

Electronic Supporting Information

First α -Deuterium Nitroxides; Synthesis and EPR Study

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Computational Section

Calculations were performed by Gaussian 09, Revision D.01¹

Optimization and energies are calculated at level of theory – PBE0/TZVP//PBE0³/TZVP², spin densities are calculated at ub3lyp/BS level, where BS denotes a mixed basis set: EPR-III⁴ for C, H, N, O atoms and TZVP for Si atoms.

Cartesian coordinates (Å), zero point energy, sum of electronic and zero-point energies [Hartree/particle]

radical (1)

ZPE = 0.988718, E+ZPE=-2648.780960

O 2

6	-3.772708000	2.082267000	3.832538000
6	-2.842974000	1.052658000	3.950691000
6	-2.005427000	0.696696000	2.881675000
6	-2.124661000	1.395032000	1.658267000
6	-3.028461000	2.477601000	1.549258000
6	-3.852588000	2.794890000	2.638019000
6	-0.990679000	-0.396689000	3.115747000
7	0.114321000	1.660967000	0.723590000
6	-1.223446000	1.066062000	0.457641000
6	0.478441000	0.513015000	-2.791826000
6	1.361851000	1.681722000	-2.425088000
6	1.795928000	1.973142000	-1.107605000
6	1.379152000	1.152572000	0.132595000
6	1.771829000	2.516230000	-3.478159000
6	2.588475000	3.621147000	-3.259937000
6	3.013447000	3.904126000	-1.965135000
6	2.635086000	3.097776000	-0.881994000
6	1.352144000	-0.352777000	0.019821000
6	2.565744000	-1.047219000	-0.041253000
6	3.155417000	3.473747000	0.486541000
6	-1.138164000	-0.403874000	0.092642000
6	0.120164000	-1.071097000	-0.010957000
6	-3.094936000	3.349740000	0.318982000
6	-2.315808000	-1.114773000	-0.172765000
6	-2.272882000	-2.522455000	-0.358666000
6	-1.074323000	-3.196272000	-0.344539000
6	0.147303000	-2.497242000	-0.198996000
6	1.394777000	-3.162253000	-0.261795000

6	2.574480000	-2.460320000	-0.174263000
1	-4.415143000	2.344541000	4.675958000
1	-2.745457000	0.512568000	4.896052000
1	-4.549632000	3.631944000	2.547724000
1	-1.636820000	1.605762000	-0.414074000
1	0.977129000	-0.451037000	-2.614869000
1	1.431834000	2.283713000	-4.490538000
1	2.890105000	4.258683000	-4.093816000
1	3.656152000	4.768021000	-1.778778000
1	3.767570000	4.383542000	0.420055000
1	2.330845000	3.654049000	1.189574000
1	-2.118840000	3.821710000	0.127707000
1	-3.835931000	4.149375000	0.457240000
1	-3.204393000	-3.067424000	-0.506504000
1	-1.052291000	-4.281566000	-0.470268000
1	1.409159000	-4.246711000	-0.395889000
1	3.529252000	-2.983005000	-0.230592000
8	0.131363000	2.852989000	1.195345000
1	2.126026000	1.388297000	0.904171000
1	0.217083000	0.565504000	-3.857725000
1	-0.460253000	0.489118000	-2.221630000
1	3.792015000	2.681070000	0.912400000
1	-3.380025000	2.789177000	-0.584175000
8	3.725375000	-0.333570000	-0.003798000
8	-3.487518000	-0.427579000	-0.234614000
14	-5.125654000	-0.873982000	-0.586715000
14	5.352309000	-0.851579000	0.316153000
6	-5.931755000	-1.735156000	0.929023000
6	-5.908699000	0.859755000	-0.823999000
6	-5.205497000	-2.017390000	-2.135561000
6	-5.792702000	-0.885856000	2.204108000
6	-5.484230000	-3.182532000	1.190037000
6	-6.648124000	-2.141792000	-2.661989000
6	-4.233273000	-1.635594000	-3.263829000
6	-7.438339000	0.892593000	-0.659976000
6	-5.488623000	1.552038000	-2.131771000
6	5.298831000	-1.792424000	1.995200000
6	4.472794000	-1.025234000	3.042861000
6	6.670401000	-2.185158000	2.573169000
6	6.259411000	0.835161000	0.382087000
6	6.122422000	1.609234000	-0.941137000
6	7.741486000	0.728268000	0.781071000
6	6.058585000	-1.895163000	-1.150371000
6	6.205902000	-3.408674000	-0.922177000
6	5.321314000	-1.616262000	-2.474365000
1	-7.005232000	-1.767888000	0.657194000
1	-4.432183000	-3.226904000	1.509715000
1	-6.085424000	-3.629383000	1.999504000
1	-5.597673000	-3.829414000	0.306461000
1	-7.009890000	-1.190845000	-3.081950000
1	-6.700128000	-2.891089000	-3.469427000

1	-7.358716000	-2.453011000	-1.880724000
1	-4.482209000	-0.658232000	-3.701727000
1	-4.279282000	-2.378836000	-4.077607000
1	-3.191202000	-1.590017000	-2.916387000
1	-4.912643000	-3.019431000	-1.773058000
1	-5.469435000	1.432535000	0.013422000
1	-7.949905000	0.323906000	-1.451751000
1	-7.806199000	1.930524000	-0.720797000
1	-7.767748000	0.486265000	0.307329000
1	-4.400084000	1.529399000	-2.288179000
1	-5.802124000	2.609403000	-2.128786000
1	-5.960828000	1.079622000	-3.007269000
1	4.758584000	-2.729699000	1.767573000
1	3.450970000	-0.814681000	2.696580000
1	4.393972000	-1.608779000	3.975262000
1	4.943839000	-0.063490000	3.301638000
1	6.542971000	-2.880352000	3.419422000
1	7.327128000	-2.677988000	1.841117000
1	7.208708000	-1.307771000	2.960284000
1	5.734959000	1.409244000	1.167956000
1	6.535871000	2.626062000	-0.833629000
1	5.078604000	1.707516000	-1.268195000
1	6.689038000	1.117863000	-1.748193000
1	8.212275000	1.725217000	0.760464000
1	8.309175000	0.094799000	0.079927000
1	7.886492000	0.319126000	1.790004000
1	7.083017000	-1.487256000	-1.254365000
1	6.780429000	-3.650640000	-0.017086000
1	6.726245000	-3.873164000	-1.776507000
1	5.231230000	-3.914631000	-0.838629000
1	0.009944000	-0.109943000	2.761919000
1	-0.917808000	-0.616795000	4.190021000
1	-1.257145000	-1.330484000	2.598158000
1	-6.337088000	-1.353175000	3.041837000
1	-4.740273000	-0.785245000	2.507639000
1	-6.188110000	0.132901000	2.080833000
1	5.848944000	-2.098113000	-3.314467000
1	4.297784000	-2.019988000	-2.454600000
1	5.243082000	-0.543715000	-2.698607000

Radical (2)

ZPE = 0.981894, E+ZPE= -2648.787785

0 2

6	-3.772708000	2.082267000	3.832538000
6	-2.842974000	1.052658000	3.950691000
6	-2.005427000	0.696696000	2.881675000
6	-2.124661000	1.395032000	1.658267000
6	-3.028461000	2.477601000	1.549258000
6	-3.852588000	2.794890000	2.638019000
6	-0.990679000	-0.396689000	3.115747000
7	0.114321000	1.660967000	0.723590000
6	-1.223446000	1.066062000	0.457641000
6	0.478441000	0.513015000	-2.791826000
6	1.361851000	1.681722000	-2.425088000
6	1.795928000	1.973142000	-1.107605000
6	1.379152000	1.152572000	0.132595000
6	1.771829000	2.516230000	-3.478159000
6	2.588475000	3.621147000	-3.259937000
6	3.013447000	3.904126000	-1.965135000
6	2.635086000	3.097776000	-0.881994000
6	1.352144000	-0.352777000	0.019821000
6	2.565744000	-1.047219000	-0.041253000
6	3.155417000	3.473747000	0.486541000
6	-1.138164000	-0.403874000	0.092642000
6	0.120164000	-1.071097000	-0.010957000
6	-3.094936000	3.349740000	0.318982000
6	-2.315808000	-1.114773000	-0.172765000
6	-2.272882000	-2.522455000	-0.358666000
6	-1.074323000	-3.196272000	-0.344539000
6	0.147303000	-2.497242000	-0.198996000
6	1.394777000	-3.162253000	-0.261795000
6	2.574480000	-2.460320000	-0.174263000
1	-4.415143000	2.344541000	4.675958000
1	-2.745457000	0.512568000	4.896052000
1	-4.549632000	3.631944000	2.547724000
1	-1.636820000	1.605762000	-0.414074000
1	0.977129000	-0.451037000	-2.614869000
1	1.431834000	2.283713000	-4.490538000
1	2.890105000	4.258683000	-4.093816000
1	3.656152000	4.768021000	-1.778778000
1	3.767570000	4.383542000	0.420055000
1	2.330845000	3.654049000	1.189574000
1	-2.118840000	3.821710000	0.127707000
1	-3.835931000	4.149375000	0.457240000
1	-3.204393000	-3.067424000	-0.506504000
1	-1.052291000	-4.281566000	-0.470268000
1	1.409159000	-4.246711000	-0.395889000
1	3.529252000	-2.983005000	-0.230592000
8	0.131363000	2.852989000	1.195345000

1	2.126026000	1.388297000	0.904171000
1	0.217083000	0.565504000	-3.857725000
1	-0.460253000	0.489118000	-2.221630000
1	3.792015000	2.681070000	0.912400000
1	-3.380025000	2.789177000	-0.584175000
8	3.725375000	-0.333570000	-0.003798000
8	-3.487518000	-0.427579000	-0.234614000
14	-5.125654000	-0.873982000	-0.586715000
14	5.352309000	-0.851579000	0.316153000
6	-5.931755000	-1.735156000	0.929023000
6	-5.908699000	0.859755000	-0.823999000
6	-5.205497000	-2.017390000	-2.135561000
6	-5.792702000	-0.885856000	2.204108000
6	-5.484230000	-3.182532000	1.190037000
6	-6.648124000	-2.141792000	-2.661989000
6	-4.233273000	-1.635594000	-3.263829000
6	-7.438339000	0.892593000	-0.659976000
6	-5.488623000	1.552038000	-2.131771000
6	5.298831000	-1.792424000	1.995200000
6	4.472794000	-1.025234000	3.042861000
6	6.670401000	-2.185158000	2.573169000
6	6.259411000	0.835161000	0.382087000
6	6.122422000	1.609234000	-0.941137000
6	7.741486000	0.728268000	0.781071000
6	6.058585000	-1.895163000	-1.150371000
6	6.205902000	-3.408674000	-0.922177000
6	5.321314000	-1.616262000	-2.474365000
1	-7.005232000	-1.767888000	0.657194000
1	-4.432183000	-3.226904000	1.509715000
1	-6.085424000	-3.629383000	1.999504000
1	-5.597673000	-3.829414000	0.306461000
1	-7.009890000	-1.190845000	-3.081950000
1	-6.700128000	-2.891089000	-3.469427000
1	-7.358716000	-2.453011000	-1.880724000
1	-4.482209000	-0.658232000	-3.701727000
1	-4.279282000	-2.378836000	-4.077607000
1	-3.191202000	-1.590017000	-2.916387000
1	-4.912643000	-3.019431000	-1.773058000
1	-5.469435000	1.432535000	0.013422000
1	-7.949905000	0.323906000	-1.451751000
1	-7.806199000	1.930524000	-0.720797000
1	-7.767748000	0.486265000	0.307329000
1	-4.400084000	1.529399000	-2.288179000
1	-5.802124000	2.609403000	-2.128786000
1	-5.960828000	1.079622000	-3.007269000
1	4.758584000	-2.729699000	1.767573000
1	3.450970000	-0.814681000	2.696580000
1	4.393972000	-1.608779000	3.975262000
1	4.943839000	-0.063490000	3.301638000
1	6.542971000	-2.880352000	3.419422000
1	7.327128000	-2.677988000	1.841117000

1	7.208708000	-1.307771000	2.960284000
1	5.734959000	1.409244000	1.167956000
1	6.535871000	2.626062000	-0.833629000
1	5.078604000	1.707516000	-1.268195000
1	6.689038000	1.117863000	-1.748193000
1	8.212275000	1.725217000	0.760464000
1	8.309175000	0.094799000	0.079927000
1	7.886492000	0.319126000	1.790004000
1	7.083017000	-1.487256000	-1.254365000
1	6.780429000	-3.650640000	-0.017086000
1	6.726245000	-3.873164000	-1.776507000
1	5.231230000	-3.914631000	-0.838629000
1	0.009944000	-0.109943000	2.761919000
1	-0.917808000	-0.616795000	4.190021000
1	-1.257145000	-1.330484000	2.598158000
1	-6.337088000	-1.353175000	3.041837000
1	-4.740273000	-0.785245000	2.507639000
1	-6.188110000	0.132901000	2.080833000
1	5.848944000	-2.098113000	-3.314467000
1	4.297784000	-2.019988000	-2.454600000
1	5.243082000	-0.543715000	-2.698607000

Hydroxylamine (13)

ZPE = 0.982891, E+ZPE= -2727.942532

0 1			
14	4.825612000	-1.344522000	0.903758000
14	-5.474640000	-0.857243000	-0.510400000
8	3.382083000	-0.802679000	0.122085000
8	-3.808377000	-0.524086000	-0.208886000
8	-0.413423000	0.983536000	-2.374020000
7	-0.204367000	1.405543000	-0.983773000
6	2.190043000	-1.443661000	-0.064107000
6	2.123244000	-2.863270000	-0.021907000
1	3.044897000	-3.431301000	0.114387000
6	0.922413000	-3.517629000	-0.170290000
1	0.883905000	-4.609797000	-0.157948000
6	-0.283143000	-2.786112000	-0.295532000
6	-0.227308000	-1.351231000	-0.332622000
6	1.043120000	-0.688994000	-0.327737000
6	-1.545723000	-3.426175000	-0.330676000
1	-1.584987000	-4.518482000	-0.325606000
6	-2.711768000	-2.694413000	-0.345261000
1	-3.674629000	-3.204094000	-0.364730000
6	-2.669608000	-1.275850000	-0.295980000
6	-1.444542000	-0.606734000	-0.278323000
6	5.925660000	0.221337000	0.981061000
1	6.849392000	-0.143239000	1.472157000
6	6.308844000	0.781971000	-0.398135000

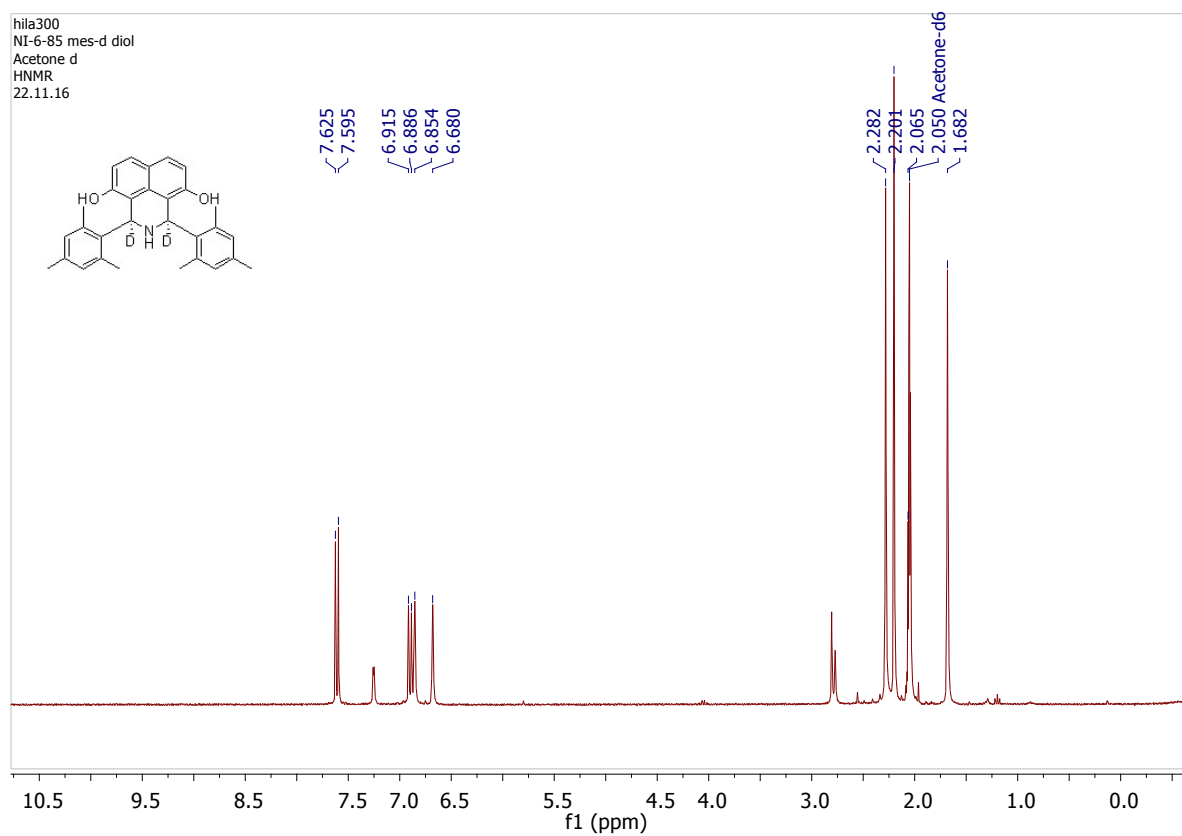
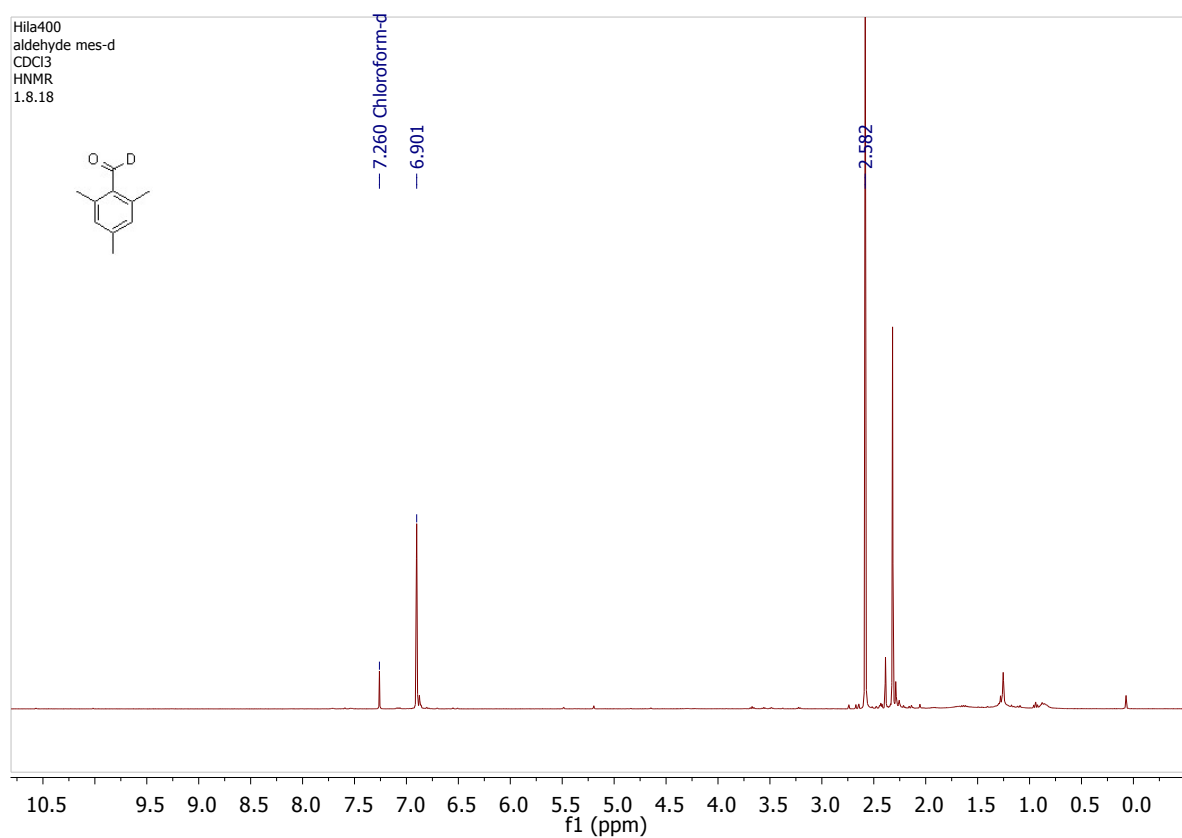
1	5.421408000	1.105259000	-0.960723000
1	6.848749000	0.047479000	-1.013550000
1	6.966139000	1.661072000	-0.285001000
6	5.331804000	1.324943000	1.871010000
1	6.023518000	2.181920000	1.934736000
1	5.140304000	0.980714000	2.897872000
1	4.385546000	1.699355000	1.454201000
6	5.689324000	-2.751987000	-0.093403000
1	5.206919000	-3.689459000	0.237965000
6	7.176687000	-2.853193000	0.295464000
1	7.641771000	-3.735151000	-0.175722000
1	7.323316000	-2.947811000	1.383075000
1	7.741966000	-1.969496000	-0.037901000
6	5.513914000	-2.659568000	-1.616955000
1	5.921563000	-1.723182000	-2.024961000
1	4.455902000	-2.710932000	-1.911646000
1	6.037222000	-3.492560000	-2.116549000
6	4.447883000	-1.922131000	2.711188000
1	5.298163000	-1.501316000	3.282493000
6	3.156442000	-1.306112000	3.278612000
1	2.269085000	-1.721554000	2.778094000
1	3.117938000	-0.213872000	3.160906000
1	3.062524000	-1.530133000	4.354565000
6	4.459871000	-3.442927000	2.936391000
1	4.341208000	-3.672777000	4.008913000
1	5.397033000	-3.912729000	2.603199000
1	3.629343000	-3.936971000	2.408943000
6	-6.354837000	0.744046000	0.087223000
1	-6.591409000	0.538186000	1.148479000
6	-5.474814000	2.002076000	0.055175000
1	-5.212978000	2.280529000	-0.977889000
1	-4.539299000	1.866918000	0.613007000
1	-6.014096000	2.858264000	0.494610000
6	-7.686332000	0.998541000	-0.644458000
1	-8.217905000	1.849442000	-0.186718000
1	-8.366624000	0.134223000	-0.617623000
1	-7.517586000	1.254564000	-1.702450000
6	-6.080110000	-2.337674000	0.563118000
1	-5.663072000	-3.254476000	0.111313000
6	-7.612888000	-2.472960000	0.522032000
1	-7.937197000	-3.370106000	1.075659000
1	-7.999614000	-2.563762000	-0.504986000
1	-8.108169000	-1.609004000	0.992065000
6	-5.570675000	-2.246145000	2.010123000
1	-5.944045000	-1.339220000	2.512388000
1	-4.472524000	-2.224005000	2.061864000
1	-5.917588000	-3.110201000	2.601464000
6	-5.744423000	-1.168940000	-2.386615000
1	-6.831804000	-1.013434000	-2.526482000
6	-5.412332000	-2.592410000	-2.864827000
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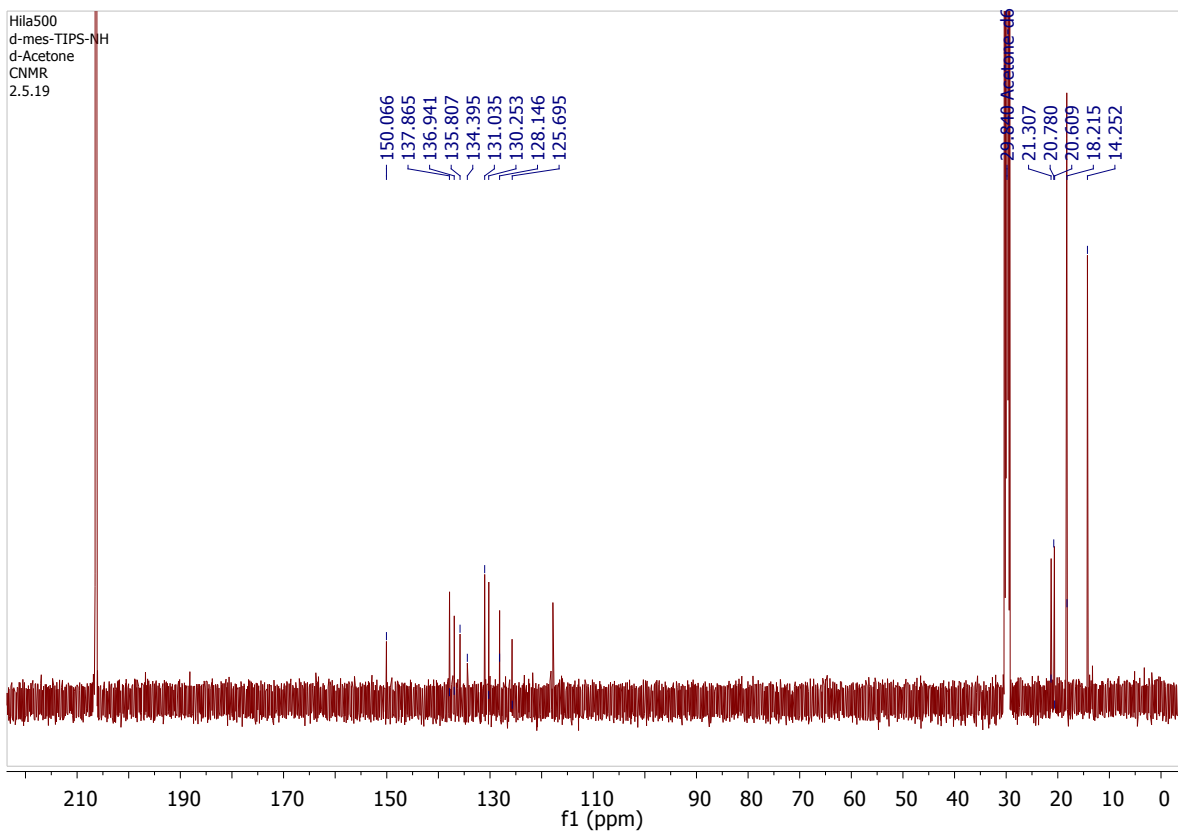
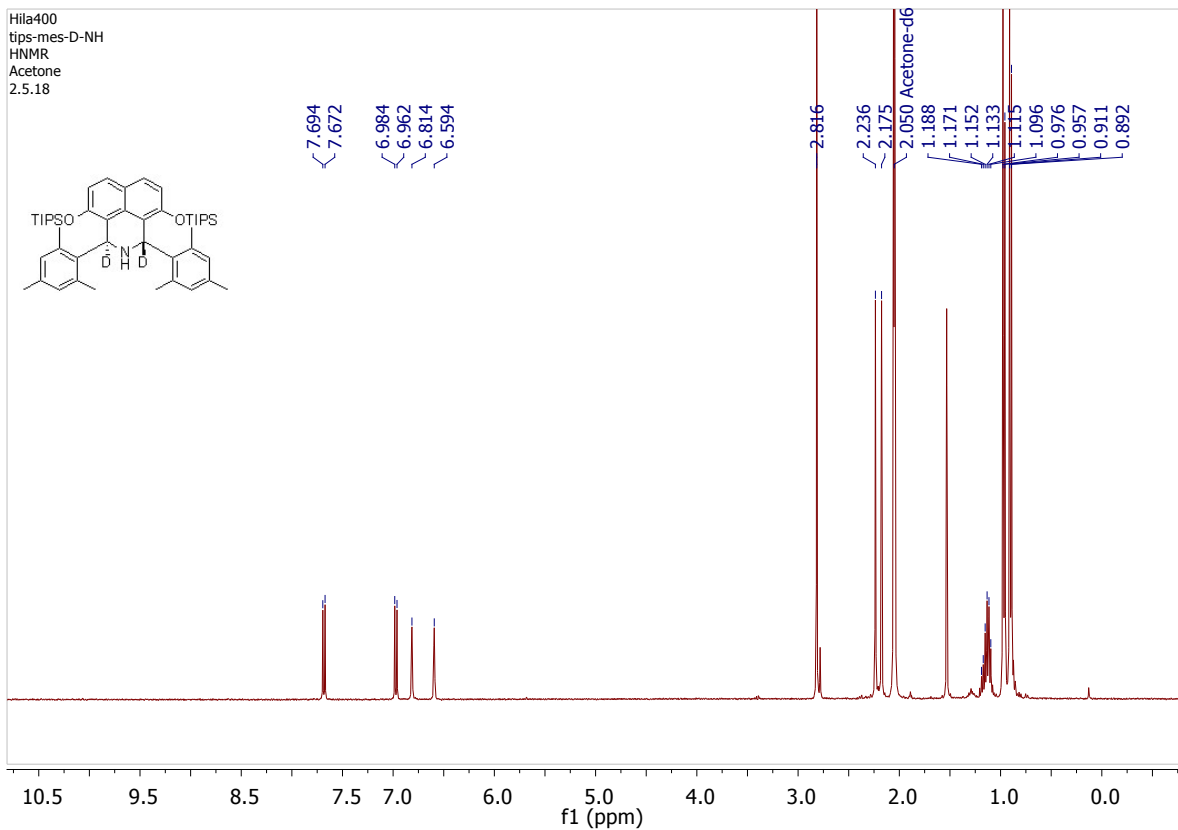
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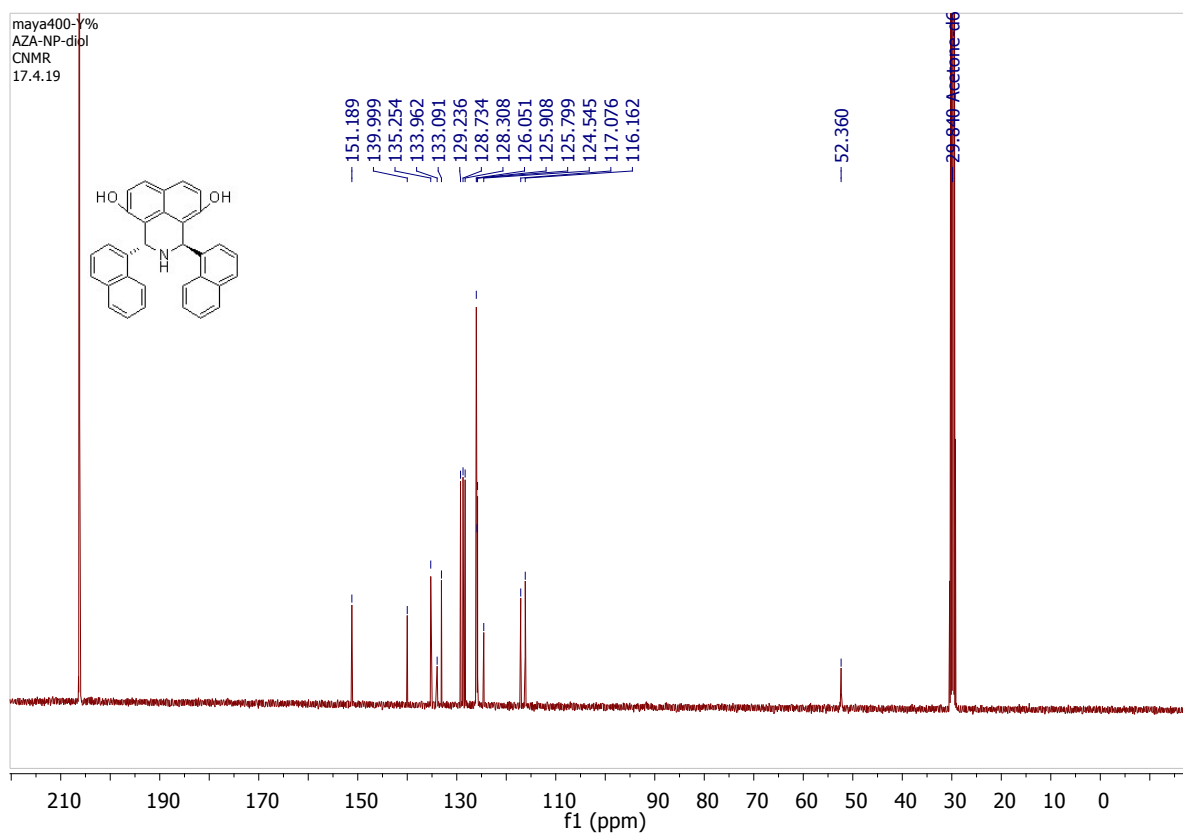
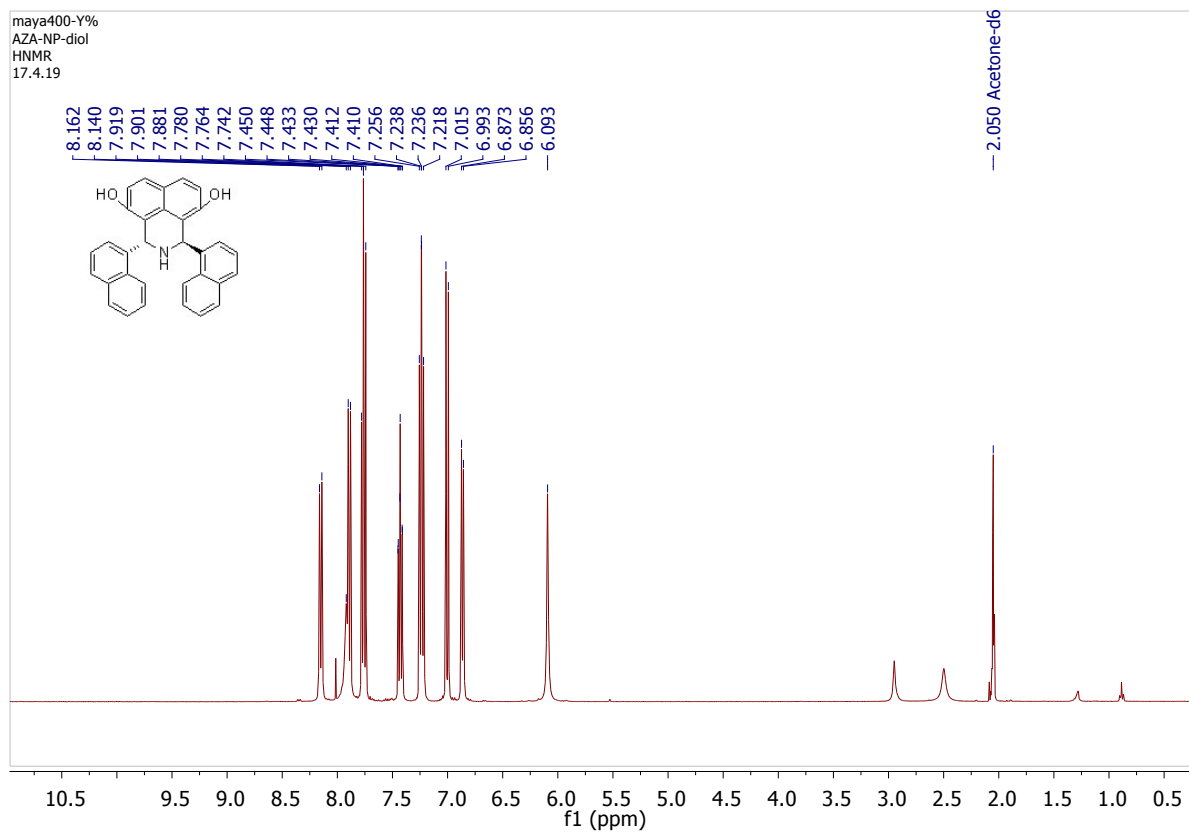
References for computational section

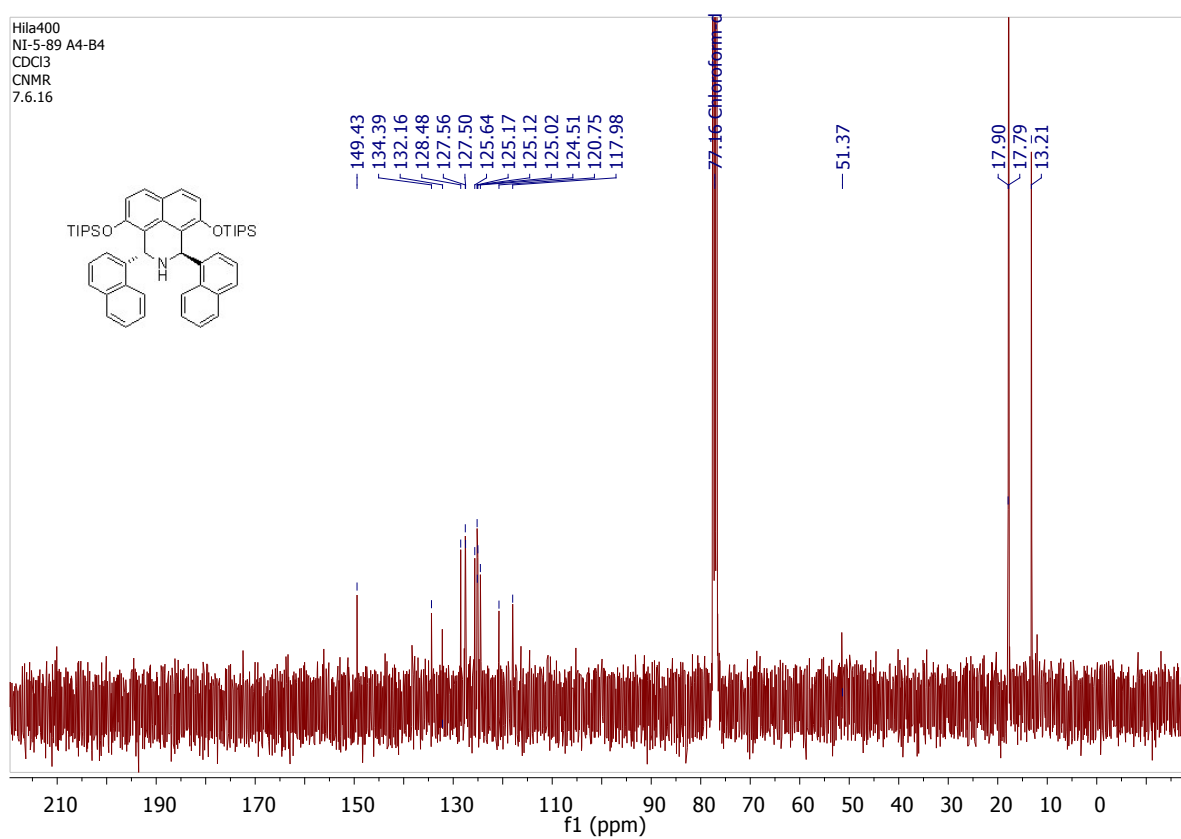
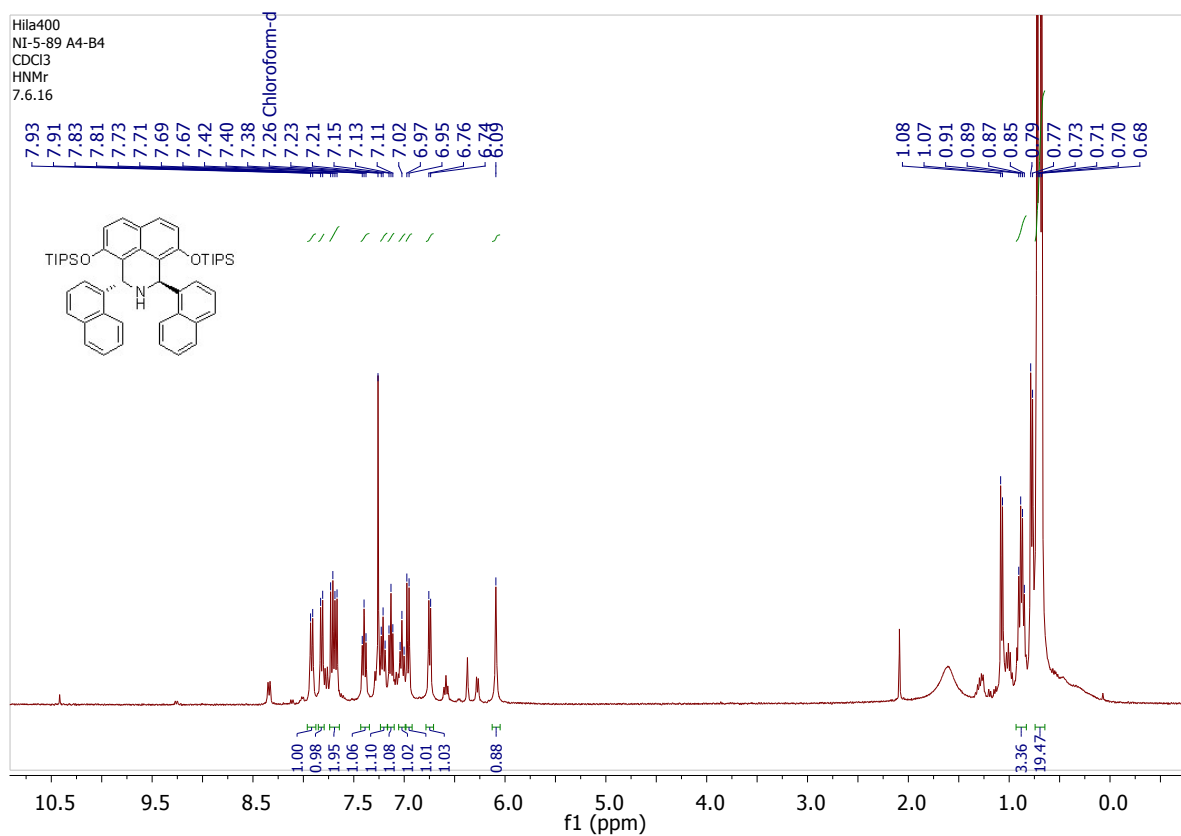
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NMR spectra:









hila300
NI-6-35-NP-D aldehyde
CDCl3
HNMR
7.8.16

