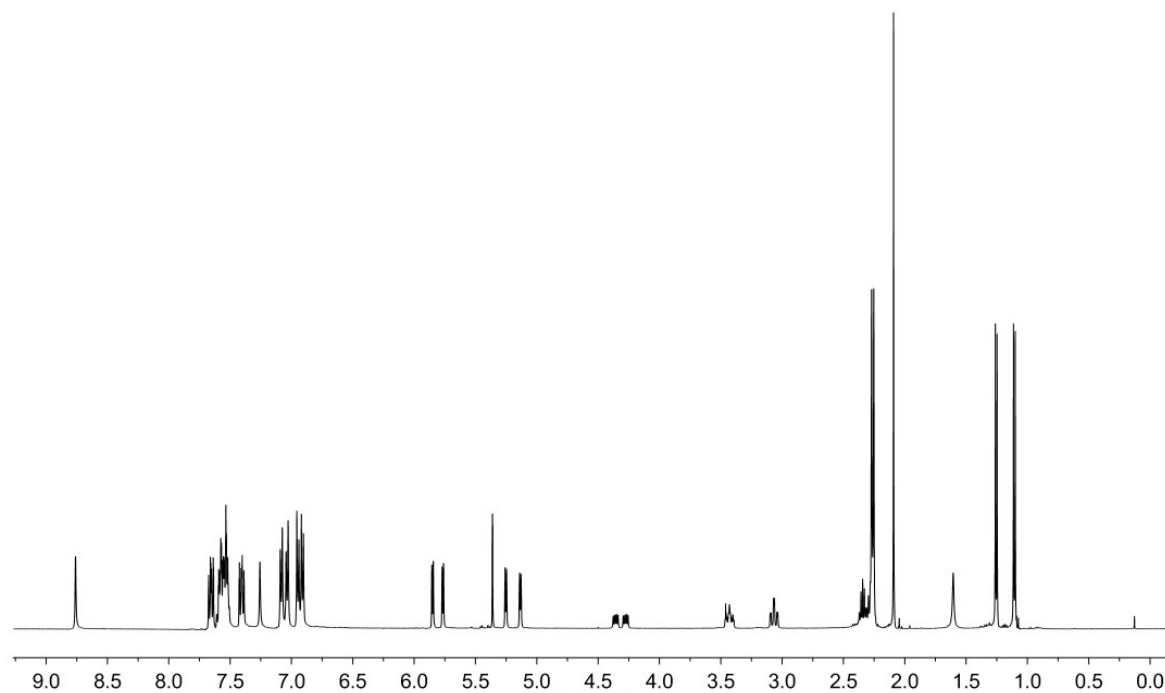
^1H NMR of **1** (500.10 MHz, CD_2Cl_2 , RT)



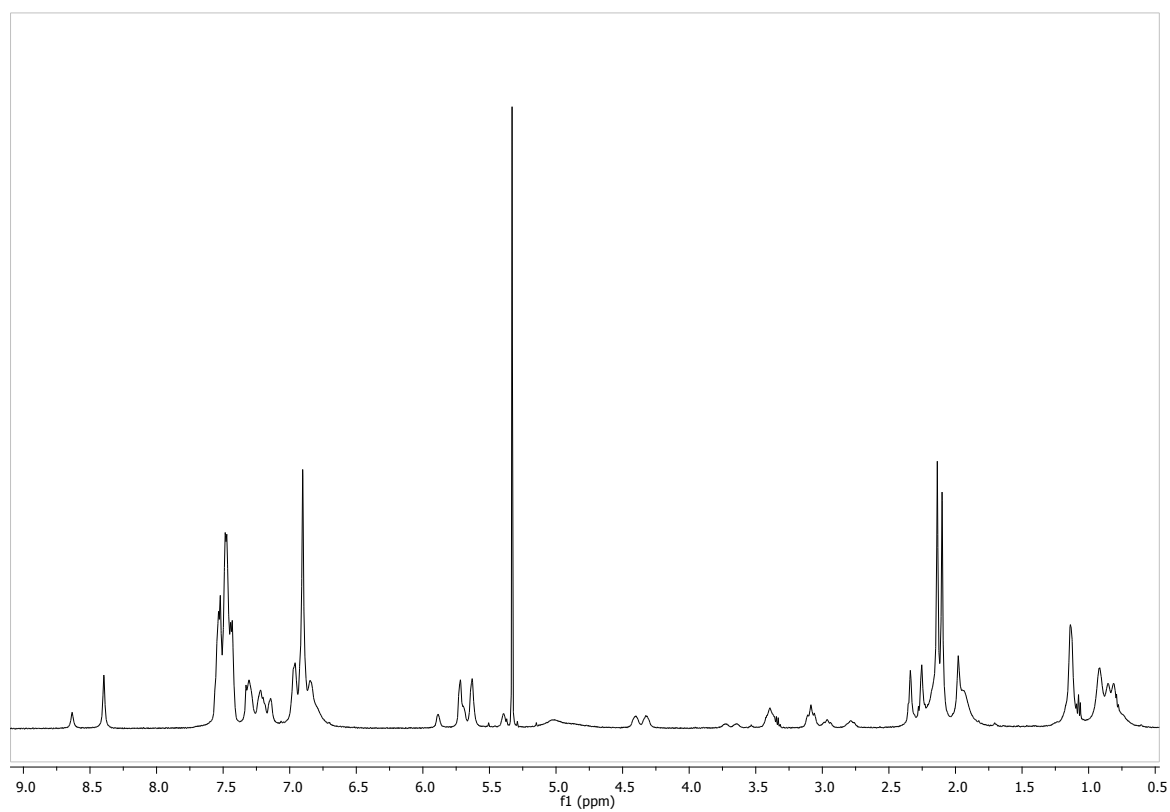
$^{13}\text{C}\{^1\text{H}\}$ NMR of **1** (125.77 MHz, CD_2Cl_2 , RT)



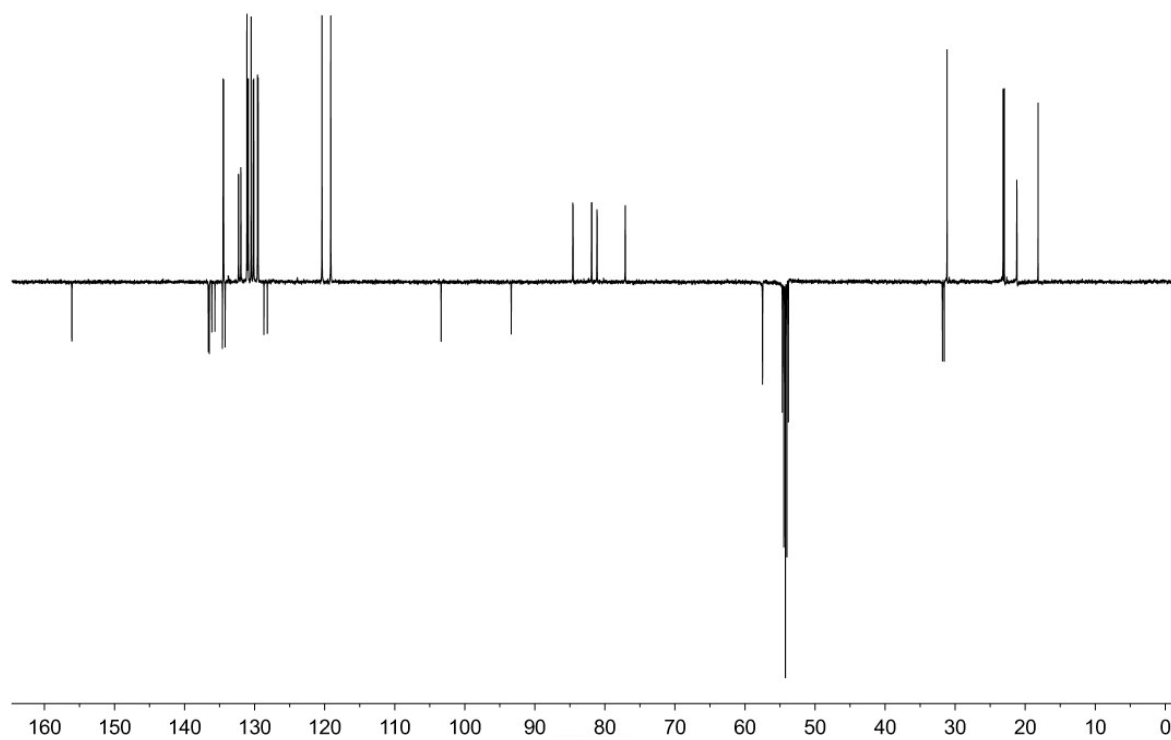
^1H NMR of 2 (500.10 MHz, CD_2Cl_2 , RT)



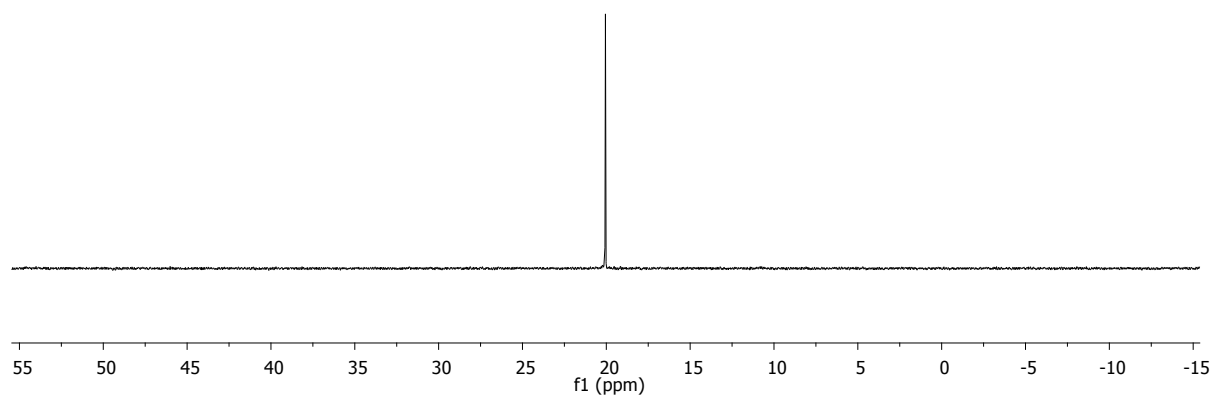
^1H NMR of 2 (500.10 MHz, CD_2Cl_2 , 183K)



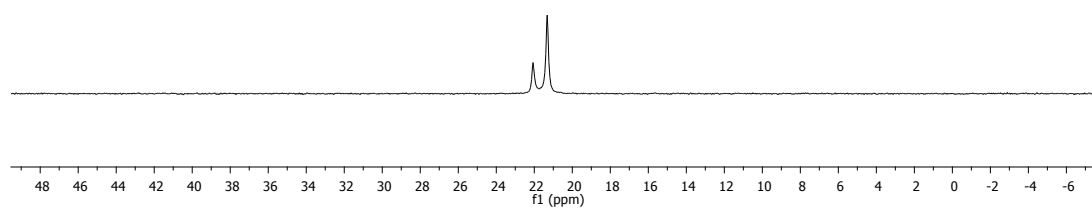
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2 (125.77 MHz, CD_2Cl_2 , RT)



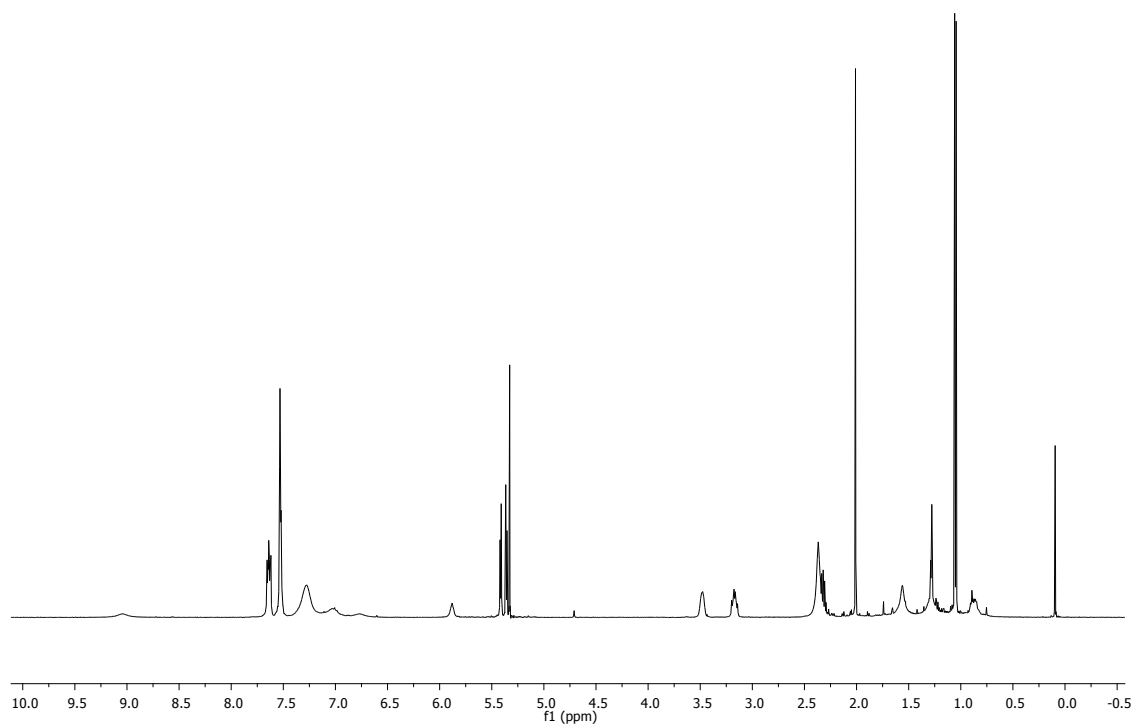
$^{31}\text{P}\{^1\text{H}\}$ NMR of 2 (202.46 MHz, CD_2Cl_2 , RT)



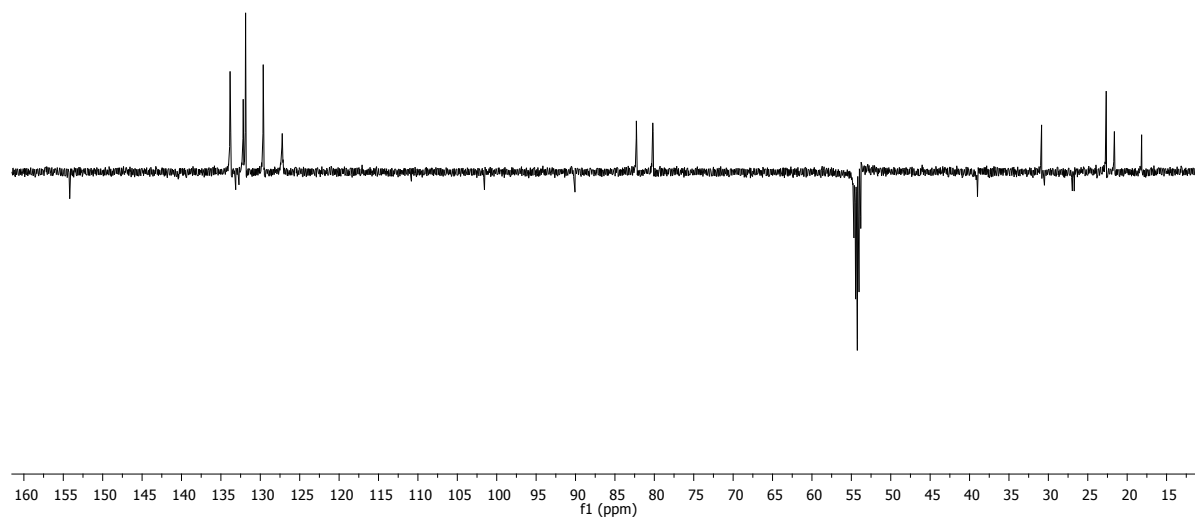
$^{31}\text{P}\{^1\text{H}\}$ NMR of 2 (202.46 MHz, CD_2Cl_2 , 183K)



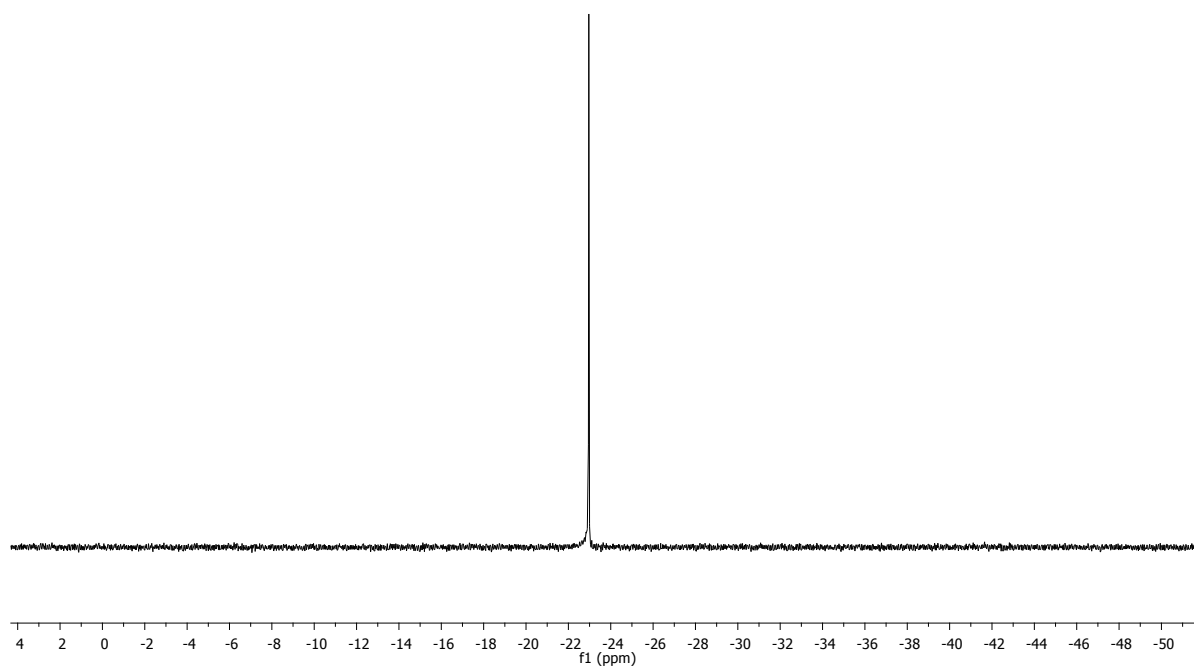
^1H NMR of 3 (500.10 MHz, CD_2Cl_2 , RT)



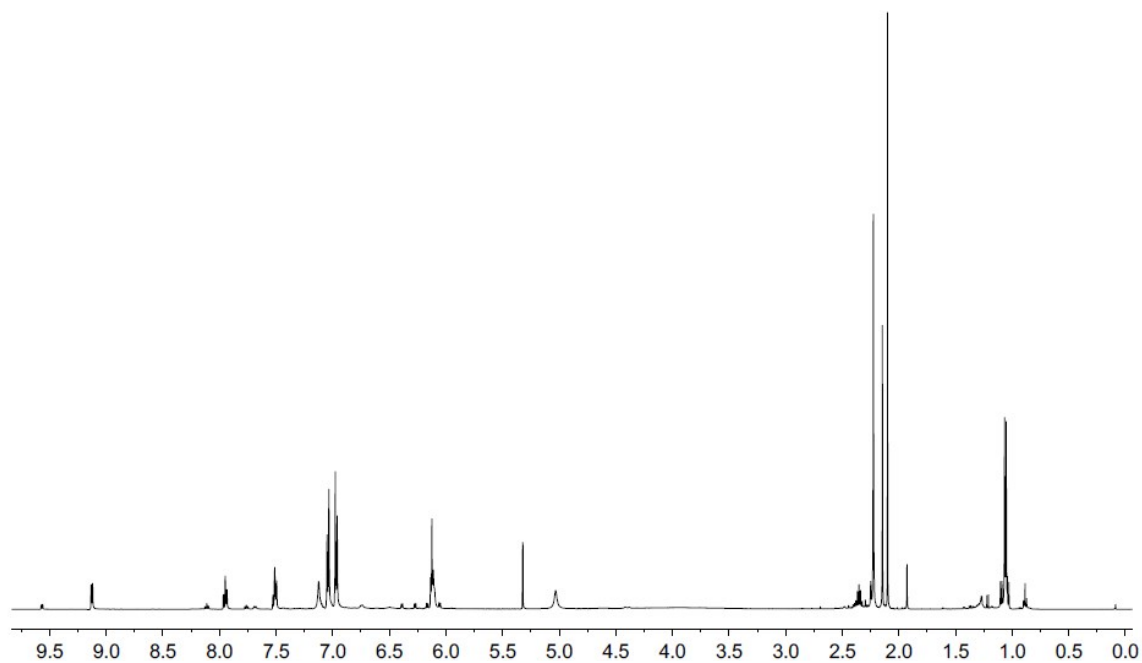
$^{13}\text{C}\{^1\text{H}\}$ NMR of 3 (125.77 MHz, CD_2Cl_2 , RT)



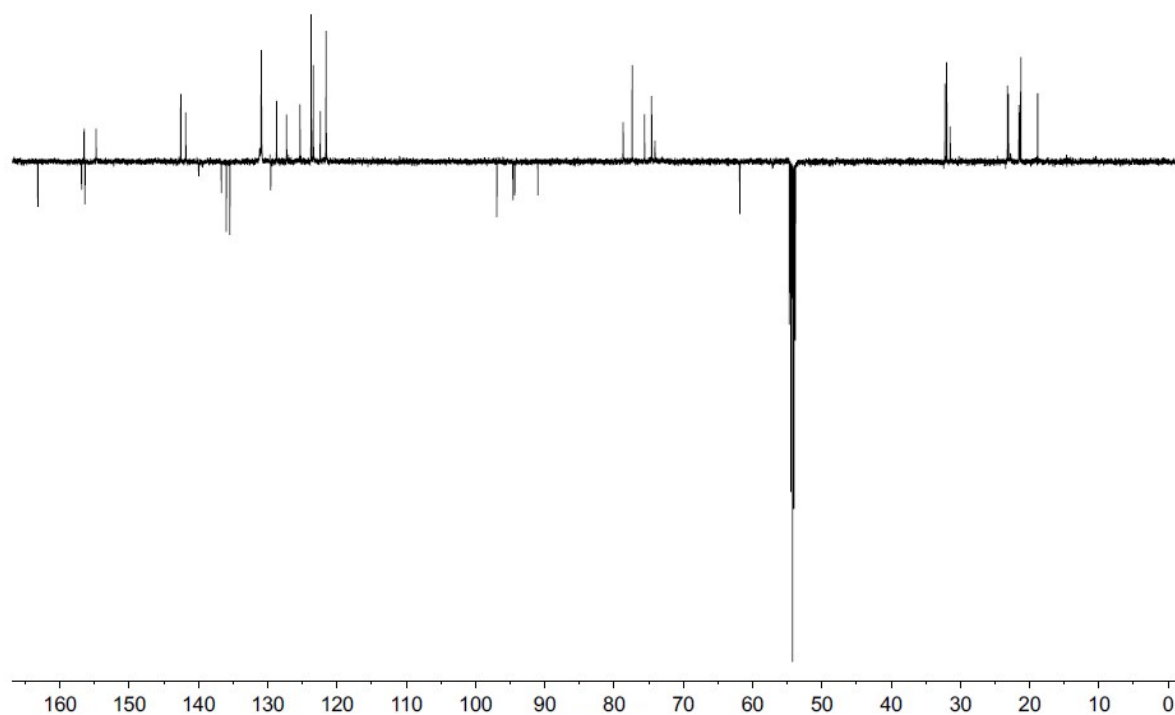
$^{31}\text{P}\{^1\text{H}\}$ NMR of 3 (202.46 MHz, CD_2Cl_2 , RT)



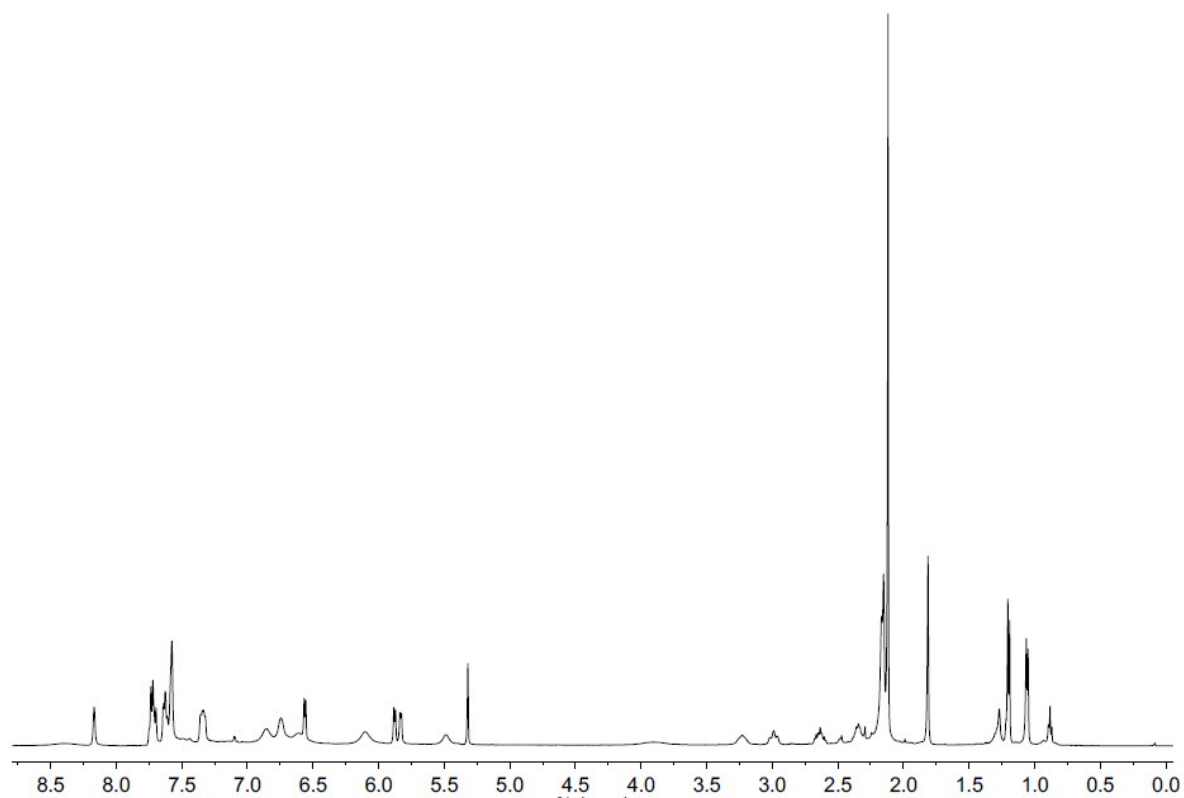
^1H NMR of 4 (500.10 MHz, CD_2Cl_2 , RT)



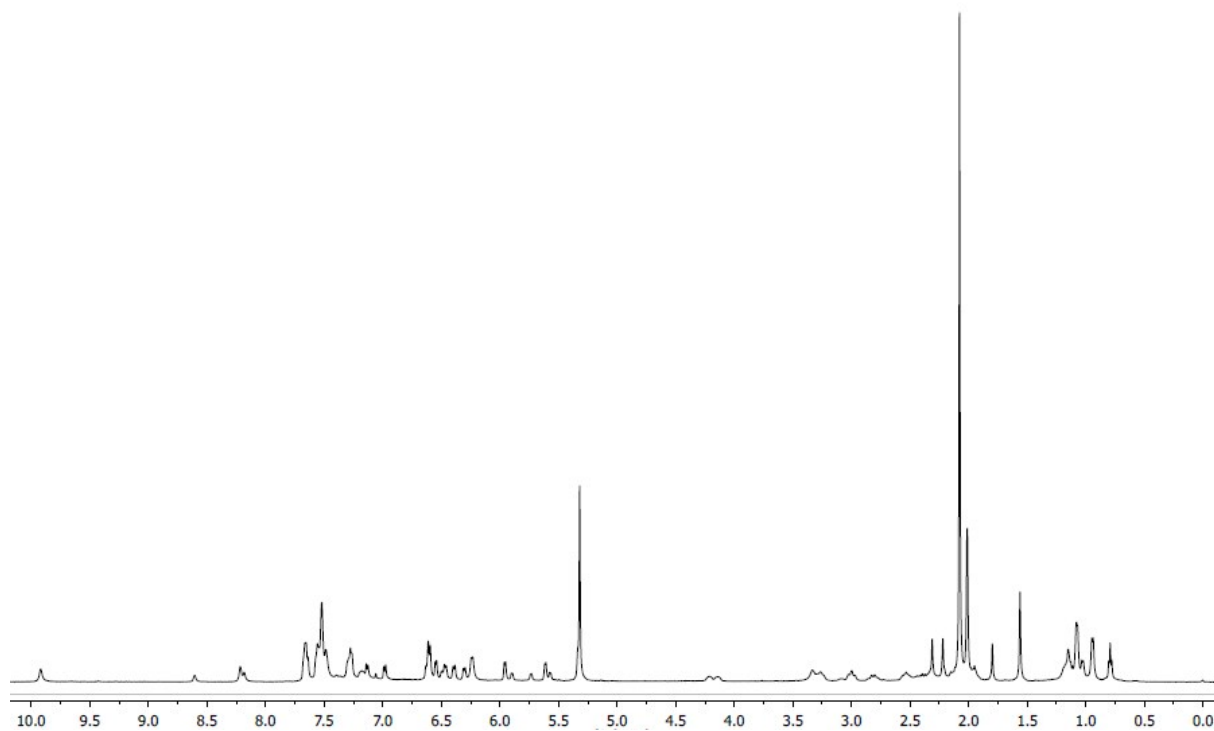
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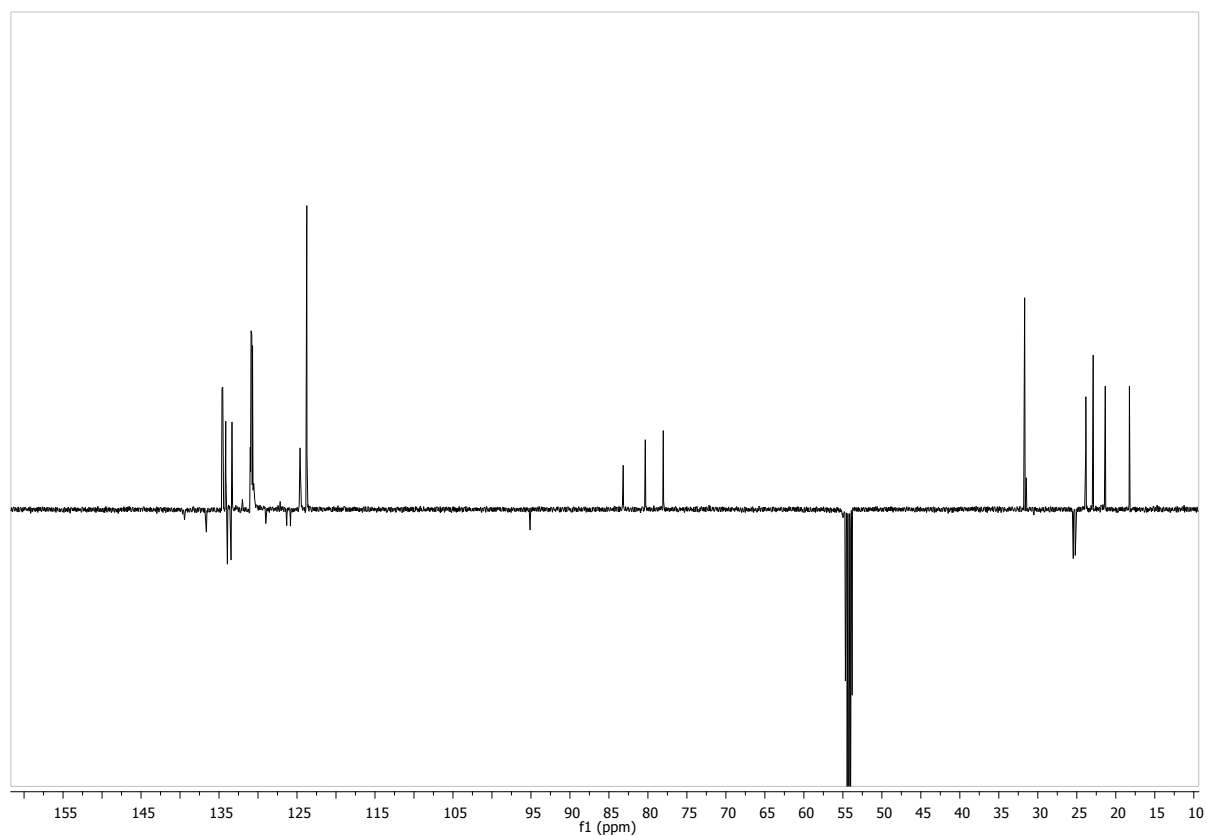
^1H NMR of 5 (500.10 MHz, CD_2Cl_2 , RT)



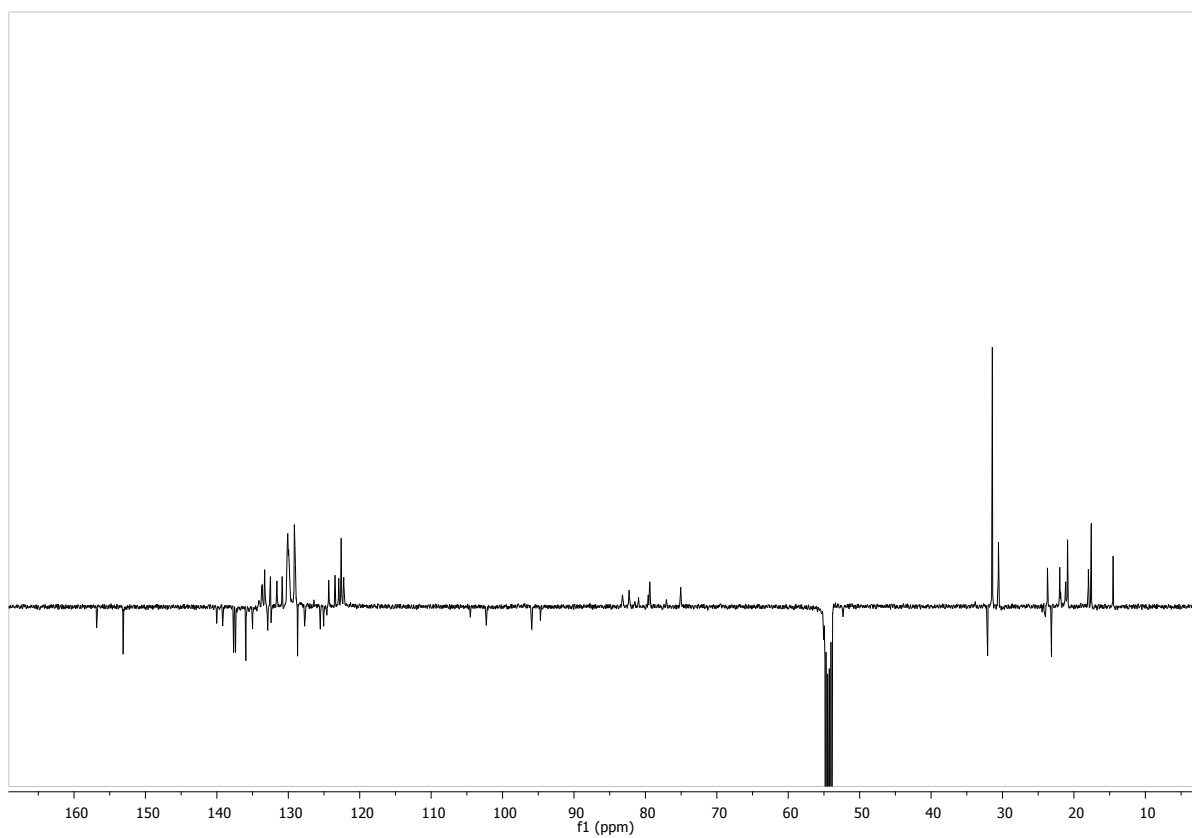
^1H NMR of 5 (500.10 MHz, CD_2Cl_2 , 193K)



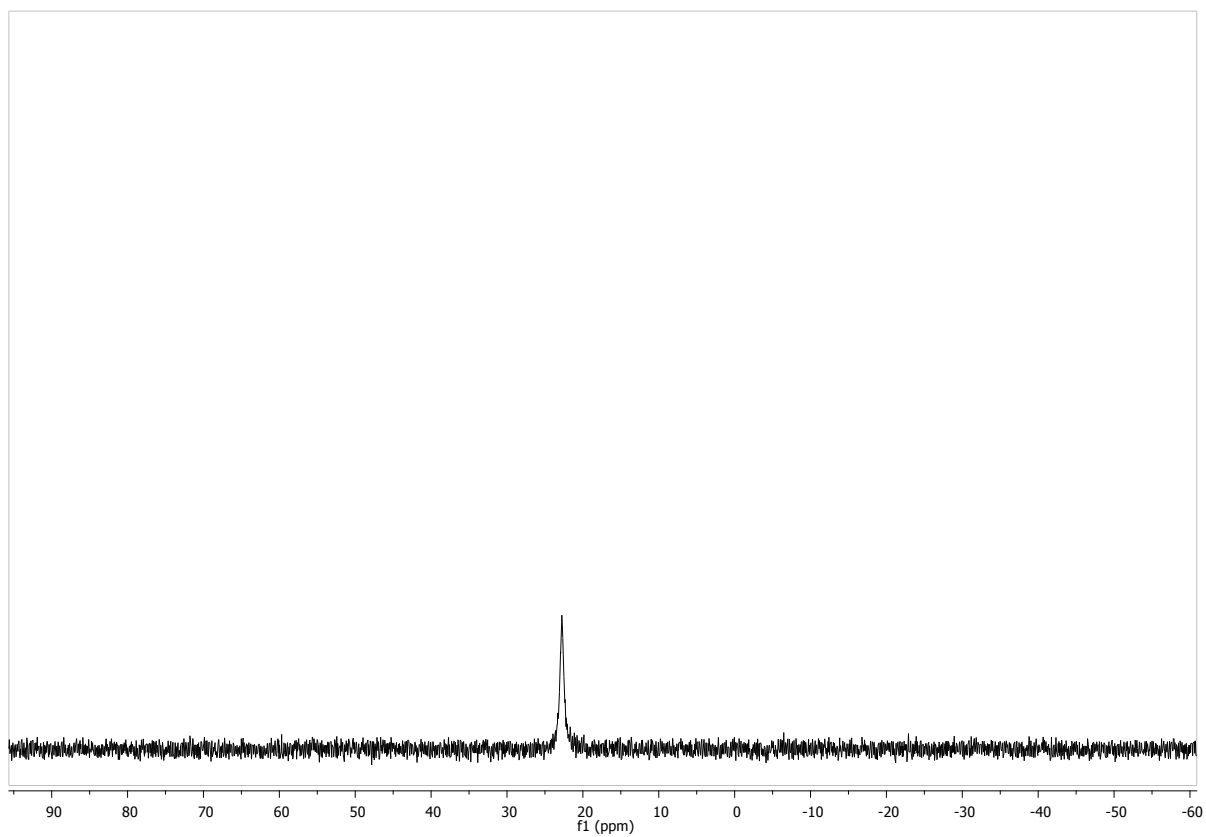
$^{13}\text{C}\{^1\text{H}\}$ NMR of 5 (125.77 MHz, CD_2Cl_2 , RT)



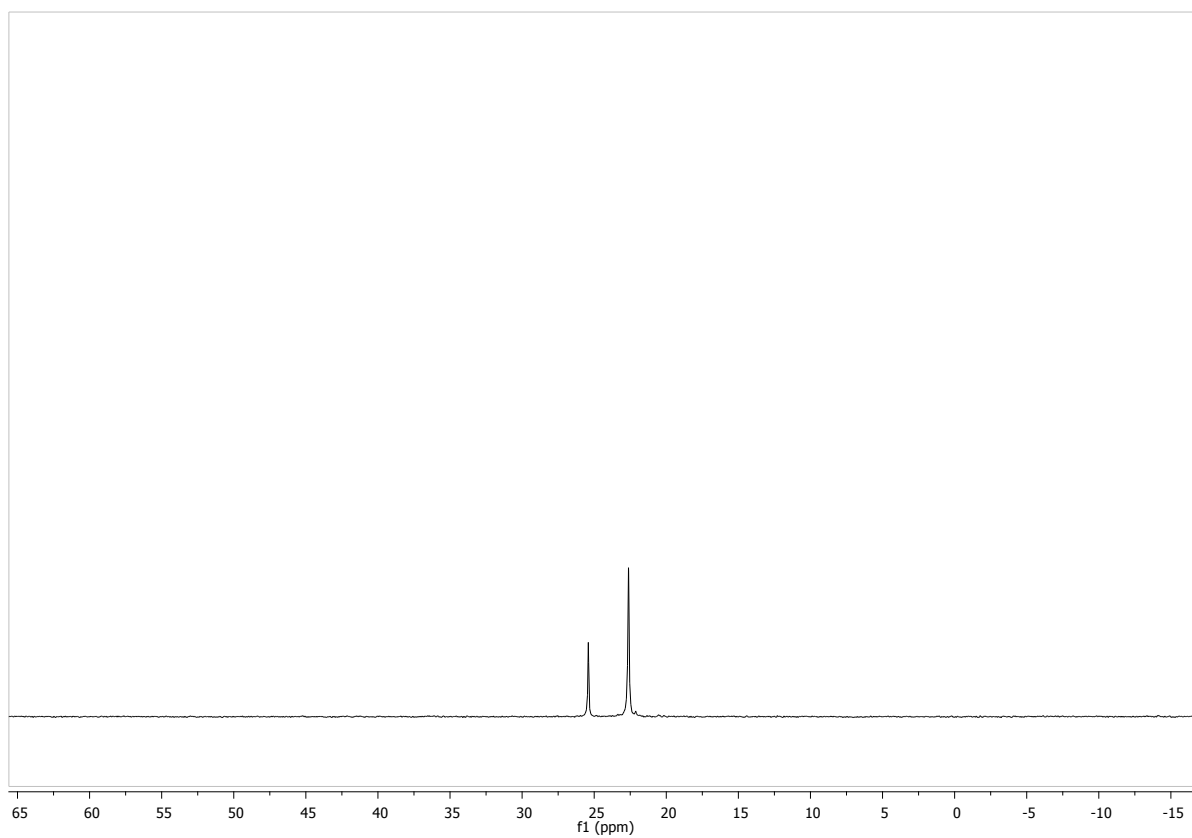
$^{13}\text{C}\{^1\text{H}\}$ NMR of 5 (125.77 MHz, CD_2Cl_2 , 193K)



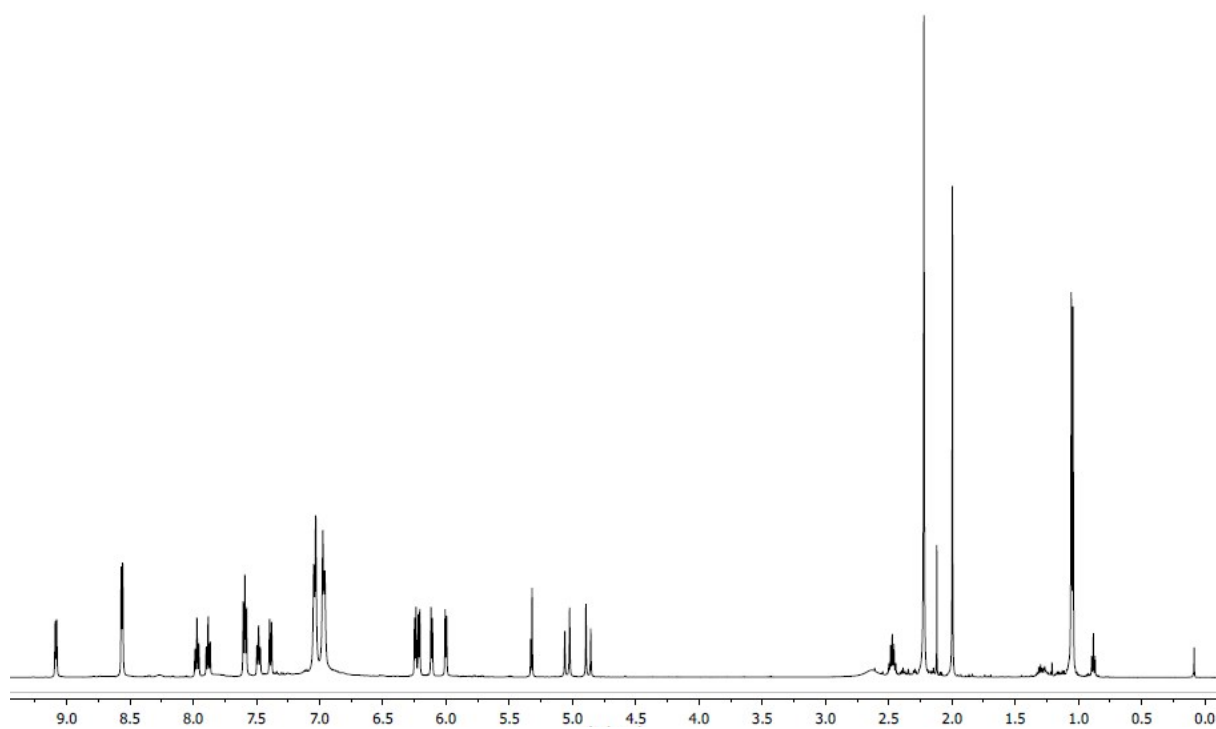
$^{31}\text{P}\{^1\text{H}\}$ NMR of 5 (202.46 MHz, CD_2Cl_2 , RT)



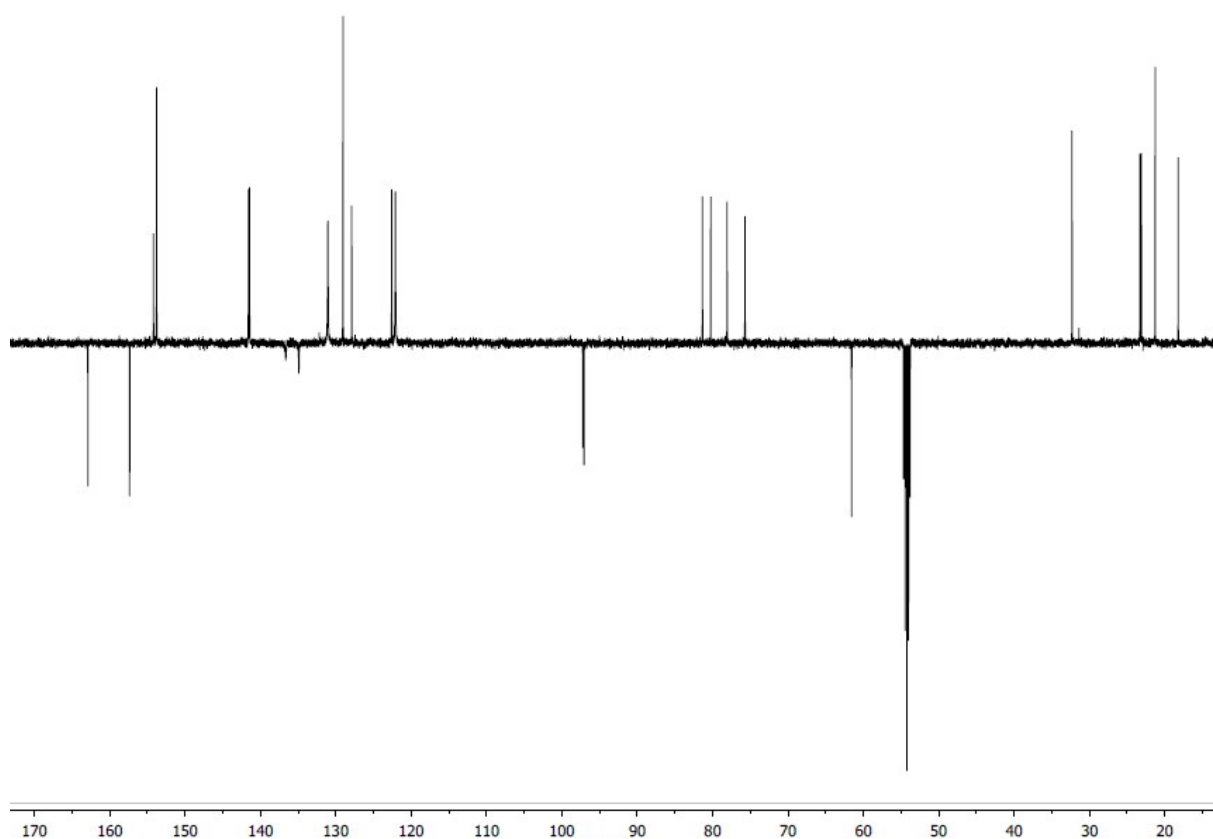
$^{31}\text{P}\{^1\text{H}\}$ NMR of 5 (202.46 MHz, CD_2Cl_2 , 193K)



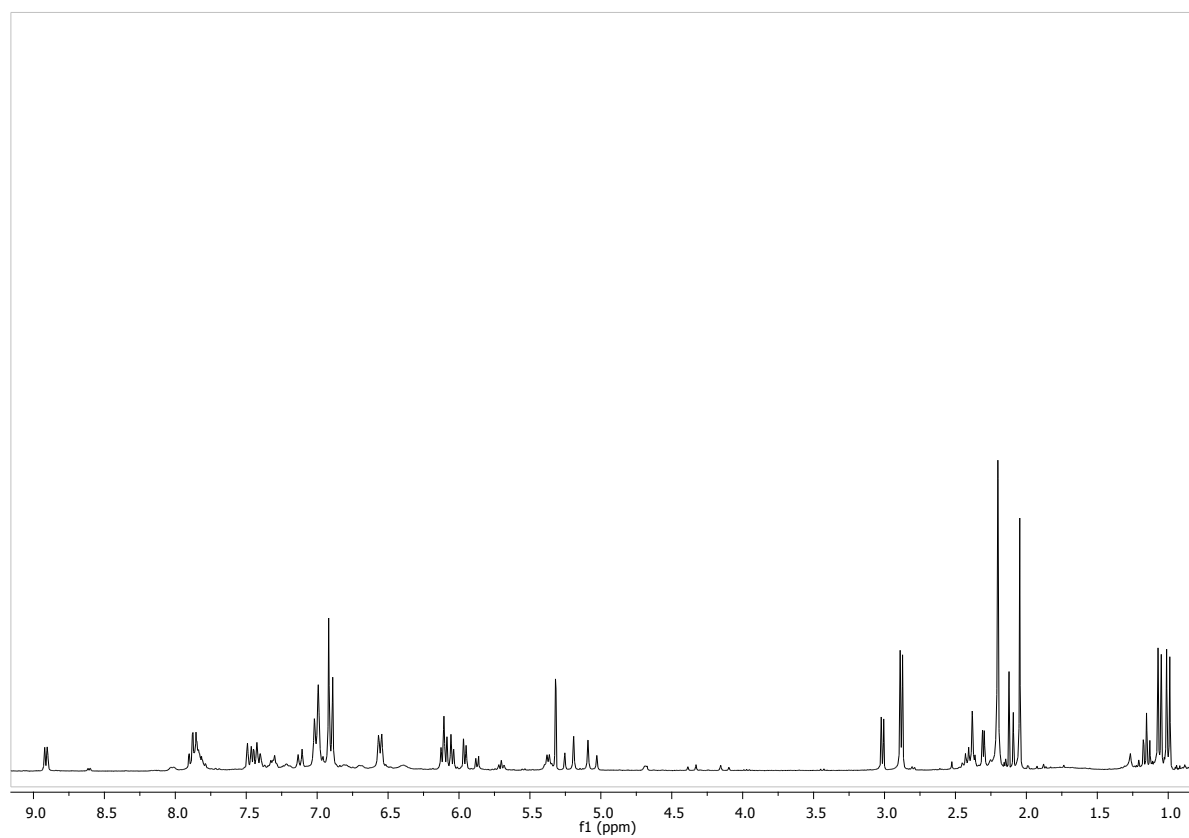
^1H NMR of 6 (500.10 MHz, CD_2Cl_2 , RT)



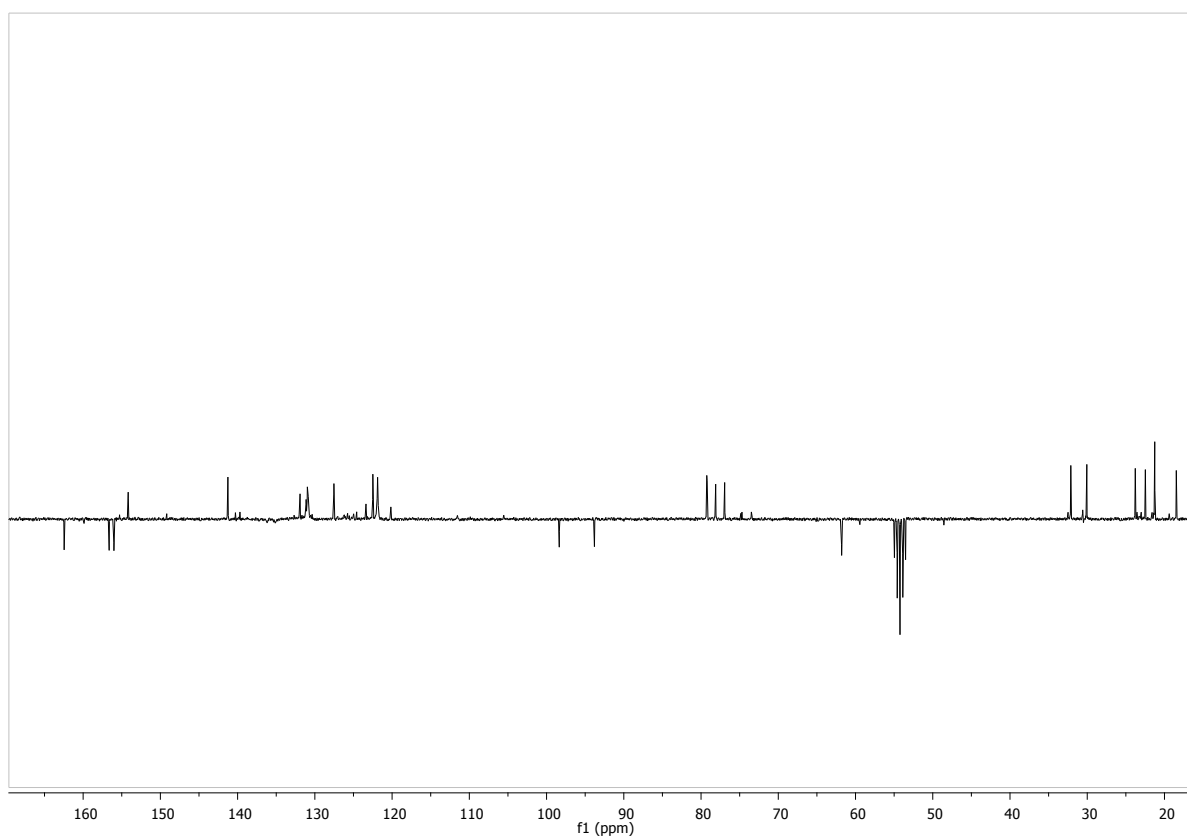
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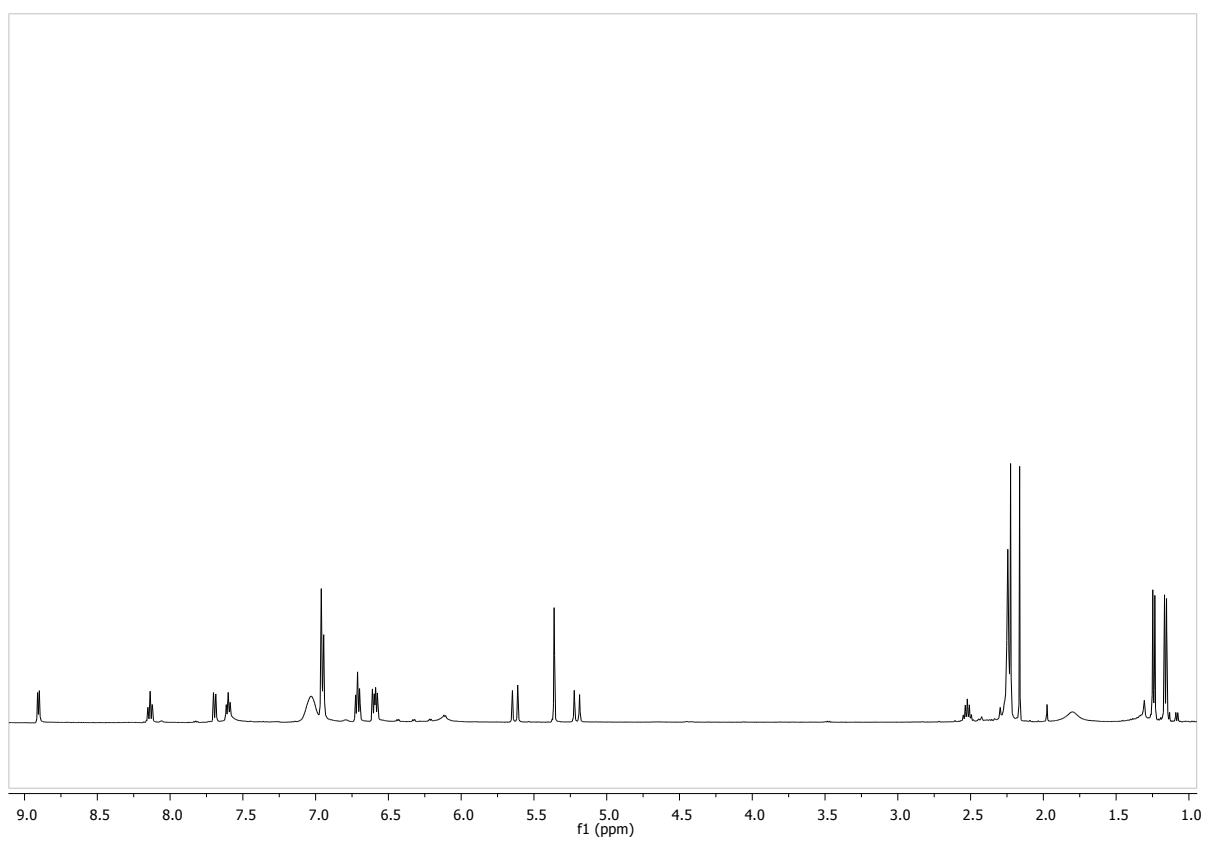
^1H NMR of 7 (300.13 MHz, CD_2Cl_2 , RT)



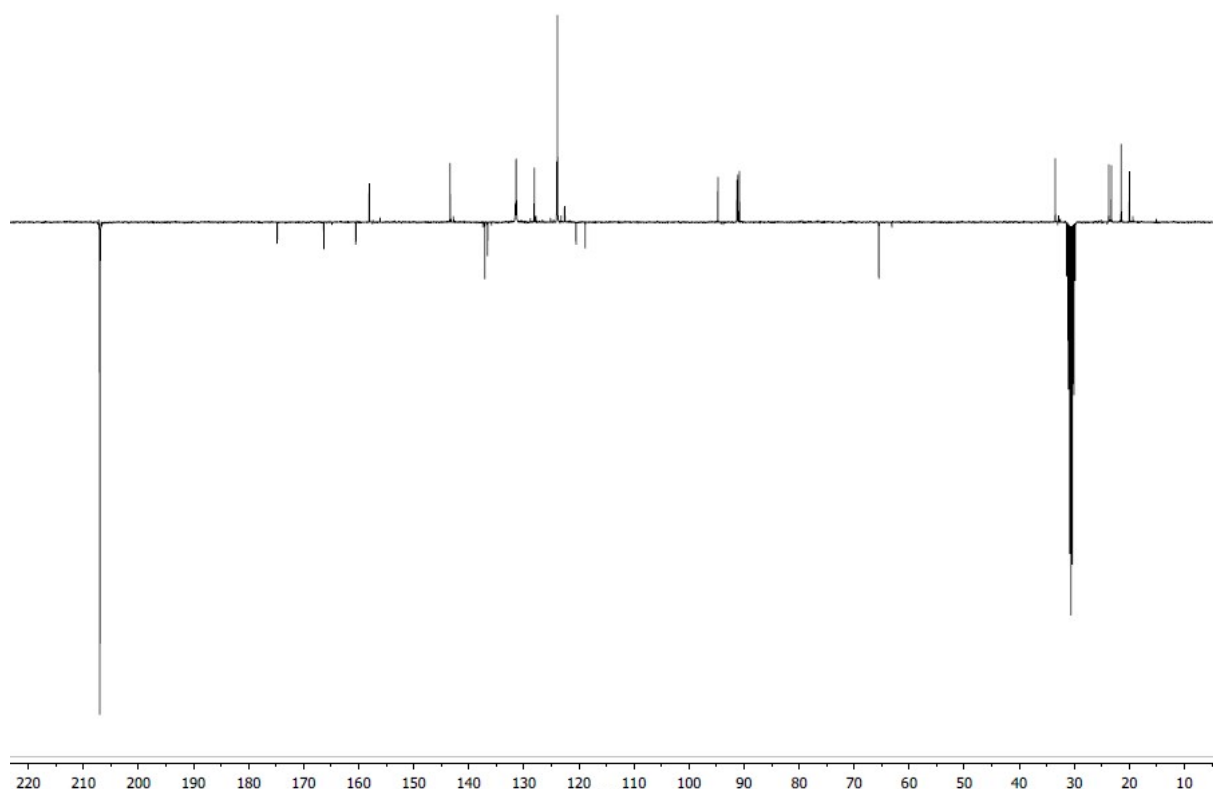
$^{13}\text{C}\{^1\text{H}\}$ NMR of 7 (100.62 MHz, CD_2Cl_2 , RT)



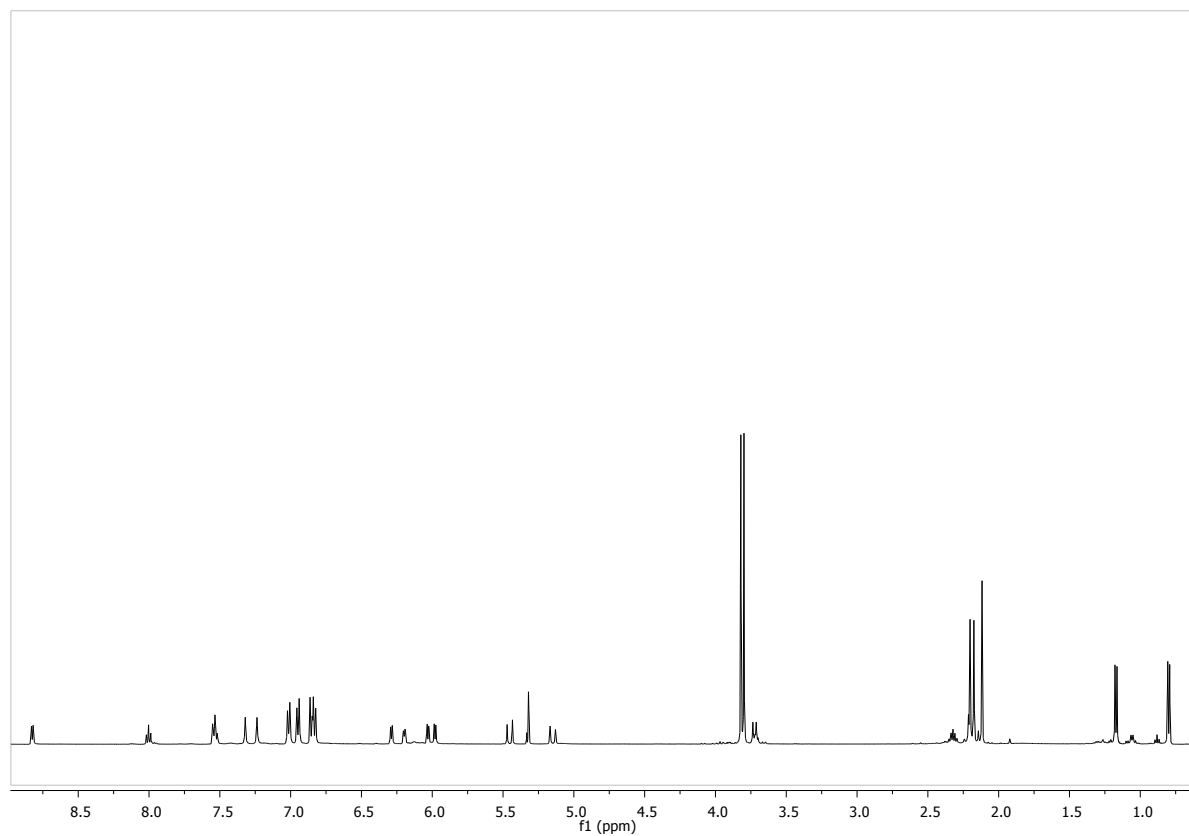
^1H NMR of 8 (300.13 MHz, CD_2Cl_2 , RT)



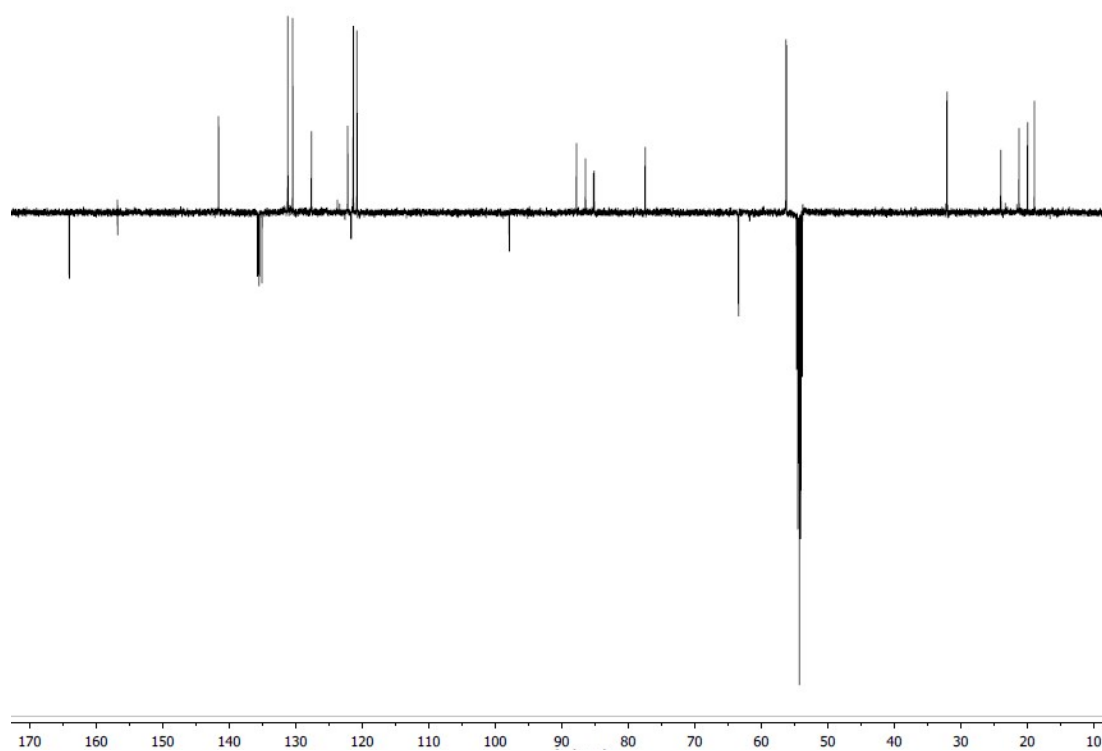
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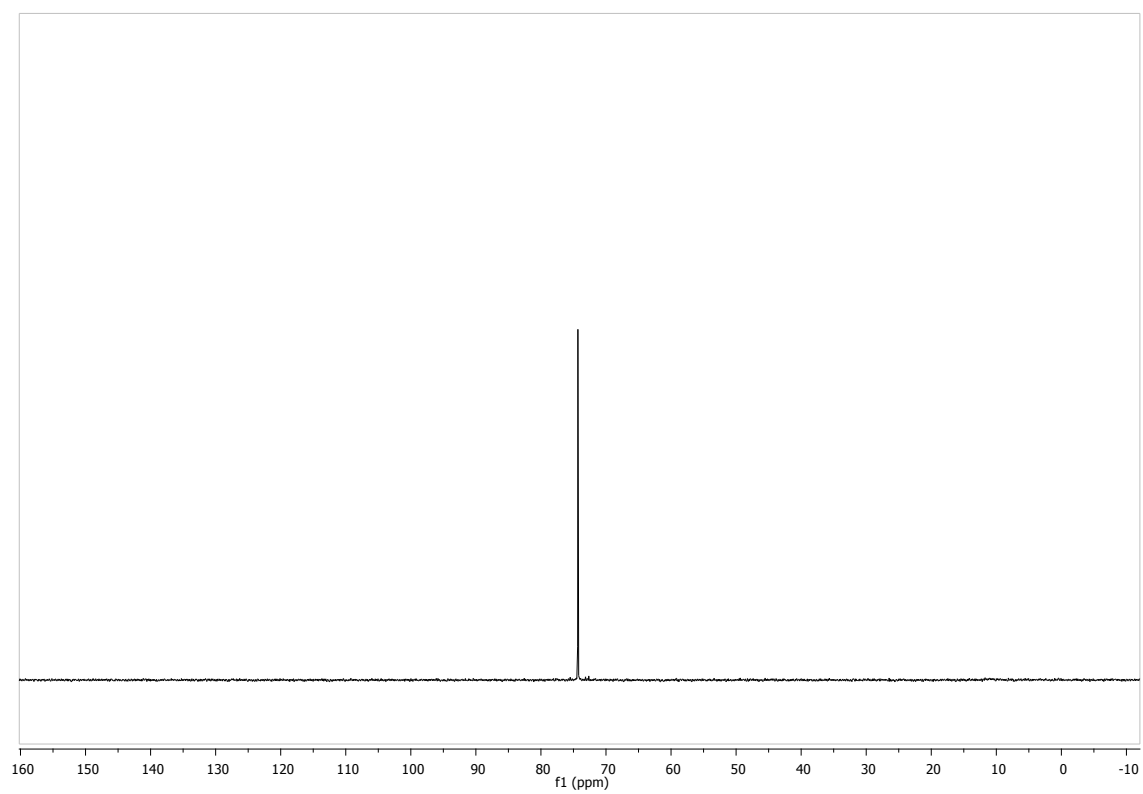
^1H NMR of 9 (500.10 MHz, CD_2Cl_2 , RT)



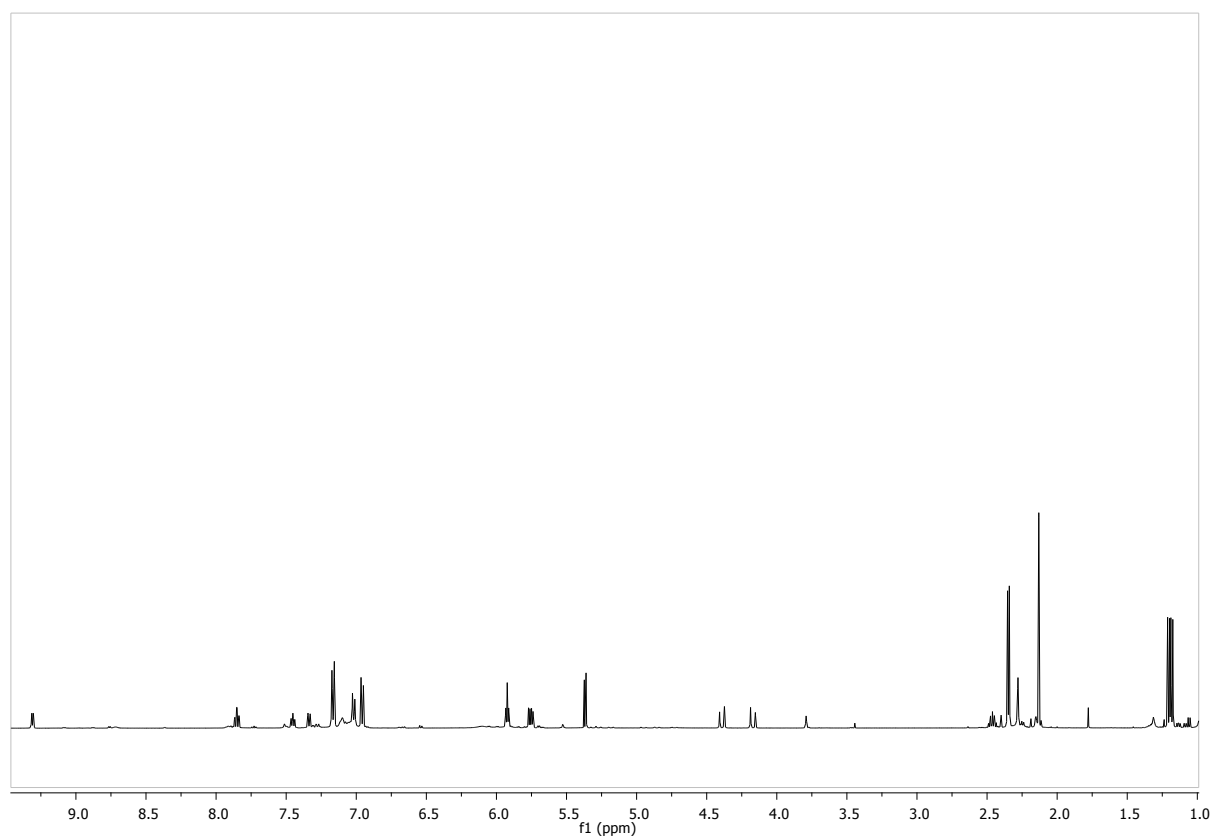
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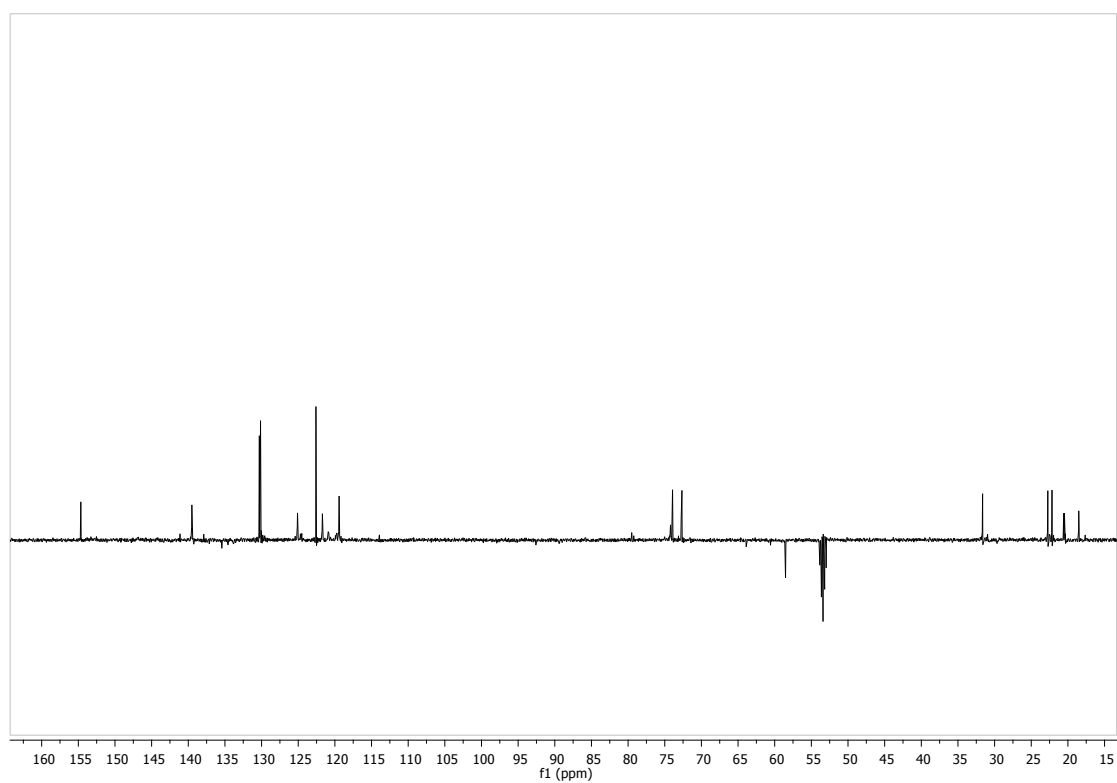
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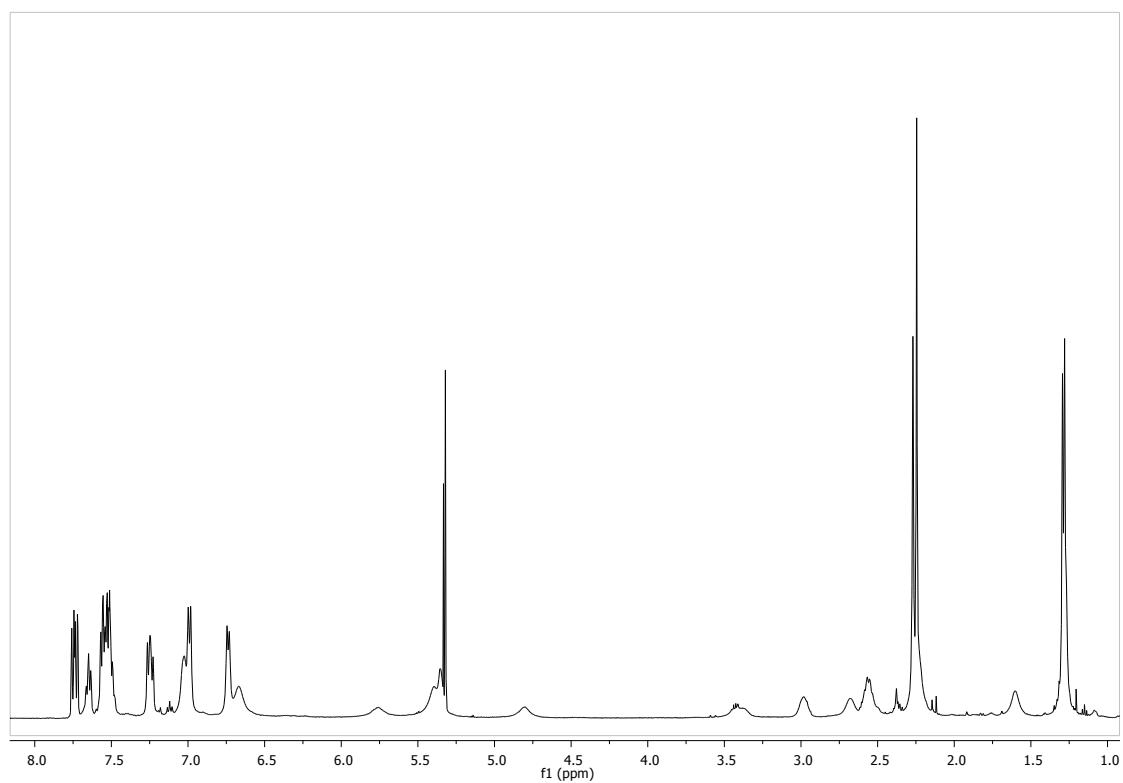
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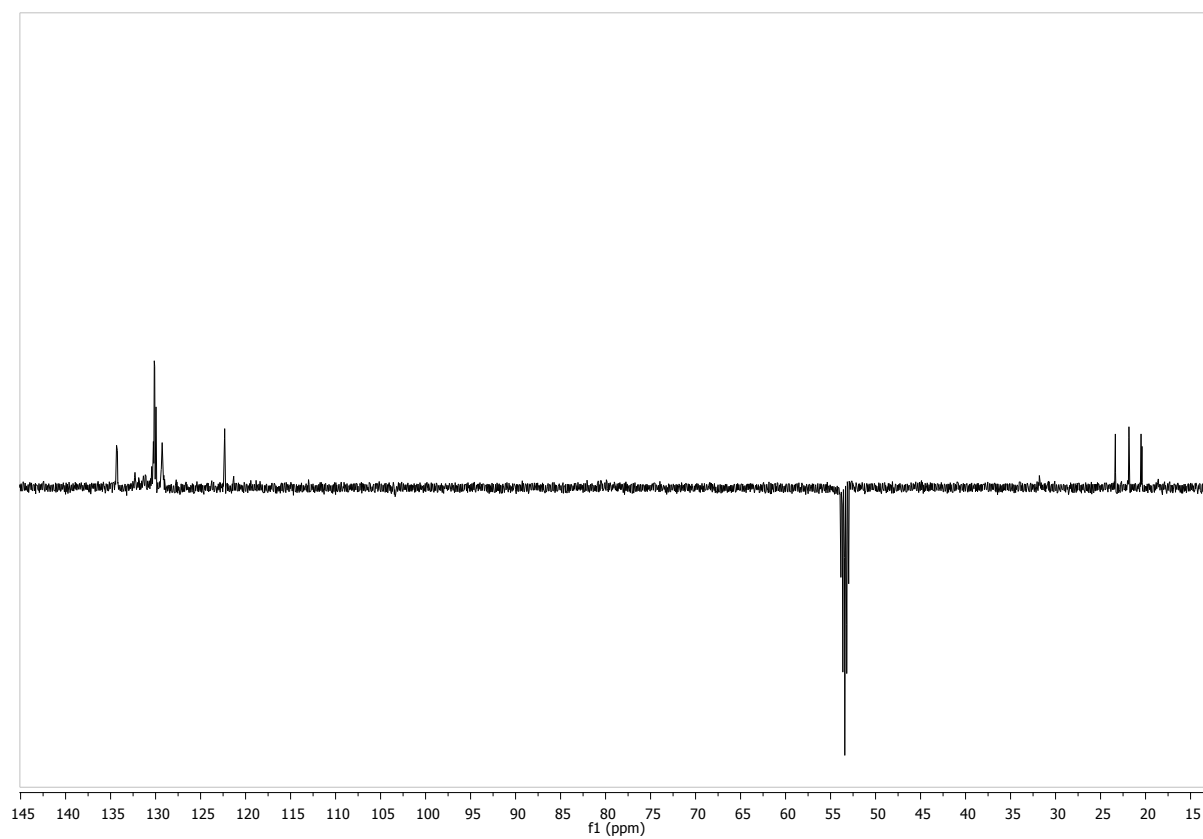
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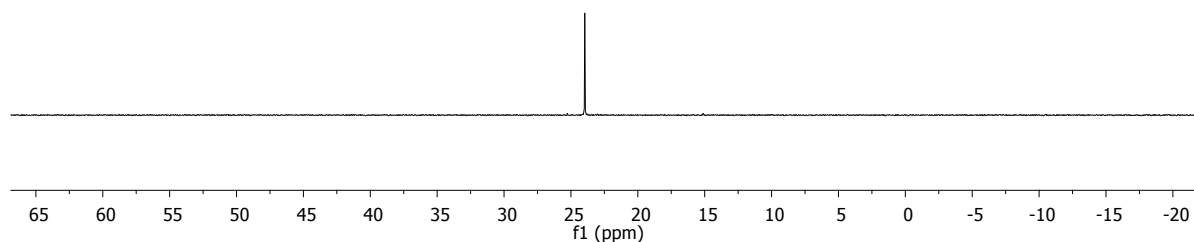
^1H NMR of 11 (500.10 MHz, CD_2Cl_2 , RT)



$^{13}\text{C}\{^1\text{H}\}$ NMR of 11 (125.77 MHz, CD_2Cl_2 , RT)



$^{31}\text{P}\{^1\text{H}\}$ NMR of 11 (202.46 MHz, CD_2Cl_2 , RT)



5- Atomic coordinates of calculated structures

```
89
2      G=-2569.444775
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H	1.318000	3.408000	-3.207000
H	0.942000	1.866000	-2.421000
C	0.261000	-1.330000	-2.158000
C	-1.149000	-1.839000	-1.889000
C	1.142000	-3.052000	0.052000
C	1.113000	-4.153000	-0.817000
H	1.148000	-4.009000	-1.891000
C	1.068000	-5.446000	-0.308000
H	1.043000	-6.291000	-0.987000
C	1.069000	-5.654000	1.071000
H	1.037000	-6.663000	1.467000
C	1.117000	-4.566000	1.937000
H	1.120000	-4.722000	3.010000
C	1.153000	-3.267000	1.432000
H	1.166000	-2.424000	2.108000
C	3.005000	-1.425000	-1.346000
C	3.321000	-0.714000	-2.512000

H	2.563000	-0.139000	-3.028000
C	4.618000	-0.731000	-3.021000
H	4.845000	-0.183000	-3.928000
C	5.617000	-1.451000	-2.369000
H	6.625000	-1.464000	-2.766000
C	5.311000	-2.164000	-1.212000
H	6.080000	-2.736000	-0.707000
C	4.013000	-2.155000	-0.705000
H	3.783000	-2.734000	0.182000
C	-1.956000	-0.115000	-0.292000
C	-1.528000	2.170000	-0.280000
C	-1.742000	2.833000	-1.486000
H	-1.502000	2.331000	-2.416000
C	-2.252000	4.129000	-1.494000
H	-2.408000	4.632000	-2.442000
C	-2.574000	4.790000	-0.304000
C	-2.380000	4.102000	0.900000
H	-2.642000	4.583000	1.837000
C	-1.866000	2.809000	0.918000
H	-1.712000	2.279000	1.852000
C	-3.098000	6.205000	-0.313000
H	-3.591000	6.443000	-1.258000
H	-2.282000	6.922000	-0.177000
H	-3.815000	6.369000	0.495000
C	-4.353000	-0.710000	-0.183000
C	-4.739000	-1.077000	-1.472000
H	-4.199000	-0.684000	-2.326000
C	-5.828000	-1.923000	-1.652000
H	-6.125000	-2.201000	-2.657000
C	-6.563000	-2.400000	-0.560000
C	-6.169000	-2.007000	0.723000
H	-6.725000	-2.359000	1.585000
C	-5.069000	-1.177000	0.919000
H	-4.758000	-0.895000	1.918000
C	-7.733000	-3.330000	-0.761000
H	-8.476000	-3.214000	0.030000
H	-7.402000	-4.374000	-0.750000
H	-8.225000	-3.152000	-1.719000
H	0.240000	-0.289000	-2.478000
H	0.730000	-1.917000	-2.950000
H	-1.817000	-1.533000	-2.704000
H	-1.145000	-2.929000	-1.865000
H	-2.363000	-2.060000	-0.217000
H	-3.414000	1.033000	0.509000
89			
2b	G=-2569.410240		
Os	-1.414000	-0.801000	0.170000
P	-1.314000	1.487000	-0.418000
N	-0.879000	-0.898000	-1.906000
N	0.629000	-1.055000	-0.341000
N	1.407000	-0.789000	-2.616000
C	-1.861000	-1.107000	2.371000
C	-2.958000	-0.468000	1.723000
H	-3.289000	0.500000	2.082000
C	-3.605000	-1.034000	0.592000
H	-4.413000	-0.489000	0.130000

C	-3.106000	-2.232000	0.008000
C	-2.012000	-2.902000	0.653000
H	-1.599000	-3.801000	0.216000
C	-1.407000	-2.333000	1.798000
H	-0.514000	-2.797000	2.203000
C	-1.274000	-0.551000	3.639000
H	-1.298000	0.540000	3.642000
H	-0.245000	-0.881000	3.783000
H	-1.854000	-0.900000	4.499000
C	-3.695000	-2.845000	-1.251000
H	-2.840000	-3.089000	-1.891000
C	-4.431000	-4.150000	-0.891000
H	-3.775000	-4.865000	-0.392000
H	-4.819000	-4.623000	-1.795000
H	-5.276000	-3.946000	-0.226000
C	-4.620000	-1.904000	-2.027000
H	-5.548000	-1.713000	-1.481000
H	-4.892000	-2.356000	-2.983000
H	-4.142000	-0.945000	-2.235000
C	-1.097000	1.529000	-2.279000
C	-1.376000	0.120000	-2.839000
C	0.056000	2.504000	0.237000
C	0.699000	2.100000	1.409000
H	0.351000	1.213000	1.919000
C	1.790000	2.814000	1.898000
H	2.302000	2.480000	2.792000
C	2.240000	3.943000	1.217000
H	3.099000	4.489000	1.586000
C	1.587000	4.367000	0.059000
H	1.931000	5.250000	-0.466000
C	0.497000	3.654000	-0.430000
H	0.001000	3.993000	-1.333000
C	-2.839000	2.427000	-0.052000
C	-3.993000	2.186000	-0.809000
H	-3.964000	1.502000	-1.650000
C	-5.187000	2.825000	-0.491000
H	-6.073000	2.641000	-1.088000
C	-5.243000	3.703000	0.592000
H	-6.173000	4.199000	0.840000
C	-4.099000	3.945000	1.349000
H	-4.136000	4.634000	2.184000
C	-2.898000	3.312000	1.029000
H	-2.009000	3.518000	1.614000
C	0.453000	-0.938000	-1.655000
C	1.751000	-1.553000	0.344000
C	1.908000	-1.239000	1.697000
H	1.170000	-0.611000	2.172000
C	2.995000	-1.720000	2.422000
H	3.087000	-1.460000	3.472000
C	3.969000	-2.528000	1.823000
C	3.788000	-2.858000	0.475000
H	4.512000	-3.499000	-0.016000
C	2.700000	-2.395000	-0.254000
H	2.589000	-2.689000	-1.288000
C	5.175000	-2.998000	2.595000
H	4.934000	-3.174000	3.645000

H	5.970000	-2.245000	2.565000
H	5.581000	-3.922000	2.179000
C	2.699000	-0.212000	-2.442000
C	2.909000	0.813000	-1.518000
H	2.092000	1.183000	-0.914000
C	4.181000	1.344000	-1.357000
H	4.331000	2.129000	-0.625000
C	5.268000	0.884000	-2.110000
C	5.032000	-0.127000	-3.045000
H	5.852000	-0.502000	-3.646000
C	3.764000	-0.679000	-3.209000
H	3.607000	-1.482000	-3.922000
C	6.641000	1.473000	-1.906000
H	7.403000	0.914000	-2.451000
H	6.909000	1.472000	-0.846000
H	6.677000	2.511000	-2.251000
H	-1.729000	2.298000	-2.726000
H	-0.055000	1.796000	-2.463000
H	-2.444000	-0.048000	-2.966000
H	-0.923000	0.017000	-3.830000
H	1.119000	-1.000000	-3.560000
Cl	5.109000	1.081000	2.059000
H	4.325000	0.096000	1.751000
89			
2c	G=-2569.446322		
Os	0.690000	-0.933000	0.313000
P	2.339000	0.417000	-0.667000
Cl	0.784000	-2.310000	-1.723000
N	-0.580000	0.290000	-0.936000
N	-2.217000	-1.345000	-1.113000
N	-2.742000	0.798000	-1.795000
C	1.208000	-2.732000	1.545000
C	1.895000	-1.611000	2.061000
H	2.975000	-1.634000	2.121000
C	1.194000	-0.408000	2.394000
H	1.763000	0.459000	2.697000
C	-0.215000	-0.319000	2.258000
C	-0.918000	-1.493000	1.813000
H	-1.991000	-1.444000	1.667000
C	-0.231000	-2.657000	1.455000
H	-0.773000	-3.487000	1.018000
C	1.924000	-3.984000	1.129000
H	3.002000	-3.828000	1.085000
H	1.579000	-4.311000	0.147000
H	1.724000	-4.780000	1.852000
C	-1.006000	0.900000	2.684000
H	-1.904000	0.919000	2.058000
C	-1.462000	0.719000	4.144000
H	-2.034000	-0.203000	4.275000
H	-2.092000	1.556000	4.451000
H	-0.599000	0.679000	4.815000
C	-0.255000	2.220000	2.492000
H	0.587000	2.312000	3.183000
H	-0.923000	3.063000	2.685000
H	0.136000	2.313000	1.479000
C	1.425000	1.212000	-2.051000

C	-0.008000	1.487000	-1.591000
C	3.849000	-0.336000	-1.363000
C	4.094000	-1.706000	-1.245000
H	3.358000	-2.345000	-0.777000
C	5.268000	-2.250000	-1.762000
H	5.452000	-3.314000	-1.673000
C	6.197000	-1.431000	-2.399000
H	7.108000	-1.857000	-2.803000
C	5.956000	-0.062000	-2.518000
H	6.679000	0.577000	-3.011000
C	4.790000	0.487000	-1.997000
H	4.621000	1.556000	-2.073000
C	3.006000	1.749000	0.402000
C	2.547000	3.068000	0.344000
H	1.814000	3.370000	-0.393000
C	3.035000	4.023000	1.235000
H	2.677000	5.044000	1.175000
C	3.982000	3.670000	2.192000
H	4.360000	4.414000	2.883000
C	4.455000	2.359000	2.248000
H	5.208000	2.083000	2.977000
C	3.975000	1.406000	1.356000
H	4.373000	0.398000	1.384000
C	-1.815000	-0.051000	-1.251000
C	-3.490000	-1.806000	-0.709000
C	-3.881000	-3.099000	-1.069000
H	-3.229000	-3.701000	-1.693000
C	-5.099000	-3.606000	-0.633000
H	-5.383000	-4.613000	-0.918000
C	-5.969000	-2.842000	0.154000
C	-5.564000	-1.551000	0.505000
H	-6.211000	-0.938000	1.123000
C	-4.338000	-1.034000	0.095000
H	-4.047000	-0.036000	0.399000
C	-7.309000	-3.386000	0.583000
H	-7.259000	-4.459000	0.778000
H	-8.059000	-3.230000	-0.199000
H	-7.670000	-2.892000	1.487000
C	-3.001000	2.158000	-1.476000
C	-2.591000	2.731000	-0.274000
H	-2.037000	2.143000	0.441000
C	-2.894000	4.062000	0.001000
H	-2.562000	4.492000	0.940000
C	-3.620000	4.848000	-0.897000
C	-4.031000	4.251000	-2.096000
H	-4.594000	4.834000	-2.816000
C	-3.723000	2.929000	-2.391000
H	-4.037000	2.495000	-3.334000
C	-3.974000	6.280000	-0.588000
H	-5.034000	6.373000	-0.332000
H	-3.790000	6.929000	-1.448000
H	-3.396000	6.664000	0.255000
H	1.913000	2.119000	-2.411000
H	1.425000	0.469000	-2.852000
H	-0.039000	2.330000	-0.895000
H	-0.613000	1.767000	-2.454000

H	-1.477000	-2.029000	-1.251000
H	-3.482000	0.327000	-2.297000
89			
2ts	G=-2569.431377		
Os	-0.998000	-0.721000	0.630000
P	-2.134000	1.022000	-0.459000
Cl	0.216000	0.983000	1.903000
N	0.457000	-0.283000	-0.886000
N	2.298000	-0.933000	0.379000
N	2.620000	-0.117000	-1.830000
C	-1.846000	-1.606000	2.502000
C	-2.816000	-1.677000	1.477000
H	-3.778000	-1.202000	1.620000
C	-2.518000	-2.274000	0.209000
H	-3.261000	-2.225000	-0.573000
C	-1.237000	-2.824000	-0.054000
C	-0.277000	-2.828000	1.023000
H	0.719000	-3.209000	0.840000
C	-0.570000	-2.232000	2.254000
H	0.206000	-2.144000	3.005000
C	-2.113000	-0.932000	3.817000
H	-3.041000	-0.360000	3.785000
H	-1.294000	-0.255000	4.068000
H	-2.201000	-1.679000	4.611000
C	-0.852000	-3.470000	-1.373000
H	0.139000	-3.076000	-1.627000
C	-0.732000	-4.994000	-1.182000
H	-0.012000	-5.254000	-0.403000
H	-0.407000	-5.466000	-2.112000
H	-1.698000	-5.424000	-0.905000
C	-1.806000	-3.143000	-2.524000
H	-2.780000	-3.620000	-2.383000
H	-1.395000	-3.514000	-3.465000
H	-1.972000	-2.071000	-2.624000
C	-0.926000	1.567000	-1.744000
C	-0.057000	0.363000	-2.116000
C	-2.666000	2.500000	0.467000
C	-2.789000	2.462000	1.857000
H	-2.485000	1.577000	2.399000
C	-3.266000	3.576000	2.544000
H	-3.354000	3.545000	3.624000
C	-3.613000	4.730000	1.847000
H	-3.978000	5.598000	2.384000
C	-3.489000	4.773000	0.458000
H	-3.760000	5.670000	-0.085000
C	-3.023000	3.660000	-0.233000
H	-2.948000	3.696000	-1.314000
C	-3.665000	0.500000	-1.324000
C	-3.667000	0.098000	-2.664000
H	-2.768000	0.163000	-3.263000
C	-4.835000	-0.381000	-3.254000
H	-4.825000	-0.681000	-4.295000
C	-6.010000	-0.469000	-2.511000
H	-6.917000	-0.842000	-2.972000
C	-6.019000	-0.060000	-1.178000
H	-6.936000	-0.106000	-0.602000

C	-4.856000	0.426000	-0.588000
H	-4.881000	0.774000	0.439000
C	1.748000	-0.459000	-0.768000
C	3.707000	-1.105000	0.564000
C	4.410000	-0.224000	1.385000
H	3.886000	0.595000	1.863000
C	5.781000	-0.382000	1.546000
H	6.323000	0.312000	2.179000
C	6.478000	-1.403000	0.888000
C	5.754000	-2.277000	0.073000
H	6.269000	-3.083000	-0.439000
C	4.376000	-2.142000	-0.080000
H	3.820000	-2.844000	-0.692000
C	7.966000	-1.562000	1.079000
H	8.406000	-2.190000	0.302000
H	8.184000	-2.028000	2.045000
H	8.472000	-0.594000	1.062000
C	3.426000	1.046000	-1.624000
C	2.966000	2.102000	-0.835000
H	2.013000	2.035000	-0.323000
C	3.761000	3.232000	-0.662000
H	3.394000	4.037000	-0.035000
C	5.014000	3.347000	-1.267000
C	5.454000	2.277000	-2.055000
H	6.428000	2.329000	-2.531000
C	4.678000	1.138000	-2.233000
H	5.052000	0.315000	-2.832000
C	5.857000	4.587000	-1.101000
H	6.922000	4.344000	-1.065000
H	5.602000	5.124000	-0.185000
H	5.709000	5.276000	-1.939000
H	-1.415000	1.994000	-2.621000
H	-0.313000	2.341000	-1.278000
H	-0.642000	-0.383000	-2.658000
H	0.770000	0.668000	-2.753000
H	1.750000	-0.757000	1.215000
H	3.157000	-0.906000	-2.166000
91			
5	G=-2185.315088		
Os	1.024000	0.406000	0.583000
P	2.652000	-0.875000	-0.530000
N	-0.281000	-0.826000	-0.580000
N	-2.156000	-0.572000	0.769000
N	-2.431000	-0.966000	-1.524000
C	1.632000	1.794000	2.257000
C	2.385000	2.097000	1.101000
H	3.466000	2.061000	1.140000
C	1.743000	2.337000	-0.155000
H	2.356000	2.463000	-1.036000
C	0.327000	2.321000	-0.265000
C	-0.437000	2.123000	0.940000
H	-1.517000	2.097000	0.886000
C	0.195000	1.840000	2.152000
H	-0.404000	1.589000	3.019000
C	2.279000	1.521000	3.587000
H	3.342000	1.299000	3.483000

H	1.790000	0.696000	4.108000
H	2.188000	2.408000	4.220000
C	-0.419000	2.588000	-1.560000
H	-1.241000	1.863000	-1.593000
C	-1.033000	4.001000	-1.501000
H	-1.698000	4.122000	-0.643000
H	-1.613000	4.194000	-2.406000
H	-0.250000	4.760000	-1.434000
C	0.433000	2.407000	-2.817000
H	1.196000	3.185000	-2.902000
H	-0.196000	2.477000	-3.706000
H	0.938000	1.440000	-2.829000
C	1.646000	-2.042000	-1.559000
C	0.265000	-1.437000	-1.816000
C	3.676000	-1.921000	0.566000
C	3.941000	-1.501000	1.878000
H	3.551000	-0.551000	2.226000
C	4.733000	-2.279000	2.721000
H	4.939000	-1.945000	3.731000
C	5.266000	-3.481000	2.258000
H	5.882000	-4.087000	2.910000
C	5.014000	-3.898000	0.951000
H	5.438000	-4.827000	0.588000
C	4.224000	-3.124000	0.105000
H	4.052000	-3.458000	-0.912000
C	3.809000	0.030000	-1.604000
C	3.509000	0.272000	-2.950000
H	2.620000	-0.146000	-3.408000
C	4.369000	1.044000	-3.728000
H	4.140000	1.216000	-4.772000
C	5.525000	1.583000	-3.167000
H	6.194000	2.180000	-3.775000
C	5.831000	1.340000	-1.828000
H	6.740000	1.741000	-1.397000
C	4.979000	0.565000	-1.046000
H	5.241000	0.355000	-0.016000
C	-1.622000	-0.779000	-0.461000
C	-3.366000	0.102000	1.117000
C	-3.974000	-0.230000	2.328000
H	-3.555000	-1.016000	2.947000
C	-5.124000	0.438000	2.731000
H	-5.585000	0.172000	3.675000
C	-5.706000	1.432000	1.935000
C	-5.081000	1.748000	0.725000
H	-5.507000	2.515000	0.088000
C	-3.919000	1.101000	0.315000
H	-3.463000	1.365000	-0.630000
C	-6.981000	2.115000	2.358000
H	-7.022000	2.248000	3.440000
H	-7.850000	1.515000	2.069000
H	-7.087000	3.095000	1.888000
C	-3.801000	-1.395000	-1.541000
C	-4.265000	-2.377000	-0.668000
H	-3.596000	-2.831000	0.052000
C	-5.596000	-2.768000	-0.729000
H	-5.952000	-3.533000	-0.047000

C	-6.481000	-2.211000	-1.660000
C	-5.985000	-1.243000	-2.539000
H	-6.644000	-0.802000	-3.278000
C	-4.659000	-0.828000	-2.480000
H	-4.297000	-0.064000	-3.160000
C	-7.928000	-2.630000	-1.698000
H	-8.371000	-2.455000	-2.679000
H	-8.511000	-2.062000	-0.966000
H	-8.042000	-3.688000	-1.455000
H	2.149000	-2.298000	-2.493000
H	1.548000	-2.960000	-0.975000
H	0.333000	-0.682000	-2.609000
H	-0.398000	-2.230000	-2.169000
H	-1.517000	-0.730000	1.534000
H	-2.021000	-0.803000	-2.432000
O	0.774000	-1.393000	1.923000
H	1.585000	-1.681000	2.375000
H	0.469000	-2.155000	1.407000
91			
5a	G=-2185.311182		
Os	0.978000	0.245000	1.000000
P	1.030000	-1.425000	-0.710000
N	-2.013000	-1.384000	0.432000
N	-1.044000	0.779000	0.332000
N	-3.361000	0.507000	0.042000
C	2.607000	0.161000	2.528000
C	3.185000	0.121000	1.240000
H	3.808000	-0.719000	0.961000
C	2.883000	1.128000	0.272000
H	3.284000	1.027000	-0.726000
C	2.040000	2.220000	0.582000
C	1.492000	2.278000	1.912000
H	0.816000	3.084000	2.161000
C	1.763000	1.282000	2.854000
H	1.293000	1.324000	3.830000
C	2.882000	-0.902000	3.553000
H	3.344000	-1.781000	3.105000
H	1.966000	-1.211000	4.062000
H	3.566000	-0.505000	4.308000
C	1.853000	3.400000	-0.347000
H	0.844000	3.782000	-0.190000
C	2.844000	4.501000	0.092000
H	2.698000	4.789000	1.135000
H	2.700000	5.391000	-0.525000
H	3.878000	4.169000	-0.029000
C	2.025000	3.064000	-1.828000
H	3.061000	2.820000	-2.075000
H	1.742000	3.926000	-2.435000
H	1.398000	2.223000	-2.121000
C	-0.564000	-1.593000	-1.640000
C	-1.692000	-2.181000	-0.803000
C	1.378000	-3.139000	-0.172000
C	1.449000	-4.151000	-1.144000
H	1.324000	-3.918000	-2.195000
C	1.715000	-5.462000	-0.767000
H	1.774000	-6.237000	-1.522000

C	1.917000	-5.777000	0.578000
H	2.129000	-6.799000	0.868000
C	1.854000	-4.777000	1.544000
H	2.014000	-5.019000	2.588000
C	1.584000	-3.460000	1.173000
H	1.522000	-2.692000	1.928000
C	2.271000	-1.101000	-2.013000
C	1.966000	-0.290000	-3.113000
H	0.969000	0.111000	-3.249000
C	2.946000	0.010000	-4.056000
H	2.698000	0.628000	-4.910000
C	4.239000	-0.488000	-3.904000
H	4.999000	-0.255000	-4.640000
C	4.548000	-1.299000	-2.813000
H	5.547000	-1.702000	-2.702000
C	3.570000	-1.609000	-1.872000
H	3.812000	-2.269000	-1.047000
C	-2.123000	0.023000	0.251000
C	-1.287000	2.171000	0.021000
C	-1.277000	2.599000	-1.306000
H	-1.062000	1.890000	-2.097000
C	-1.531000	3.933000	-1.610000
H	-1.511000	4.254000	-2.645000
C	-1.806000	4.868000	-0.604000
C	-1.832000	4.416000	0.722000
H	-2.054000	5.116000	1.520000
C	-1.584000	3.082000	1.036000
H	-1.623000	2.743000	2.065000
C	-2.102000	6.307000	-0.938000
H	-1.630000	6.607000	-1.874000
H	-1.760000	6.979000	-0.149000
H	-3.181000	6.458000	-1.051000
C	-4.543000	-0.303000	-0.123000
C	-4.919000	-0.732000	-1.395000
H	-4.324000	-0.452000	-2.257000
C	-6.069000	-1.499000	-1.547000
H	-6.361000	-1.828000	-2.538000
C	-6.863000	-1.846000	-0.445000
C	-6.468000	-1.398000	0.821000
H	-7.071000	-1.647000	1.687000
C	-5.321000	-0.627000	0.989000
H	-5.039000	-0.266000	1.972000
C	-8.127000	-2.644000	-0.624000
H	-8.358000	-3.234000	0.264000
H	-8.058000	-3.319000	-1.479000
H	-8.974000	-1.973000	-0.803000
H	-0.837000	-0.613000	-2.034000
H	-0.391000	-2.250000	-2.494000
H	-2.592000	-2.257000	-1.419000
H	-1.429000	-3.182000	-0.458000
H	-2.909000	-1.729000	0.775000
H	-3.461000	1.514000	-0.009000
O	-0.170000	-1.138000	2.265000
H	-0.941000	-1.445000	1.687000
H	-0.539000	-0.726000	3.054000

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5b  G=-2185.276704
Os   -1.245000   -0.828000    0.079000
P    -1.206000    1.490000   -0.308000
N    -0.511000   -0.720000   -1.924000
N     0.869000   -0.971000   -0.263000
N     1.820000   -0.644000   -2.473000
C    -1.873000   -1.407000    2.189000
C    -2.919000   -0.699000    1.533000
H    -3.298000    0.214000    1.976000
C    -3.459000   -1.129000    0.290000
H    -4.235000   -0.539000   -0.171000
C    -2.908000   -2.253000   -0.384000
C    -1.855000   -2.982000    0.264000
H    -1.403000   -3.829000   -0.236000
C    -1.356000   -2.555000    1.514000
H    -0.504000   -3.070000    1.942000
C    -1.417000   -1.021000    3.569000
H    -1.495000    0.055000    3.730000
H    -0.391000   -1.340000    3.760000
H    -2.051000   -1.512000    4.313000
C    -3.404000   -2.729000   -1.737000
H    -2.508000   -2.913000   -2.340000
C    -4.155000   -4.064000   -1.556000
H    -3.528000   -4.829000   -1.094000
H    -4.481000   -4.441000   -2.528000
H    -5.041000   -3.928000   -0.931000
C    -4.284000   -1.713000   -2.472000
H    -5.250000   -1.587000   -1.976000
H    -4.484000   -2.063000   -3.486000
H    -3.807000   -0.734000   -2.544000
C    -0.856000    1.706000   -2.141000
C    -0.970000    0.331000   -2.839000
C     0.095000    2.461000    0.566000
C     0.514000    2.023000    1.825000
H     0.074000    1.125000    2.242000
C     1.479000    2.737000    2.543000
H     1.749000    2.425000    3.547000
C     2.045000    3.892000    1.992000
H     2.784000    4.455000    2.550000
C     1.626000    4.337000    0.737000
H     2.042000    5.245000    0.317000
C     0.644000    3.638000    0.037000
H     0.308000    4.020000   -0.920000
C    -2.761000    2.381000    0.038000
C    -3.847000    2.203000   -0.832000
H    -3.742000    1.607000   -1.732000
C    -5.074000    2.794000   -0.548000
H    -5.905000    2.663000   -1.230000
C    -5.230000    3.559000    0.608000
H    -6.186000    4.020000    0.827000
C    -4.156000    3.737000    1.476000
H    -4.273000    4.339000    2.369000
C    -2.922000    3.151000    1.195000
H    -2.091000    3.309000    1.873000
C     0.784000   -0.790000   -1.587000
C     1.919000   -1.540000    0.461000

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C	1.950000	-1.344000	1.855000
H	1.138000	-0.794000	2.312000
C	2.952000	-1.922000	2.648000
H	2.930000	-1.766000	3.721000
C	3.970000	-2.692000	2.082000
C	3.928000	-2.883000	0.692000
H	4.689000	-3.495000	0.222000
C	2.933000	-2.332000	-0.106000
H	2.925000	-2.540000	-1.166000
C	5.052000	-3.324000	2.918000
H	4.977000	-3.030000	3.965000
H	6.045000	-3.042000	2.556000
H	4.990000	-4.415000	2.870000
C	3.039000	0.043000	-2.214000
C	3.045000	1.255000	-1.521000
H	2.114000	1.684000	-1.174000
C	4.250000	1.935000	-1.305000
H	4.228000	2.908000	-0.822000
C	5.470000	1.430000	-1.782000
C	5.436000	0.219000	-2.484000
H	6.360000	-0.195000	-2.872000
C	4.245000	-0.468000	-2.697000
H	4.250000	-1.406000	-3.239000
C	6.759000	2.185000	-1.596000
H	7.026000	2.710000	-2.518000
H	7.584000	1.510000	-1.359000
H	6.684000	2.929000	-0.802000
H	-1.526000	2.452000	-2.570000
H	0.164000	2.079000	-2.243000
H	-2.002000	0.110000	-3.103000
H	-0.398000	0.338000	-3.771000
H	1.609000	-0.856000	-3.438000
H	3.175000	0.028000	1.579000
O	3.655000	0.913000	1.415000
H	3.047000	1.639000	1.711000
H	3.834000	1.032000	0.434000
91			
5c	G=-2185.315718		
Os	0.677000	-0.907000	0.343000
P	2.349000	0.397000	-0.688000
N	-0.569000	0.201000	-0.997000
N	-2.266000	-1.393000	-1.035000
N	-2.771000	0.732000	-1.752000
C	1.102000	-2.726000	1.601000
C	1.885000	-1.651000	2.078000
H	2.962000	-1.748000	2.126000
C	1.277000	-0.396000	2.384000
H	1.912000	0.441000	2.645000
C	-0.129000	-0.211000	2.296000
C	-0.922000	-1.343000	1.902000
H	-1.994000	-1.227000	1.791000
C	-0.328000	-2.558000	1.548000
H	-0.943000	-3.369000	1.177000
C	1.710000	-4.045000	1.211000
H	2.789000	-3.975000	1.080000
H	1.262000	-4.432000	0.293000

H	1.519000	-4.775000	2.002000
C	-0.813000	1.059000	2.759000
H	-1.800000	1.073000	2.287000
C	-1.028000	0.961000	4.283000
H	-1.583000	0.061000	4.557000
H	-1.593000	1.826000	4.637000
H	-0.071000	0.945000	4.810000
C	-0.073000	2.342000	2.376000
H	0.893000	2.424000	2.878000
H	-0.663000	3.212000	2.668000
H	0.100000	2.391000	1.301000
C	1.417000	1.294000	-2.011000
C	-0.042000	1.457000	-1.590000
C	3.633000	-0.571000	-1.561000
C	3.947000	-1.872000	-1.144000
H	3.441000	-2.298000	-0.285000
C	4.931000	-2.606000	-1.804000
H	5.173000	-3.609000	-1.472000
C	5.610000	-2.044000	-2.883000
H	6.377000	-2.611000	-3.396000
C	5.310000	-0.746000	-3.296000
H	5.845000	-0.304000	-4.128000
C	4.327000	-0.009000	-2.640000
H	4.117000	1.003000	-2.967000
C	3.236000	1.598000	0.350000
C	2.807000	2.925000	0.461000
H	1.969000	3.292000	-0.120000
C	3.465000	3.798000	1.323000
H	3.138000	4.829000	1.396000
C	4.545000	3.352000	2.082000
H	5.057000	4.035000	2.749000
C	4.978000	2.031000	1.972000
H	5.830000	1.688000	2.547000
C	4.330000	1.154000	1.107000
H	4.694000	0.138000	1.003000
C	-1.846000	-0.115000	-1.238000
C	-3.584000	-1.809000	-0.663000
C	-4.060000	-3.032000	-1.136000
H	-3.458000	-3.621000	-1.819000
C	-5.312000	-3.487000	-0.735000
H	-5.669000	-4.442000	-1.104000
C	-6.123000	-2.732000	0.120000
C	-5.628000	-1.505000	0.577000
H	-6.233000	-0.901000	1.245000
C	-4.369000	-1.045000	0.206000
H	-4.010000	-0.093000	0.580000
C	-7.497000	-3.211000	0.510000
H	-7.541000	-4.300000	0.563000
H	-8.238000	-2.888000	-0.229000
H	-7.802000	-2.808000	1.478000
C	-2.947000	2.124000	-1.470000
C	-2.676000	2.644000	-0.207000
H	-2.308000	1.993000	0.574000
C	-2.879000	3.998000	0.043000
H	-2.663000	4.392000	1.029000
C	-3.377000	4.852000	-0.946000

C	-3.656000	4.303000	-2.205000
H	-4.045000	4.942000	-2.990000
C	-3.439000	2.957000	-2.475000
H	-3.648000	2.555000	-3.459000
C	-3.639000	6.309000	-0.668000
H	-4.711000	6.486000	-0.534000
H	-3.309000	6.937000	-1.499000
H	-3.132000	6.645000	0.238000
H	1.868000	2.259000	-2.245000
H	1.492000	0.674000	-2.909000
H	-0.143000	2.269000	-0.868000
H	-0.633000	1.737000	-2.462000
H	-1.544000	-2.098000	-0.994000
H	-3.577000	0.271000	-2.157000
O	0.799000	-2.163000	-1.541000
H	1.690000	-2.499000	-1.742000
H	0.510000	-1.675000	-2.327000
91			
5ts	G=-2185.295678		
Os	0.841000	-0.886000	-0.483000
P	2.026000	1.014000	0.265000
N	-0.517000	-0.237000	1.028000
N	-2.414000	-0.990000	-0.081000
N	-2.711000	0.240000	1.869000
C	1.462000	-2.032000	-2.328000
C	2.572000	-1.906000	-1.465000
H	3.481000	-1.441000	-1.820000
C	2.475000	-2.293000	-0.089000
H	3.312000	-2.090000	0.565000
C	1.285000	-2.858000	0.439000
C	0.188000	-3.062000	-0.471000
H	-0.741000	-3.468000	-0.091000
C	0.269000	-2.651000	-1.807000
H	-0.597000	-2.745000	-2.453000
C	1.512000	-1.598000	-3.766000
H	2.369000	-0.954000	-3.965000
H	0.597000	-1.075000	-4.054000
H	1.604000	-2.480000	-4.407000
C	1.139000	-3.327000	1.875000
H	0.150000	-2.994000	2.208000
C	1.160000	-4.870000	1.894000
H	0.377000	-5.301000	1.267000
H	1.008000	-5.230000	2.914000
H	2.124000	-5.247000	1.544000
C	2.192000	-2.756000	2.827000
H	3.185000	-3.160000	2.617000
H	1.946000	-3.026000	3.855000
H	2.253000	-1.669000	2.767000
C	0.944000	1.677000	1.611000
C	0.085000	0.528000	2.146000
C	2.177000	2.331000	-0.994000
C	2.313000	1.982000	-2.347000
H	2.343000	0.936000	-2.633000
C	2.444000	2.972000	-3.320000
H	2.555000	2.696000	-4.362000
C	2.443000	4.315000	-2.948000

H	2.547000	5.086000	-3.702000
C	2.318000	4.667000	-1.605000
H	2.328000	5.711000	-1.315000
C	2.185000	3.683000	-0.628000
H	2.101000	3.977000	0.412000
C	3.699000	0.728000	0.920000
C	3.915000	0.489000	2.282000
H	3.103000	0.548000	2.996000
C	5.195000	0.188000	2.742000
H	5.359000	0.016000	3.799000
C	6.262000	0.116000	1.848000
H	7.256000	-0.114000	2.209000
C	6.052000	0.359000	0.491000
H	6.884000	0.325000	-0.202000
C	4.777000	0.666000	0.025000
H	4.632000	0.885000	-1.027000
C	-1.835000	-0.353000	0.953000
C	-3.804000	-1.284000	-0.287000
C	-4.331000	-1.055000	-1.558000
H	-3.708000	-0.627000	-2.337000
C	-5.659000	-1.372000	-1.823000
H	-6.059000	-1.194000	-2.814000
C	-6.485000	-1.908000	-0.830000
C	-5.930000	-2.135000	0.437000
H	-6.546000	-2.563000	1.219000
C	-4.601000	-1.837000	0.713000
H	-4.191000	-2.031000	1.695000
C	-7.934000	-2.218000	-1.100000
H	-8.242000	-3.143000	-0.607000
H	-8.132000	-2.318000	-2.168000
H	-8.574000	-1.416000	-0.717000
C	-3.070000	1.604000	1.615000
C	-3.252000	2.081000	0.314000
H	-3.227000	1.406000	-0.532000
C	-3.578000	3.422000	0.107000
H	-3.735000	3.771000	-0.908000
C	-3.744000	4.311000	1.170000
C	-3.570000	3.808000	2.465000
H	-3.701000	4.467000	3.316000
C	-3.232000	2.478000	2.692000
H	-3.105000	2.120000	3.709000
C	-4.142000	5.748000	0.945000
H	-3.938000	6.066000	-0.079000
H	-3.612000	6.420000	1.624000
H	-5.213000	5.883000	1.126000
H	1.523000	2.149000	2.405000
H	0.299000	2.438000	1.165000
H	0.689000	-0.167000	2.733000
H	-0.674000	0.945000	2.804000
H	-1.797000	-1.261000	-0.833000
H	-2.504000	0.049000	2.839000
O	-0.385000	0.587000	-1.662000
H	0.158000	1.216000	-2.170000
H	-0.995000	1.129000	-1.133000

73

1 G=-1973.168599

Os	-1.231000	-0.977000	-0.078000
N	-2.548000	0.084000	1.179000
N	0.018000	0.434000	0.868000
N	1.887000	-0.909000	1.053000
H	1.263000	-1.664000	1.330000
N	2.127000	1.396000	1.303000
H	3.006000	1.170000	1.749000
C	-0.274000	-2.475000	-1.434000
C	-1.667000	-2.794000	-1.251000
H	-1.932000	-3.752000	-0.822000
C	-2.678000	-1.851000	-1.512000
H	-3.711000	-2.111000	-1.319000
C	-2.350000	-0.509000	-1.920000
C	-0.980000	-0.187000	-2.115000
H	-0.694000	0.817000	-2.389000
C	0.038000	-1.166000	-1.866000
H	1.080000	-0.873000	-1.925000
C	0.789000	-3.483000	-1.101000
H	0.559000	-3.977000	-0.155000
H	1.770000	-3.014000	-1.020000
H	0.838000	-4.246000	-1.884000
C	-3.471000	0.490000	-2.135000
H	-4.251000	0.242000	-1.405000
C	-4.058000	0.293000	-3.545000
H	-3.311000	0.526000	-4.309000
H	-4.915000	0.954000	-3.696000
H	-4.391000	-0.735000	-3.702000
C	-3.060000	1.947000	-1.898000
H	-2.597000	2.075000	-0.919000
H	-3.939000	2.593000	-1.945000
H	-2.361000	2.299000	-2.661000
C	-3.788000	-0.344000	1.492000
H	-4.082000	-1.291000	1.063000
C	-4.625000	0.371000	2.331000
H	-5.611000	-0.013000	2.554000
C	-4.164000	1.563000	2.884000
H	-4.793000	2.142000	3.549000
C	-2.875000	1.987000	2.586000
H	-2.473000	2.897000	3.013000
C	-2.085000	1.225000	1.734000
C	-0.687000	1.619000	1.347000
H	-0.735000	2.386000	0.561000
H	-0.172000	2.072000	2.198000
C	1.316000	0.322000	1.056000
C	3.202000	-1.239000	0.640000
C	3.827000	-2.347000	1.216000
H	3.320000	-2.902000	1.998000
C	5.089000	-2.736000	0.783000
H	5.556000	-3.604000	1.236000
C	5.770000	-2.028000	-0.213000
C	5.130000	-0.920000	-0.777000
H	5.627000	-0.358000	-1.561000
C	3.858000	-0.530000	-0.372000
H	3.379000	0.319000	-0.846000
C	7.158000	-2.432000	-0.643000
H	7.290000	-3.515000	-0.595000

H	7.913000	-1.981000	0.009000
H	7.370000	-2.109000	-1.664000
C	2.089000	2.641000	0.613000
C	2.634000	3.769000	1.229000
H	3.047000	3.689000	2.228000
C	2.641000	4.988000	0.562000
H	3.073000	5.854000	1.053000
C	2.093000	5.125000	-0.719000
C	1.544000	3.987000	-1.315000
H	1.117000	4.059000	-2.310000
C	1.548000	2.754000	-0.668000
H	1.129000	1.882000	-1.156000
C	2.123000	6.452000	-1.434000
H	1.419000	6.476000	-2.267000
H	3.121000	6.652000	-1.838000
H	1.877000	7.274000	-0.757000
Cl	-0.891000	-2.350000	1.903000
73			
1b	G=-1973.164690		
Os	1.728000	-0.445000	-0.306000
N	2.695000	1.410000	-0.554000
N	0.255000	0.958000	0.262000
N	-1.564000	-0.211000	-0.540000
H	-0.998000	-0.422000	-1.359000
N	-1.892000	1.566000	0.969000
H	-1.511000	1.980000	1.806000
C	1.163000	-2.610000	-0.375000
C	2.486000	-2.426000	-0.914000
H	2.680000	-2.722000	-1.937000
C	3.494000	-1.777000	-0.178000
H	4.465000	-1.618000	-0.631000
C	3.221000	-1.221000	1.122000
C	1.920000	-1.400000	1.663000
H	1.663000	-0.965000	2.618000
C	0.909000	-2.088000	0.913000
H	-0.102000	-2.132000	1.302000
C	0.093000	-3.271000	-1.197000
H	0.106000	-2.881000	-2.217000
H	-0.897000	-3.105000	-0.772000
H	0.272000	-4.349000	-1.241000
C	4.330000	-0.489000	1.854000
H	4.943000	-0.006000	1.085000
C	5.210000	-1.517000	2.589000
H	4.638000	-2.028000	3.368000
H	6.060000	-1.021000	3.062000
H	5.599000	-2.275000	1.904000
C	3.835000	0.604000	2.806000
H	3.178000	1.309000	2.293000
H	4.684000	1.163000	3.204000
H	3.296000	0.185000	3.660000
C	3.844000	1.564000	-1.242000
H	4.250000	0.668000	-1.687000
C	4.455000	2.797000	-1.391000
H	5.377000	2.871000	-1.953000
C	3.854000	3.919000	-0.827000
H	4.304000	4.899000	-0.931000

C	2.651000	3.764000	-0.147000
H	2.140000	4.616000	0.284000
C	2.091000	2.499000	-0.030000
C	0.795000	2.245000	0.692000
H	0.994000	2.247000	1.775000
H	0.096000	3.061000	0.484000
C	-1.053000	0.774000	0.240000
C	-2.688000	-1.031000	-0.282000
C	-3.377000	-1.577000	-1.367000
H	-3.070000	-1.328000	-2.377000
C	-4.451000	-2.431000	-1.149000
H	-4.973000	-2.850000	-2.002000
C	-4.879000	-2.749000	0.145000
C	-4.175000	-2.195000	1.218000
H	-4.477000	-2.431000	2.233000
C	-3.085000	-1.354000	1.016000
H	-2.553000	-0.945000	1.865000
C	-6.077000	-3.636000	0.371000
H	-6.161000	-4.401000	-0.404000
H	-7.002000	-3.049000	0.353000
H	-6.027000	-4.139000	1.339000
C	-3.266000	1.843000	0.698000
C	-3.720000	2.034000	-0.606000
H	-3.028000	1.966000	-1.437000
C	-5.065000	2.298000	-0.832000
H	-5.410000	2.434000	-1.851000
C	-5.978000	2.403000	0.223000
C	-5.497000	2.226000	1.524000
H	-6.181000	2.298000	2.362000
C	-4.158000	1.938000	1.765000
H	-3.810000	1.774000	2.779000
C	-7.428000	2.726000	-0.037000
H	-7.568000	3.805000	-0.157000
H	-8.065000	2.400000	0.787000
H	-7.783000	2.247000	-0.952000
Cl	0.963000	-0.039000	-2.582000
73			
1ts	G=-1973.153480		
Os	1.728000	-0.489000	-0.308000
N	2.101000	1.587000	-0.302000
N	0.161000	0.299000	0.863000
N	-1.508000	-1.161000	0.206000
H	-0.950000	-1.369000	-0.615000
N	-2.010000	0.607000	1.729000
H	-2.411000	0.033000	2.458000
C	1.692000	-2.697000	-0.668000
C	2.688000	-2.076000	-1.499000
H	2.598000	-2.164000	-2.575000
C	3.702000	-1.263000	-0.958000
H	4.409000	-0.780000	-1.620000
C	3.745000	-0.985000	0.454000
C	2.774000	-1.598000	1.290000
H	2.754000	-1.387000	2.349000
C	1.757000	-2.432000	0.721000
H	0.968000	-2.807000	1.362000
C	0.605000	-3.537000	-1.278000

H	0.221000	-3.065000	-2.186000
H	-0.222000	-3.683000	-0.581000
H	0.998000	-4.521000	-1.547000
C	4.833000	-0.070000	0.984000
H	5.016000	0.678000	0.204000
C	6.124000	-0.889000	1.171000
H	5.987000	-1.654000	1.939000
H	6.943000	-0.238000	1.482000
H	6.422000	-1.389000	0.246000
C	4.457000	0.678000	2.266000
H	3.522000	1.228000	2.148000
H	5.240000	1.395000	2.520000
H	4.355000	-0.001000	3.117000
C	2.892000	2.212000	-1.196000
H	3.344000	1.582000	-1.948000
C	3.093000	3.582000	-1.167000
H	3.739000	4.042000	-1.903000
C	2.439000	4.338000	-0.198000
H	2.569000	5.413000	-0.157000
C	1.596000	3.696000	0.701000
H	1.048000	4.252000	1.452000
C	1.444000	2.318000	0.627000
C	0.569000	1.526000	1.557000
H	1.151000	1.252000	2.446000
H	-0.290000	2.108000	1.886000
C	-1.080000	-0.098000	0.927000
C	-2.871000	-1.603000	0.188000
C	-3.658000	-1.365000	-0.937000
H	-3.234000	-0.840000	-1.785000
C	-4.986000	-1.774000	-0.943000
H	-5.595000	-1.583000	-1.820000
C	-5.557000	-2.406000	0.169000
C	-4.747000	-2.643000	1.283000
H	-5.161000	-3.149000	2.148000
C	-3.408000	-2.257000	1.292000
H	-2.780000	-2.475000	2.149000
C	-7.013000	-2.800000	0.161000
H	-7.650000	-1.920000	0.291000
H	-7.245000	-3.500000	0.966000
H	-7.292000	-3.267000	-0.787000
C	-2.998000	1.354000	1.010000
C	-2.675000	1.971000	-0.200000
H	-1.688000	1.856000	-0.634000
C	-3.645000	2.703000	-0.880000
H	-3.383000	3.163000	-1.827000
C	-4.939000	2.851000	-0.377000
C	-5.237000	2.229000	0.841000
H	-6.236000	2.317000	1.255000
C	-4.286000	1.485000	1.529000
H	-4.550000	0.991000	2.457000
C	-5.976000	3.671000	-1.103000
H	-6.973000	3.238000	-0.997000
H	-5.751000	3.745000	-2.169000
H	-6.019000	4.690000	-0.704000
C1	0.329000	0.055000	-2.218000

2c-delta G=-2569.440168

Os	0.680000	-0.971000	0.240000
P	2.315000	0.574000	-0.421000
Cl	0.730000	-2.173000	-1.897000
N	-0.562000	0.345000	-0.938000
N	-2.307000	-1.173000	-1.109000
N	-2.721000	1.025000	-1.681000
C	1.334000	-2.800000	1.323000
C	1.854000	-1.665000	1.988000
H	2.925000	-1.558000	2.104000
C	1.005000	-0.592000	2.403000
H	1.458000	0.292000	2.828000
C	-0.393000	-0.636000	2.160000
C	-0.935000	-1.848000	1.597000
H	-1.999000	-1.913000	1.413000
C	-0.099000	-2.888000	1.187000
H	-0.519000	-3.729000	0.649000
C	2.217000	-3.906000	0.819000
H	3.258000	-3.585000	0.773000
H	1.905000	-4.212000	-0.182000
H	2.154000	-4.772000	1.484000
C	-1.351000	0.468000	2.565000
H	-2.047000	0.590000	1.729000
C	-2.165000	0.023000	3.794000
H	-2.712000	-0.904000	3.604000
H	-2.893000	0.792000	4.063000
H	-1.510000	-0.140000	4.654000
C	-0.670000	1.814000	2.817000
H	-0.050000	1.789000	3.717000
H	-1.423000	2.592000	2.958000
H	-0.036000	2.102000	1.978000
C	1.312000	1.959000	-1.113000
C	0.130000	1.316000	-1.825000
C	3.552000	0.108000	-1.683000
C	3.900000	-1.235000	-1.851000
H	3.367000	-2.001000	-1.305000
C	4.911000	-1.590000	-2.741000
H	5.169000	-2.634000	-2.872000
C	5.575000	-0.608000	-3.471000
H	6.356000	-0.885000	-4.169000
C	5.237000	0.735000	-3.304000
H	5.757000	1.502000	-3.865000
C	4.235000	1.094000	-2.408000
H	4.005000	2.144000	-2.269000
C	3.351000	1.255000	0.934000
C	2.942000	2.347000	1.709000
H	2.026000	2.877000	1.482000
C	3.715000	2.779000	2.784000
H	3.392000	3.634000	3.368000
C	4.900000	2.122000	3.104000
H	5.500000	2.459000	3.941000
C	5.318000	1.037000	2.336000
H	6.246000	0.529000	2.570000
C	4.552000	0.608000	1.255000
H	4.901000	-0.220000	0.649000
C	-1.831000	0.095000	-1.216000

C	-3.612000	-1.586000	-0.749000
C	-4.070000	-2.828000	-1.199000
H	-3.447000	-3.423000	-1.858000
C	-5.319000	-3.292000	-0.805000
H	-5.656000	-4.260000	-1.159000
C	-6.151000	-2.535000	0.027000
C	-5.677000	-1.296000	0.468000
H	-6.293000	-0.691000	1.124000
C	-4.421000	-0.823000	0.100000
H	-4.075000	0.133000	0.475000
C	-7.523000	-3.030000	0.413000
H	-7.538000	-4.117000	0.523000
H	-8.258000	-2.770000	-0.355000
H	-7.858000	-2.588000	1.353000
C	-2.859000	2.388000	-1.315000
C	-2.156000	2.963000	-0.256000
H	-1.449000	2.372000	0.305000
C	-2.371000	4.297000	0.078000
H	-1.817000	4.724000	0.907000
C	-3.281000	5.092000	-0.622000
C	-3.979000	4.497000	-1.680000
H	-4.696000	5.084000	-2.243000
C	-3.773000	3.169000	-2.030000
H	-4.325000	2.736000	-2.857000
C	-3.491000	6.545000	-0.276000
H	-4.548000	6.814000	-0.321000
H	-2.959000	7.194000	-0.979000
H	-3.126000	6.774000	0.727000
H	0.962000	2.584000	-0.291000
H	1.889000	2.582000	-1.796000
H	-0.545000	2.091000	-2.182000
H	0.484000	0.748000	-2.692000
H	-1.609000	-1.889000	-1.288000
H	-3.518000	0.631000	-2.160000
89			
2ts-ld G=-2569.434727			
Os	0.723000	-0.863000	0.317000
P	2.313000	0.598000	-0.555000
Cl	0.725000	-2.145000	-1.778000
N	-0.617000	0.409000	-0.805000
N	-2.208000	-1.283000	-0.977000
N	-2.781000	0.830000	-1.710000
C	1.456000	-2.643000	1.442000
C	2.000000	-1.473000	2.024000
H	3.074000	-1.353000	2.074000
C	1.163000	-0.391000	2.438000
H	1.626000	0.515000	2.800000
C	-0.245000	-0.461000	2.275000
C	-0.807000	-1.699000	1.798000
H	-1.878000	-1.778000	1.665000
C	0.018000	-2.746000	1.383000
H	-0.421000	-3.612000	0.903000
C	2.318000	-3.770000	0.949000
H	3.362000	-3.462000	0.875000
H	1.981000	-4.101000	-0.035000
H	2.260000	-4.616000	1.639000

C	-1.179000	0.649000	2.713000
H	-2.087000	0.536000	2.111000
C	-1.565000	0.435000	4.188000
H	-1.997000	-0.556000	4.349000
H	-2.300000	1.180000	4.501000
H	-0.688000	0.531000	4.834000
C	-0.617000	2.052000	2.474000
H	0.254000	2.249000	3.102000
H	-1.369000	2.805000	2.720000
H	-0.331000	2.180000	1.429000
C	1.352000	1.948000	-1.378000
C	-0.142000	1.622000	-1.536000
C	3.560000	-0.008000	-1.750000
C	3.917000	-1.359000	-1.765000
H	3.380000	-2.063000	-1.147000
C	4.943000	-1.802000	-2.597000
H	5.206000	-2.853000	-2.609000
C	5.615000	-0.901000	-3.418000
H	6.408000	-1.249000	-4.070000
C	5.268000	0.449000	-3.402000
H	5.794000	1.154000	-4.035000
C	4.250000	0.897000	-2.567000
H	4.013000	1.955000	-2.546000
C	3.363000	1.419000	0.718000
C	2.881000	2.493000	1.476000
H	1.902000	2.911000	1.281000
C	3.650000	3.037000	2.502000
H	3.268000	3.876000	3.071000
C	4.906000	2.507000	2.792000
H	5.504000	2.931000	3.589000
C	5.392000	1.437000	2.045000
H	6.372000	1.026000	2.257000
C	4.629000	0.897000	1.011000
H	5.030000	0.080000	0.423000
C	-1.841000	0.021000	-1.121000
C	-3.490000	-1.780000	-0.656000
C	-3.840000	-3.066000	-1.082000
H	-3.149000	-3.633000	-1.696000
C	-5.068000	-3.608000	-0.723000
H	-5.320000	-4.608000	-1.059000
C	-5.988000	-2.889000	0.048000
C	-5.623000	-1.605000	0.466000
H	-6.309000	-1.027000	1.074000
C	-4.389000	-1.054000	0.135000
H	-4.129000	-0.064000	0.489000
C	-7.337000	-3.470000	0.392000
H	-7.749000	-3.017000	1.296000
H	-7.277000	-4.549000	0.549000
H	-8.052000	-3.297000	-0.419000
C	-3.115000	2.175000	-1.386000
C	-3.014000	2.658000	-0.083000
H	-2.661000	2.006000	0.703000
C	-3.359000	3.976000	0.201000
H	-3.268000	4.339000	1.219000
C	-3.837000	4.832000	-0.795000
C	-3.947000	4.323000	-2.095000

H	-4.312000	4.966000	-2.890000
C	-3.583000	3.017000	-2.396000
H	-3.650000	2.648000	-3.413000
C	-4.251000	6.248000	-0.483000
H	-5.340000	6.325000	-0.406000
H	-3.931000	6.937000	-1.268000
H	-3.828000	6.591000	0.463000
H	1.488000	2.855000	-0.790000
H	1.793000	2.138000	-2.356000
H	-0.709000	2.493000	-1.207000
H	-0.371000	1.473000	-2.593000
H	-1.463000	-1.951000	-1.159000
H	-3.494000	0.322000	-2.215000