

## Supporting Information

# A Pseudo-Dearomatized PN<sup>3</sup>P\*Ni-H Complex as a Ligand and σ-Nucleophilic Catalyst

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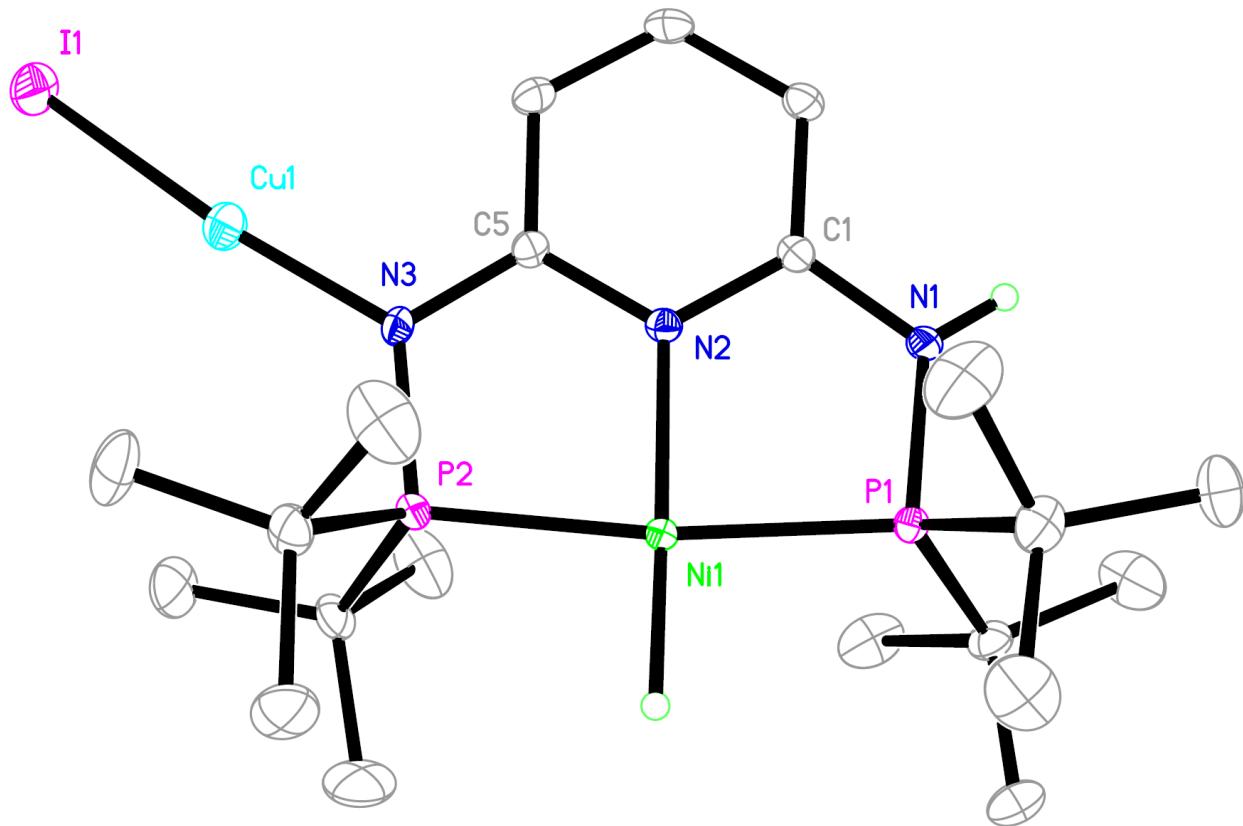
<sup>#</sup>College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China.

### Table of Contents:

Crystallographic data for complex <b>9</b> .....	S2
The ORTEP diagram of complex <b>9</b> at 30% ellipsoid probability.....	S3
NMR Spectra.....	S4
Computational details.....	S29
References.....	S73

**Table S1** Crystallographic data for complex **9**:

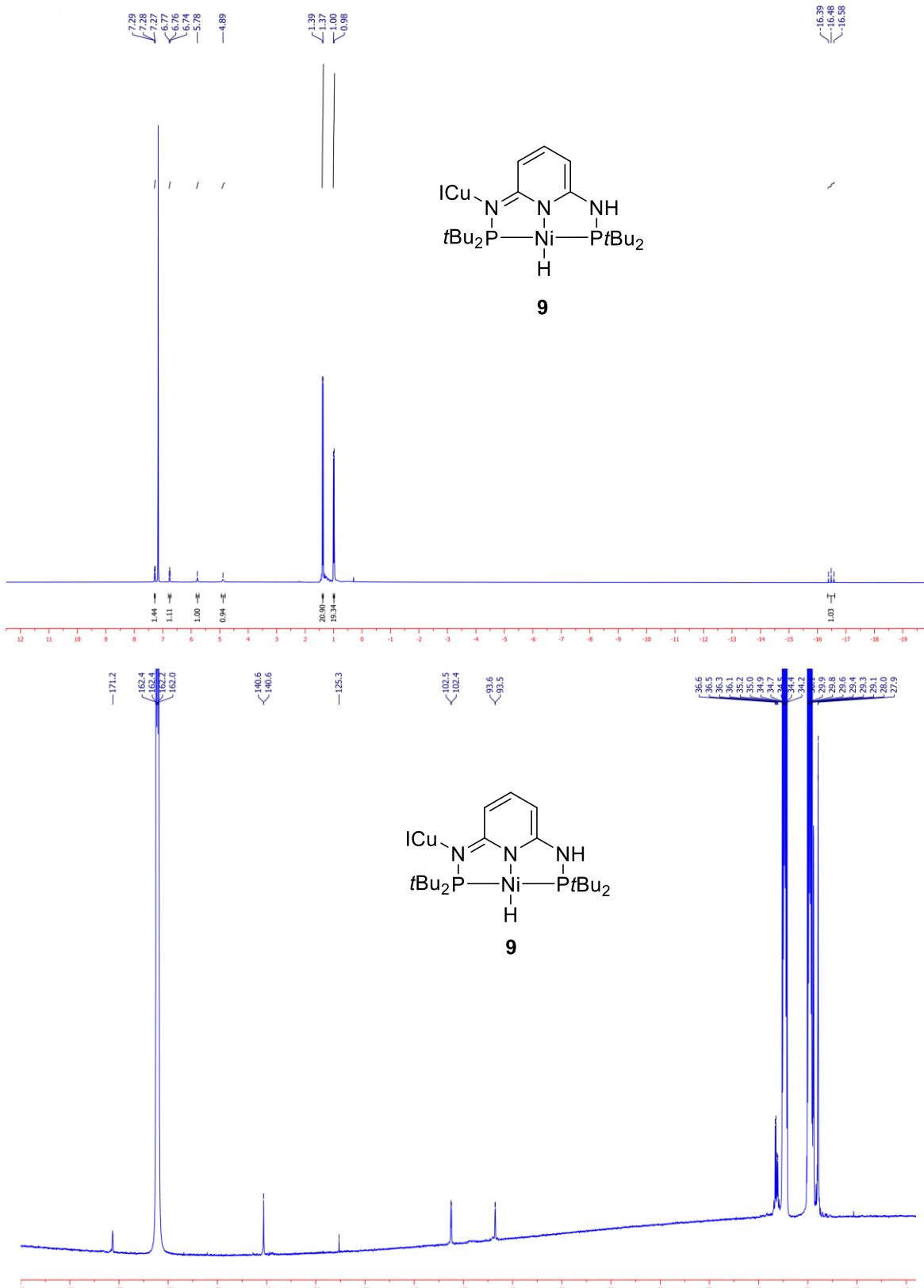
	<b>9</b>
Formula	C <sub>21</sub> H <sub>41</sub> N <sub>3</sub> NiP <sub>2</sub> CuI
Formula weight	646.65
Crystsyst	monoclinic
Space group	P21/c
T[K]	150
a[Å]	12.3898(3)
b[Å]	8.3356(2)
c[Å]	29.3057(6)
α[deg]	90
β[deg]	114.300(1)
λ[deg]	90
V[Å <sup>3</sup> ]	2758.44(11)
Z	4
Density[gcm <sup>-3</sup> ]	1.557
F(000)	1312
θ range (°)	4.0 to 70.1
Data collected ( <i>hkl</i> )	-15 ≤ <i>h</i> ≤ 15 -10 ≤ <i>k</i> ≤ 10 -35 ≤ <i>l</i> ≤ 35
Refns collected/unique	35925/5216
Data/restrains/para	5216/0/278
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.081
Final <i>R</i> <sub>1</sub> , <i>wR</i> <sub>2</sub> [ <i>I</i> >2σ( <i>I</i> )]	0.0595, 0.1523
<i>R</i> <sub>1</sub> , <i>wR</i> <sub>2</sub> (all data)	0.0639, 0.1553
Δρmax, min/e Å <sup>-3</sup>	-1.53, 4.43



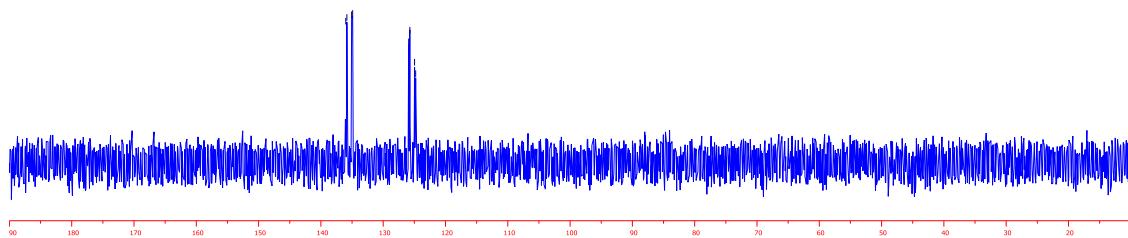
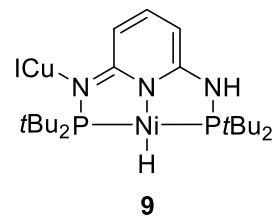
**Figure S1.** The ORTEP diagram of complex **9** at 30% ellipsoid probability.

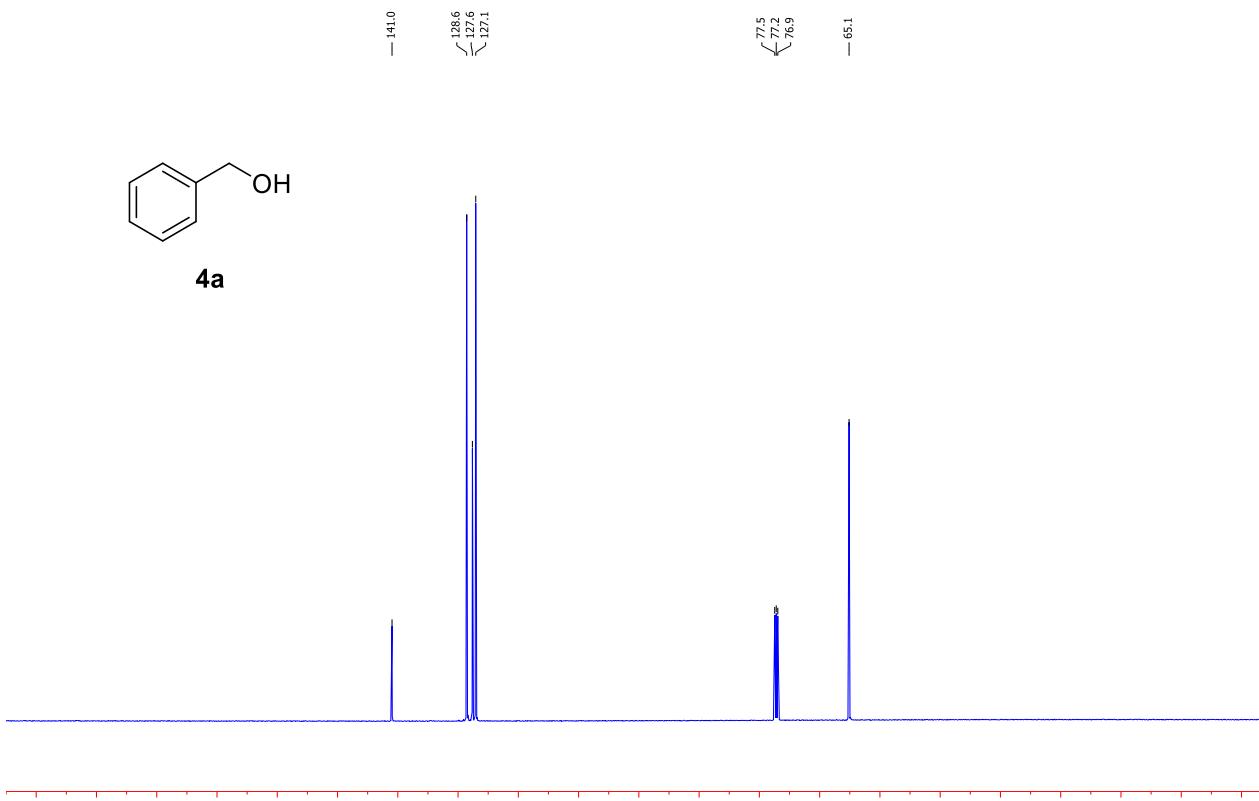
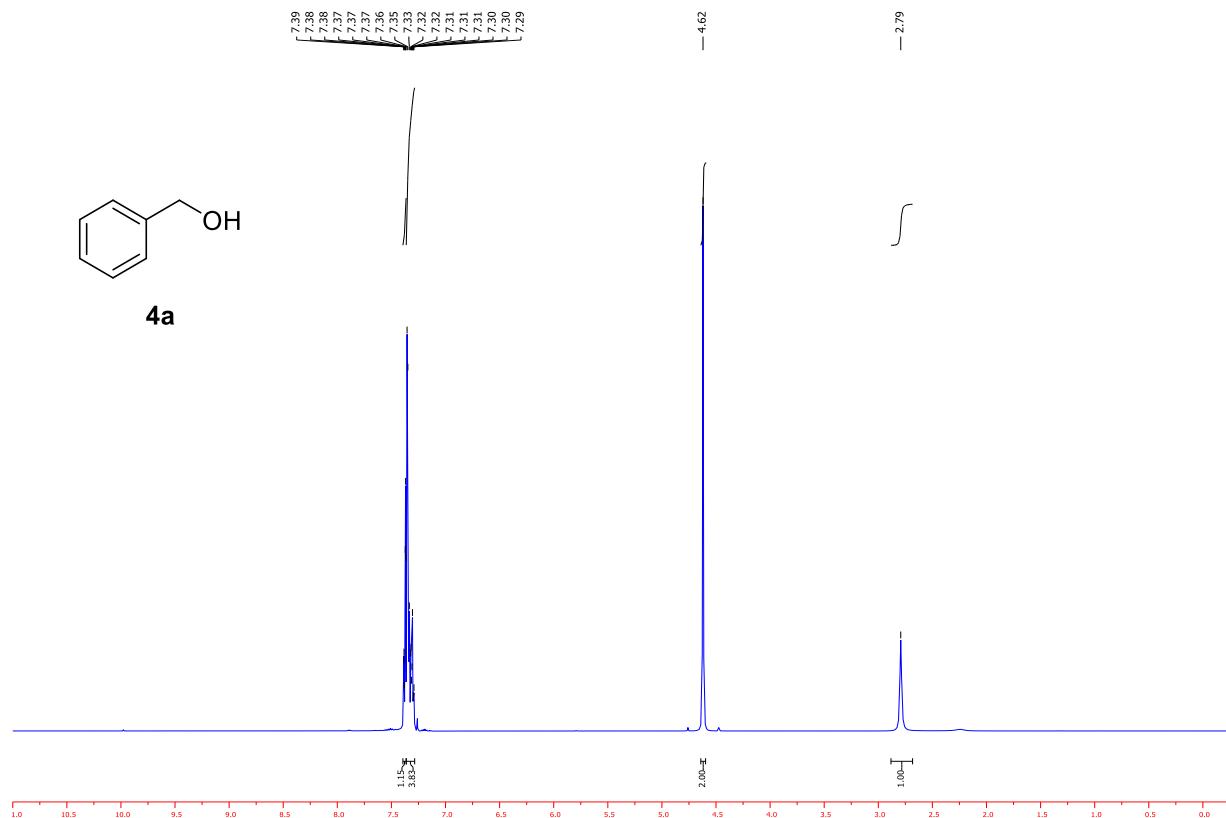
Hydrogen atoms (except for pincer arms and  $\text{Ni}-\text{H}$ ) are omitted for clarity. Selected bond lengths ( $\text{\AA}$ )  $\text{Ni1-N2}$  1.901(5);  $\text{Ni1-P1}$  2.1645(16);  $\text{Ni1-P2}$  2.1649(16);  $\text{N3-C5}$  1.364(7);  $\text{N1-C1}$  1.388(7).

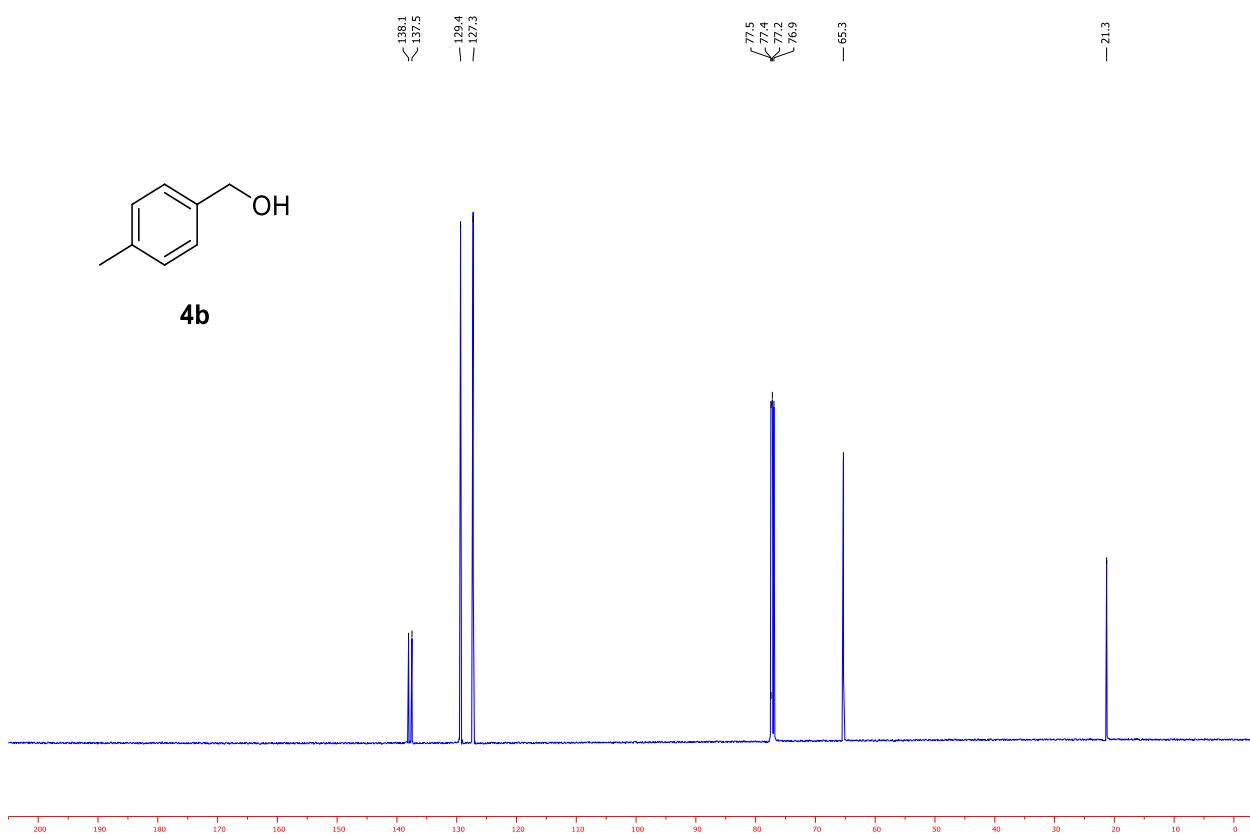
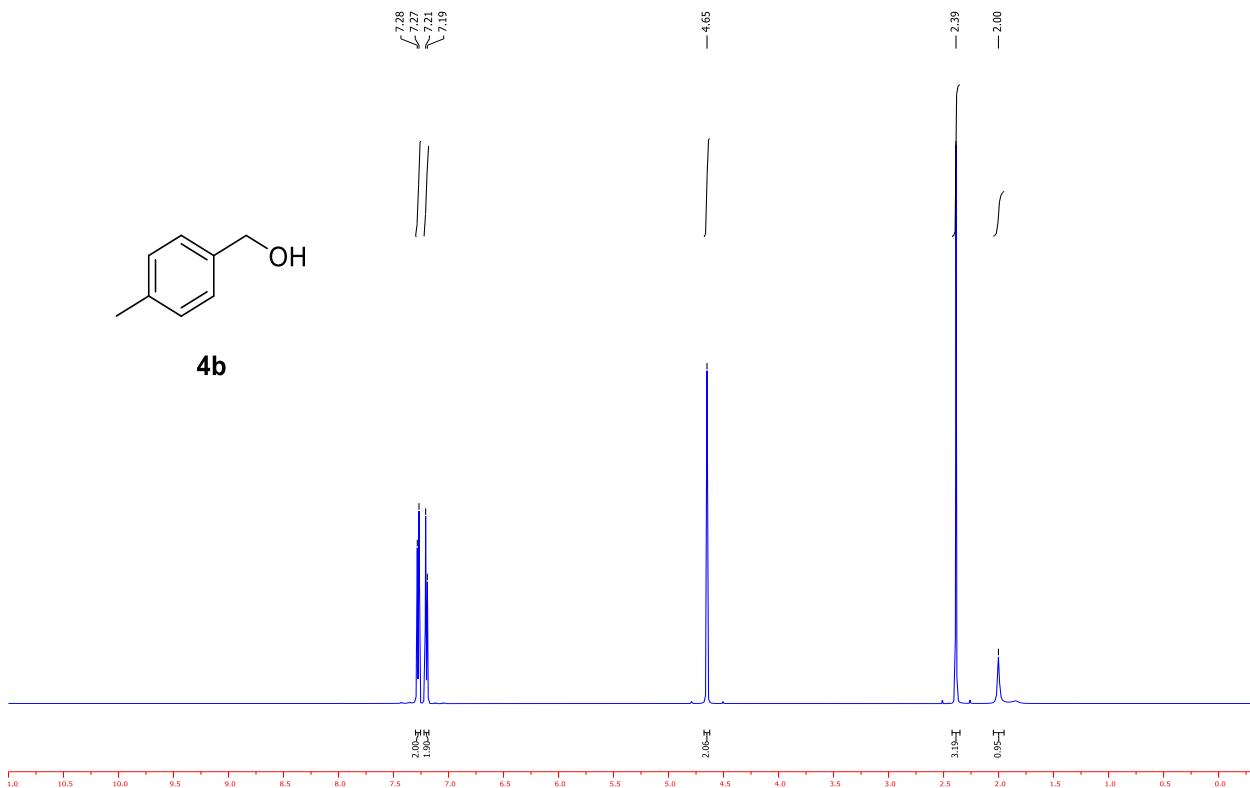
## NMR Spectra

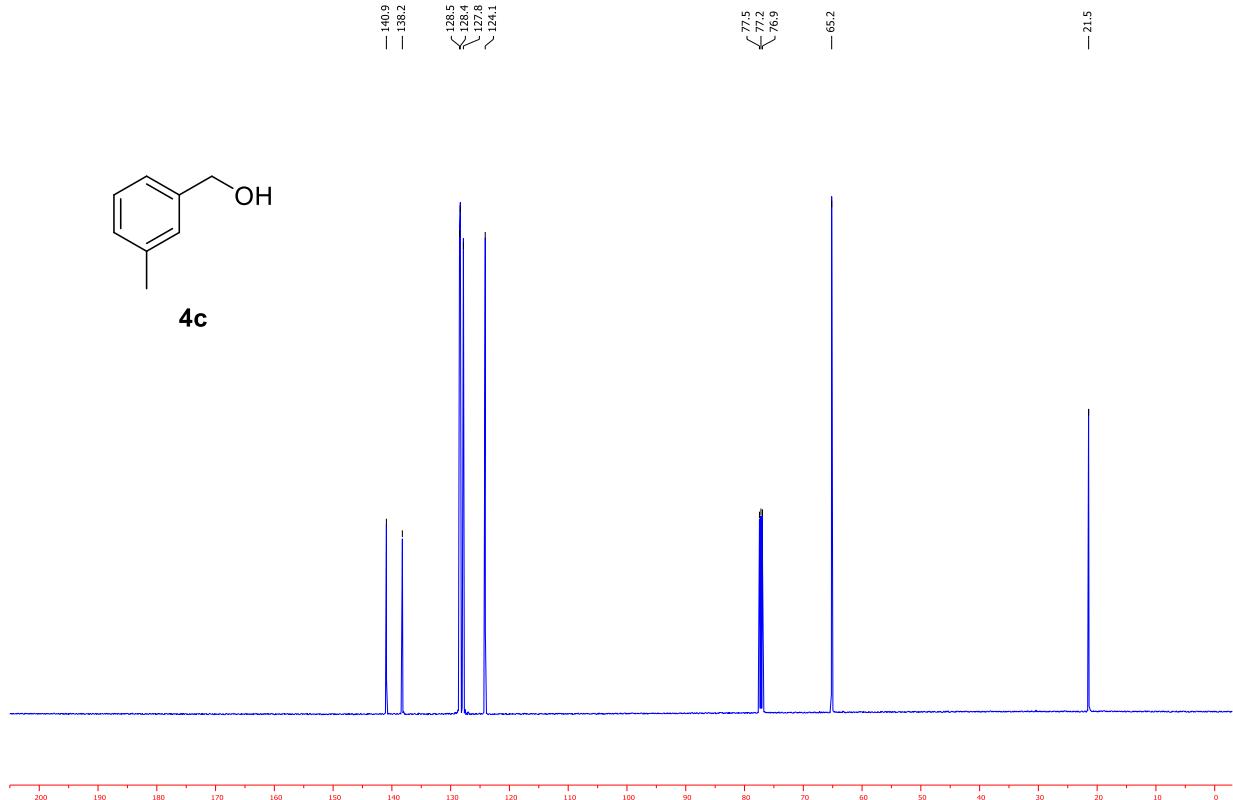
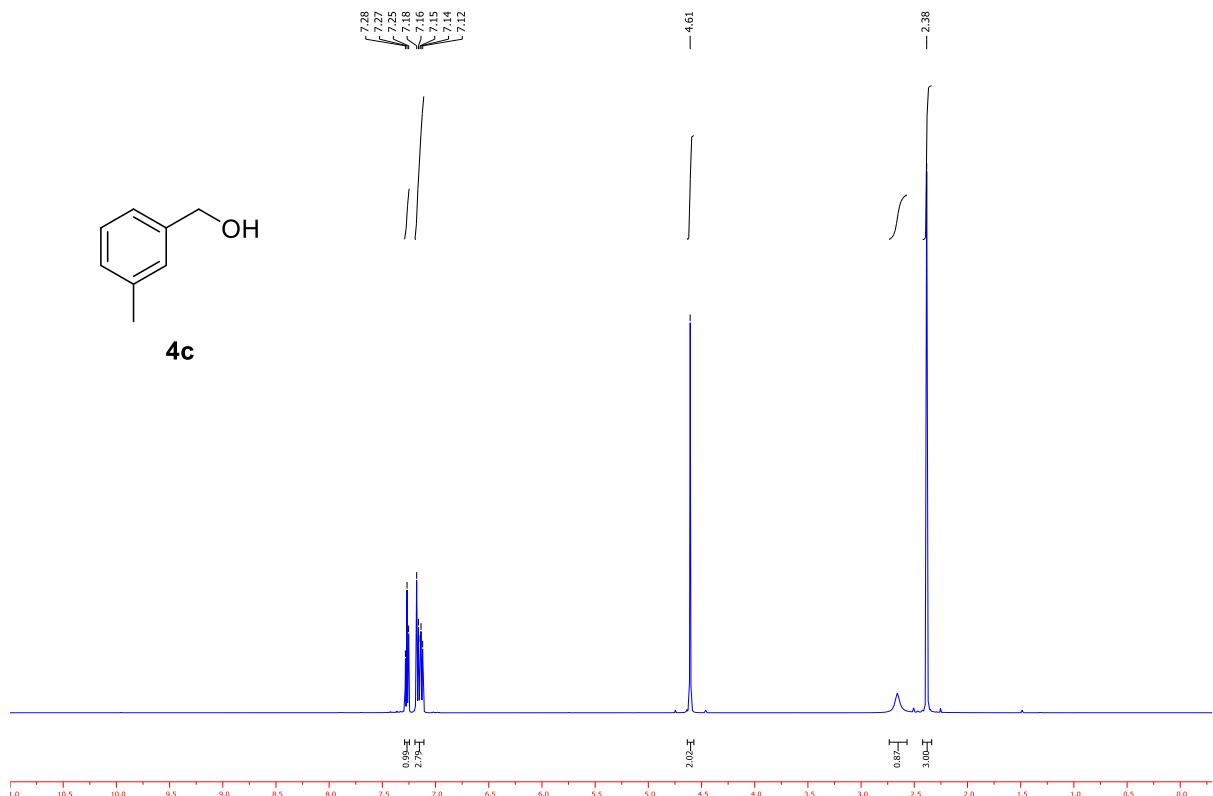


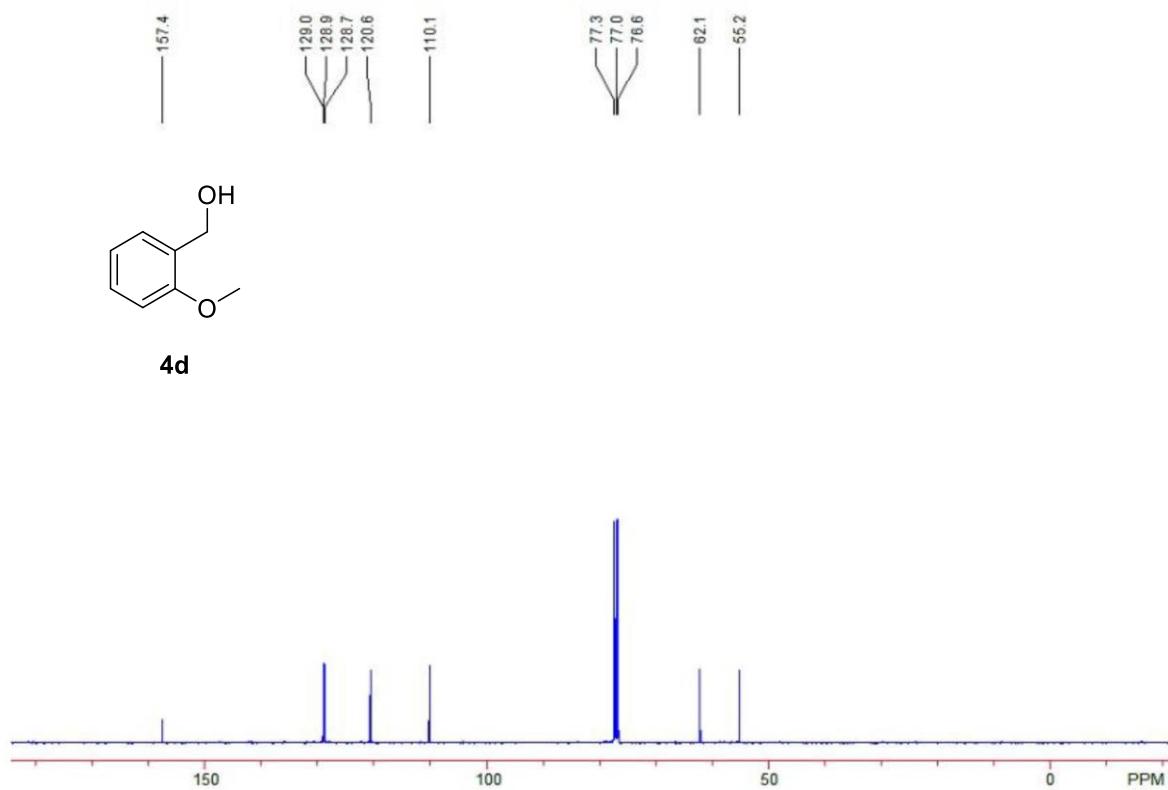
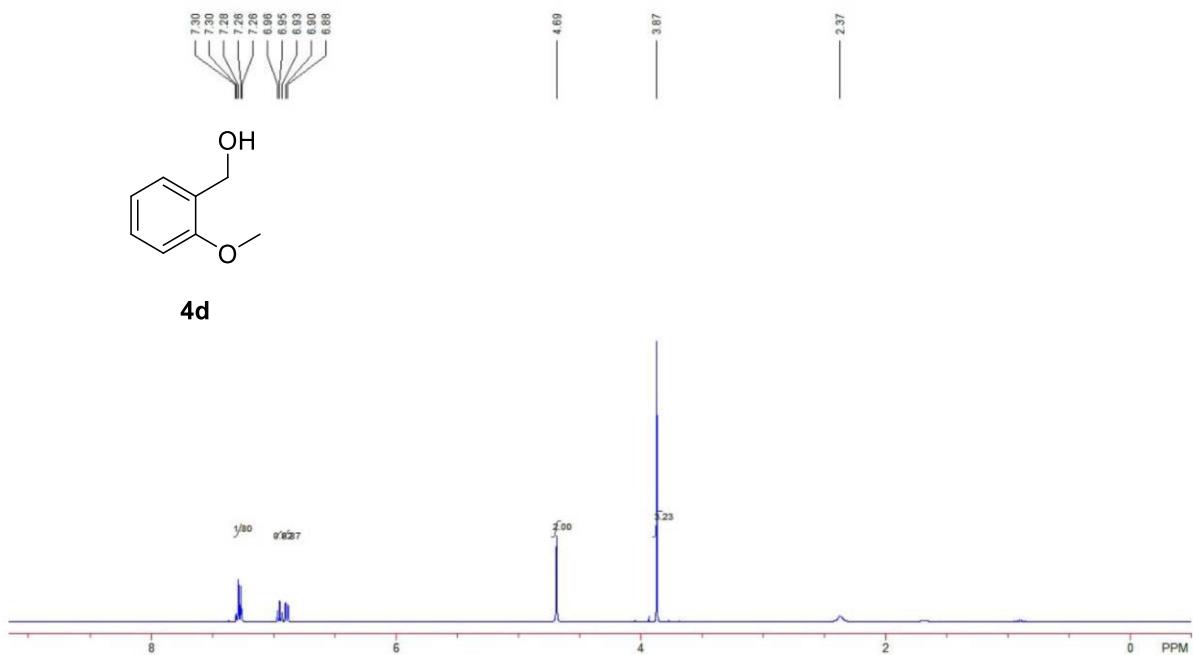
136.01  
135.83  
135.07  
134.90  
125.91  
125.72  
124.97  
124.79

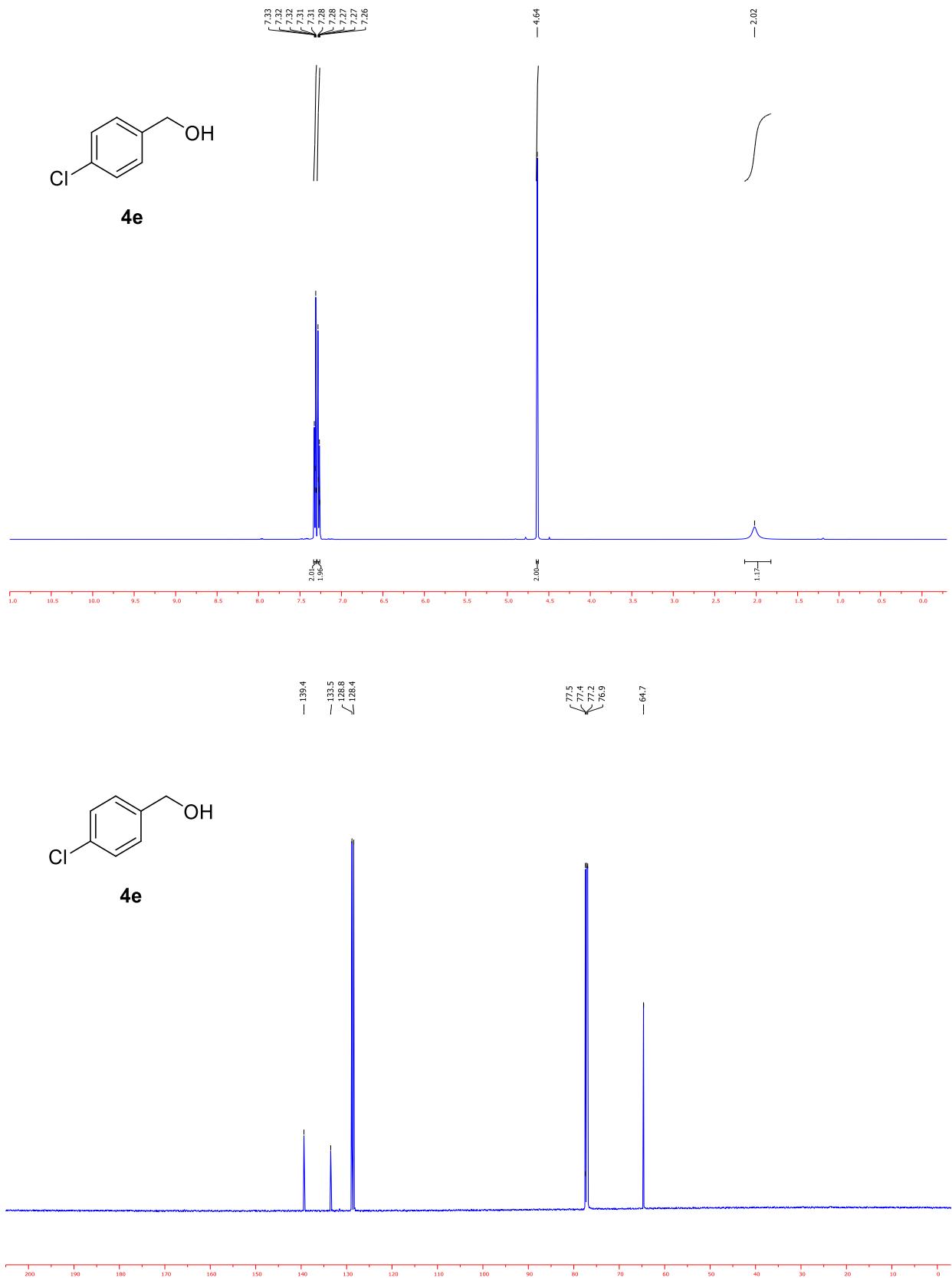


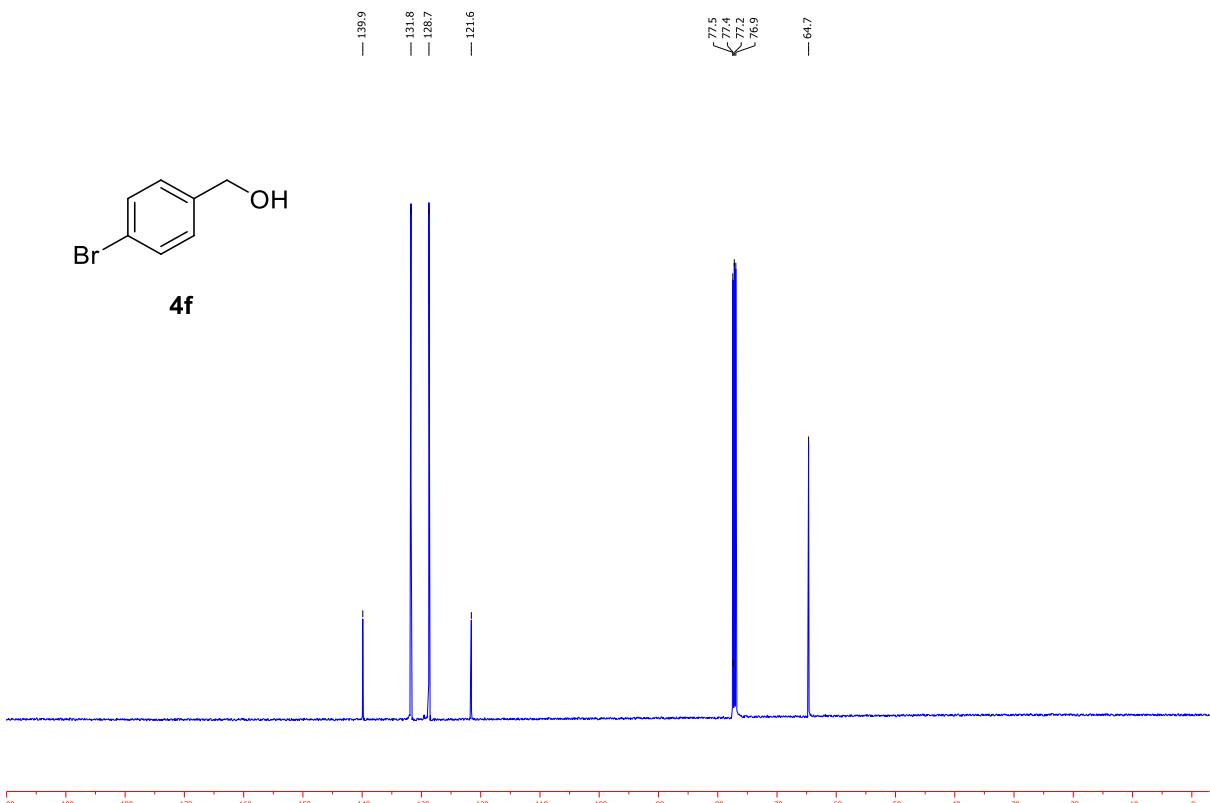
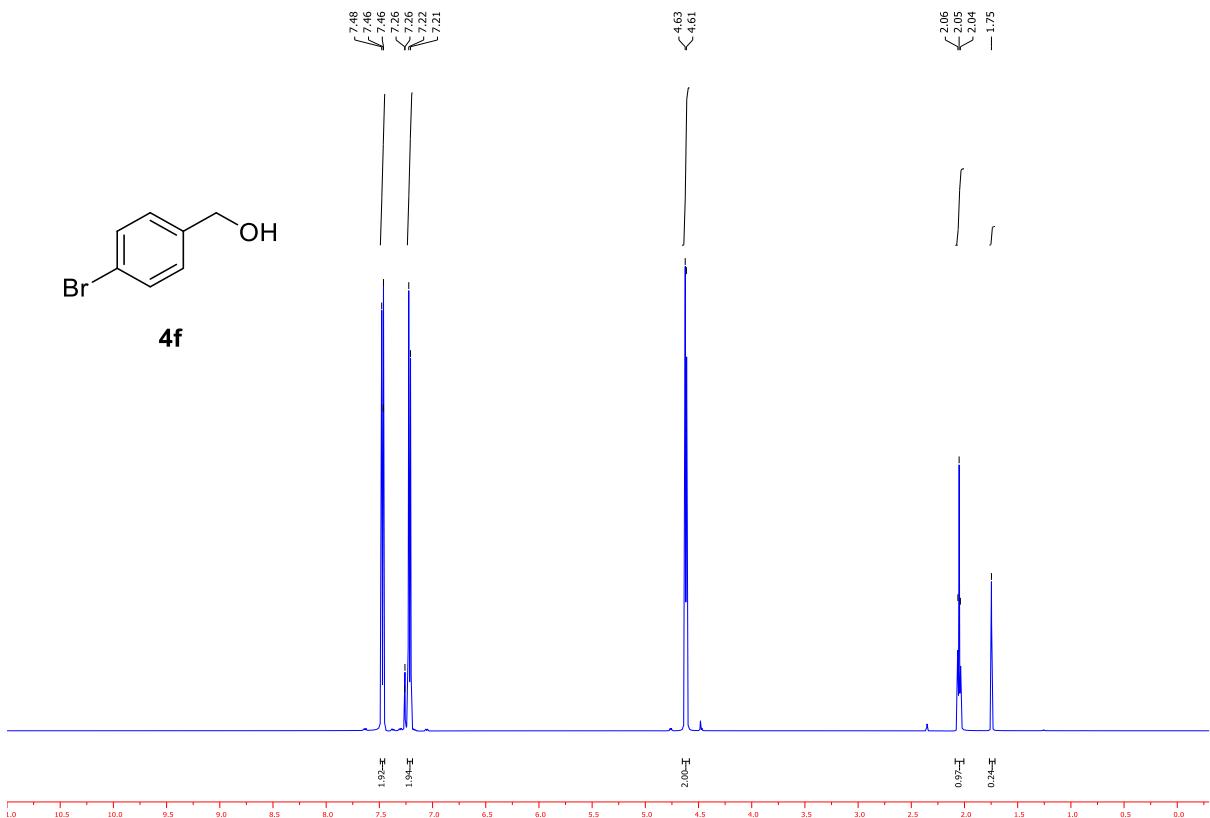






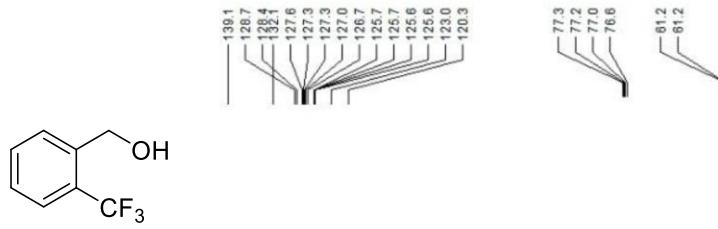
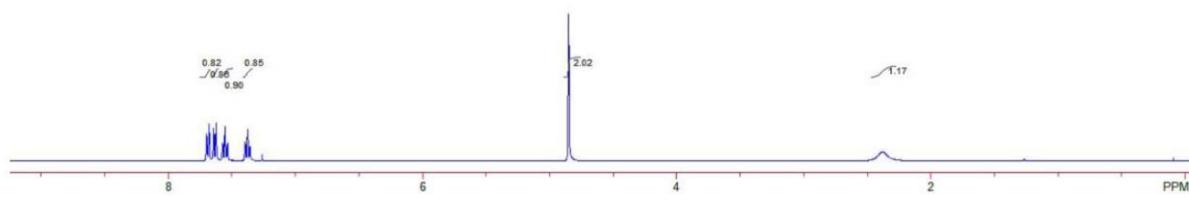




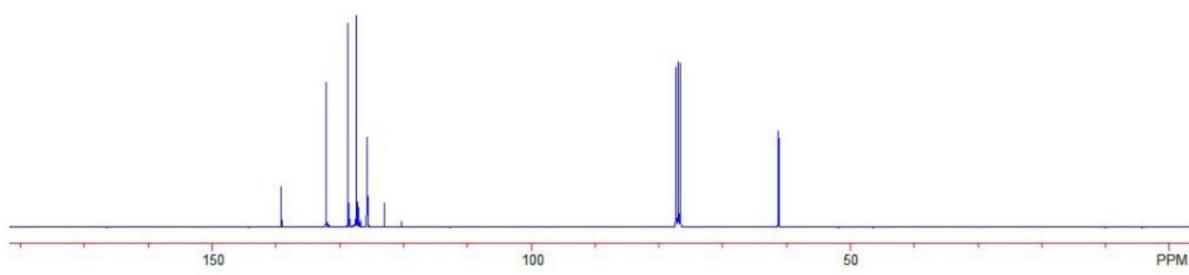


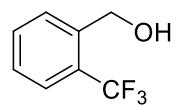


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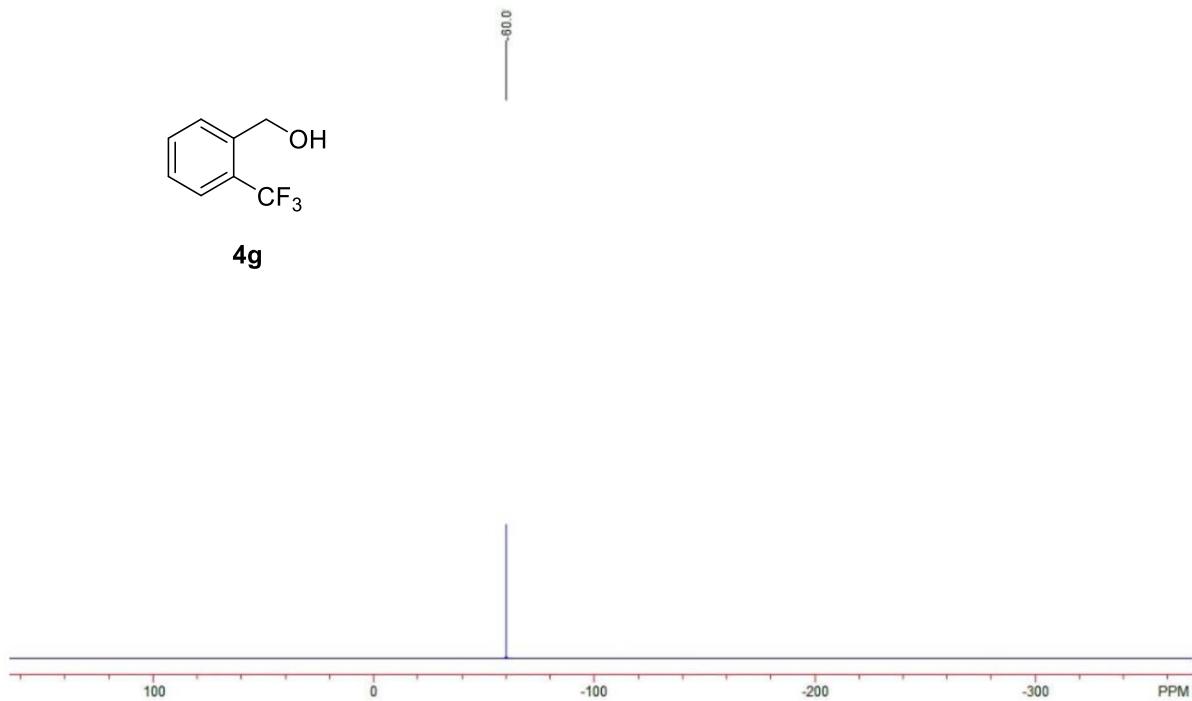


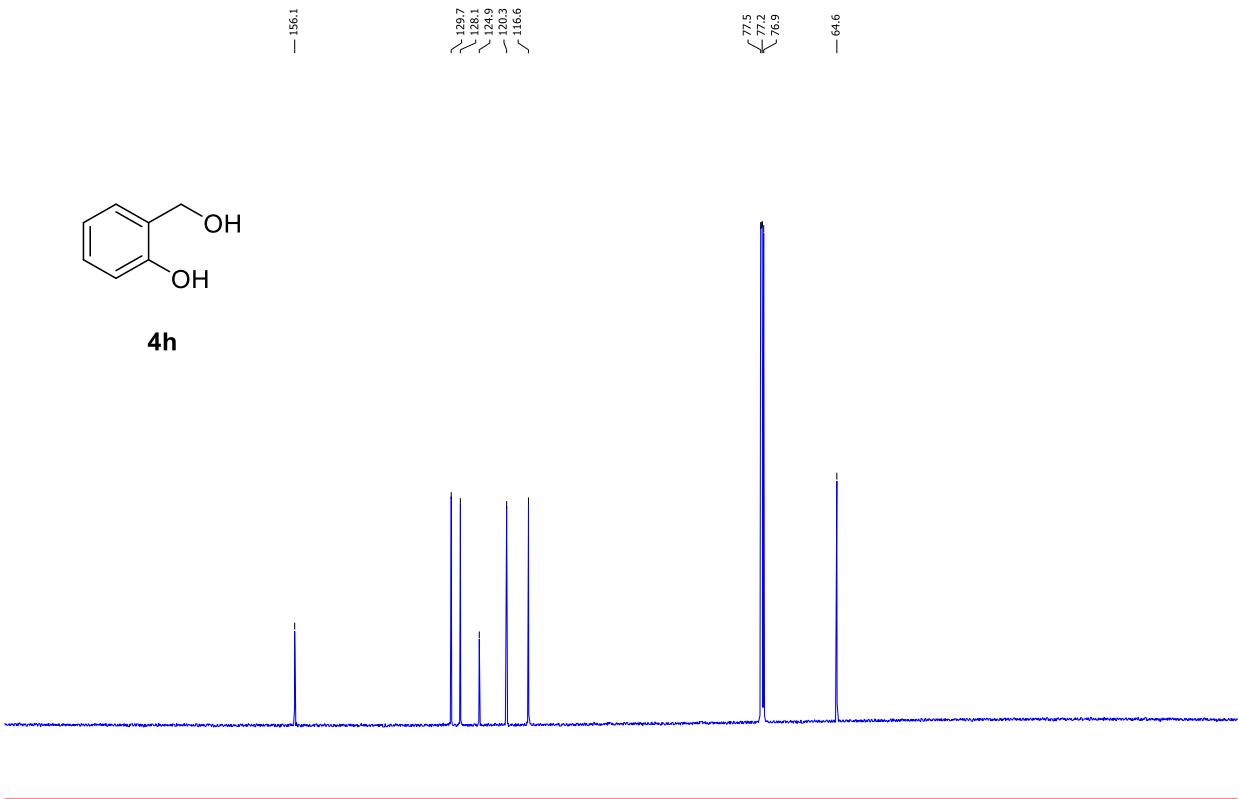
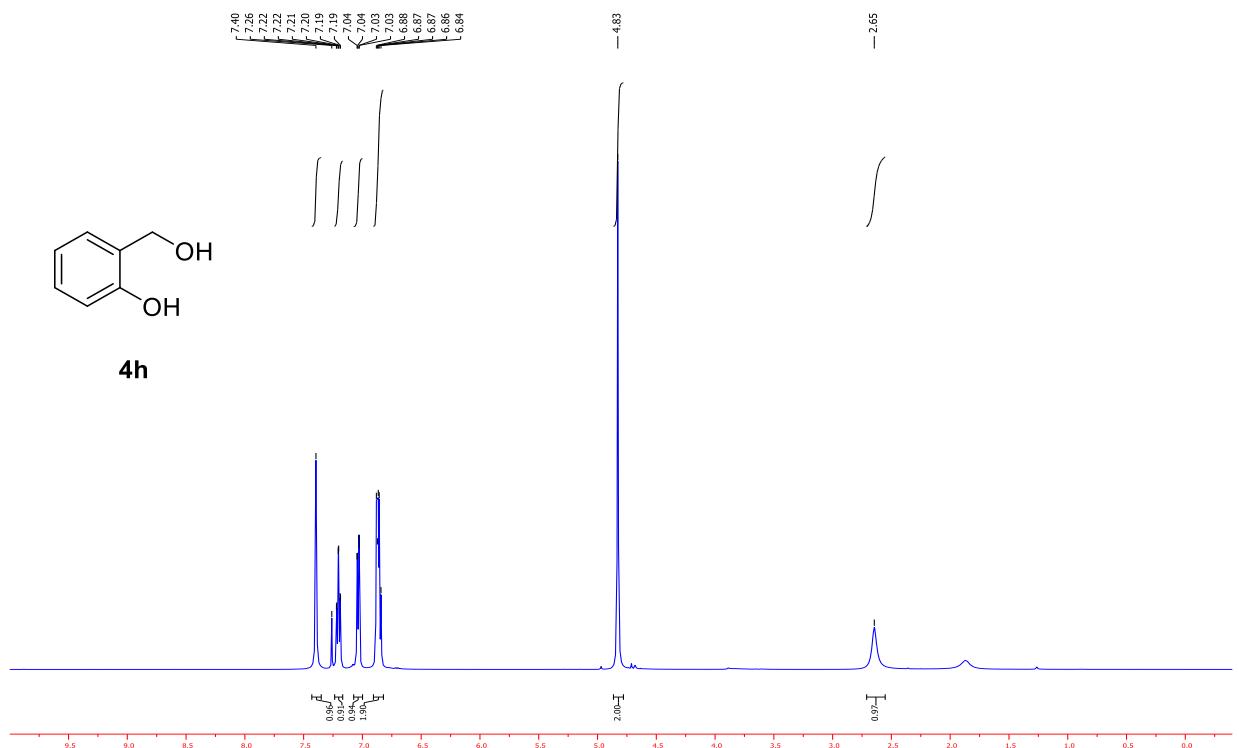
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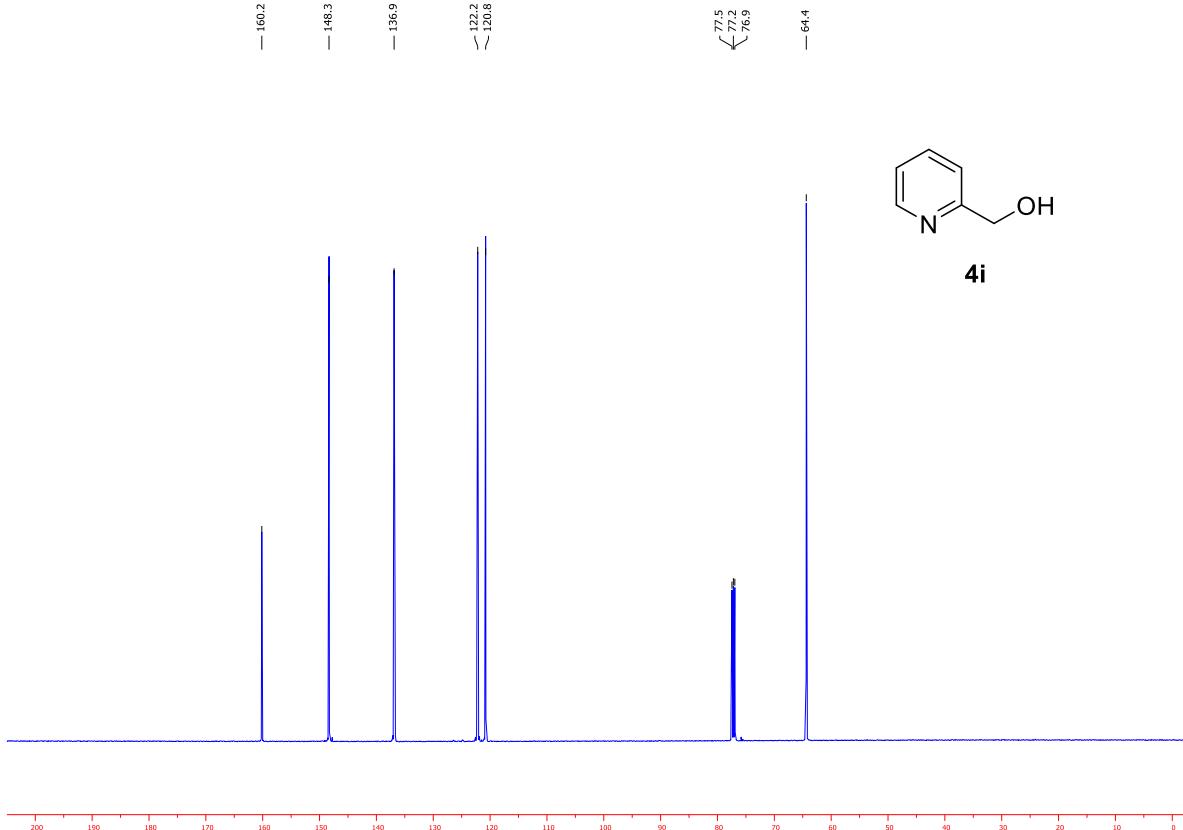
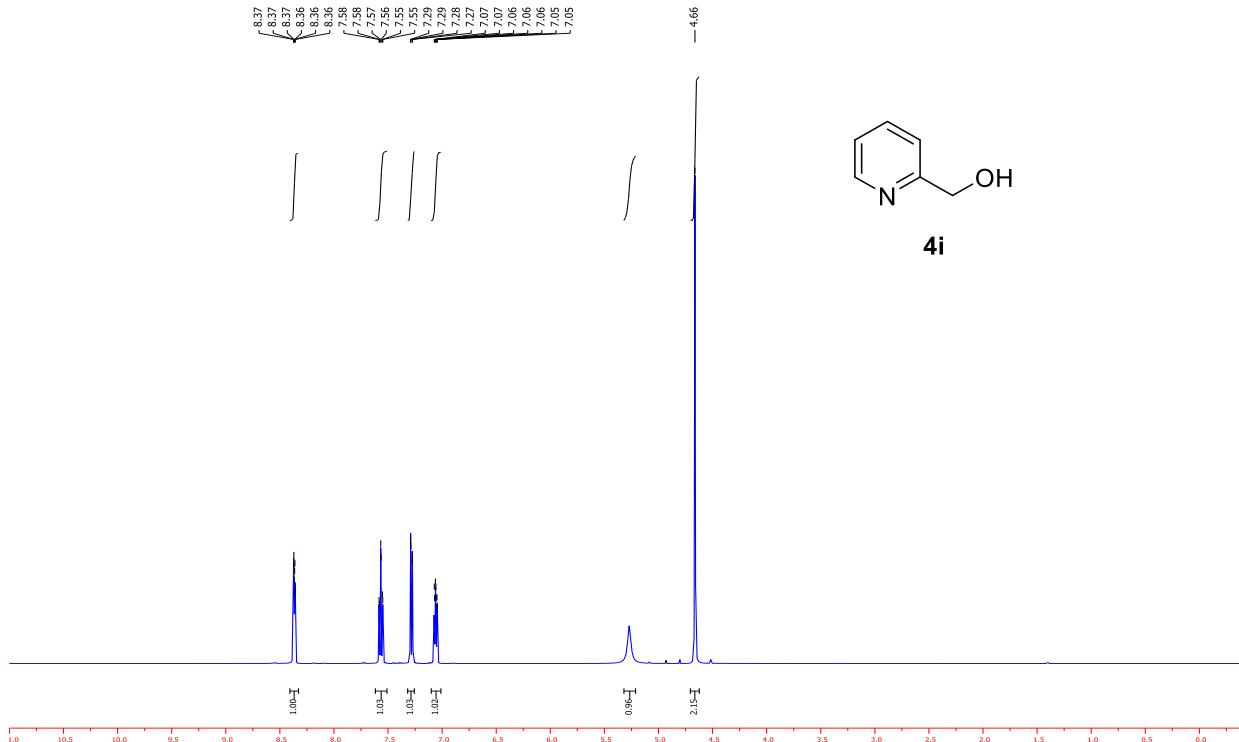


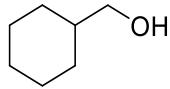
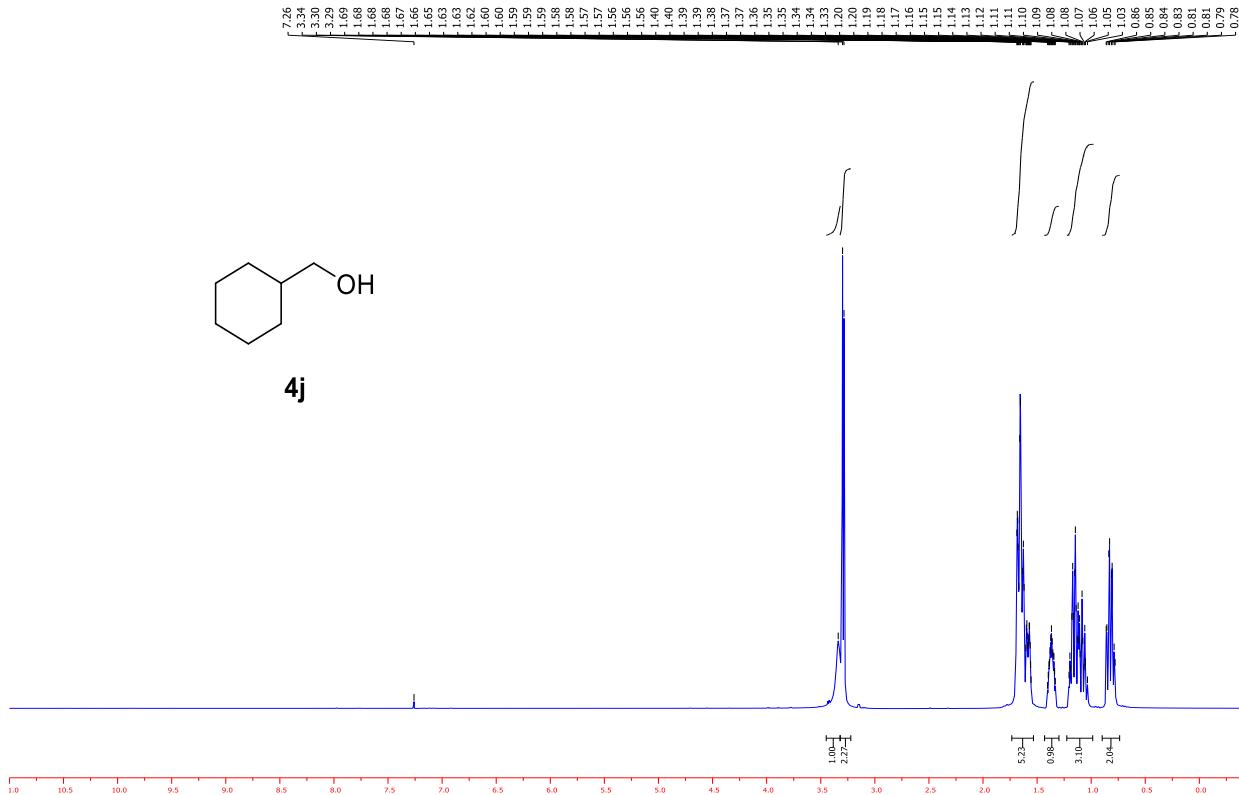


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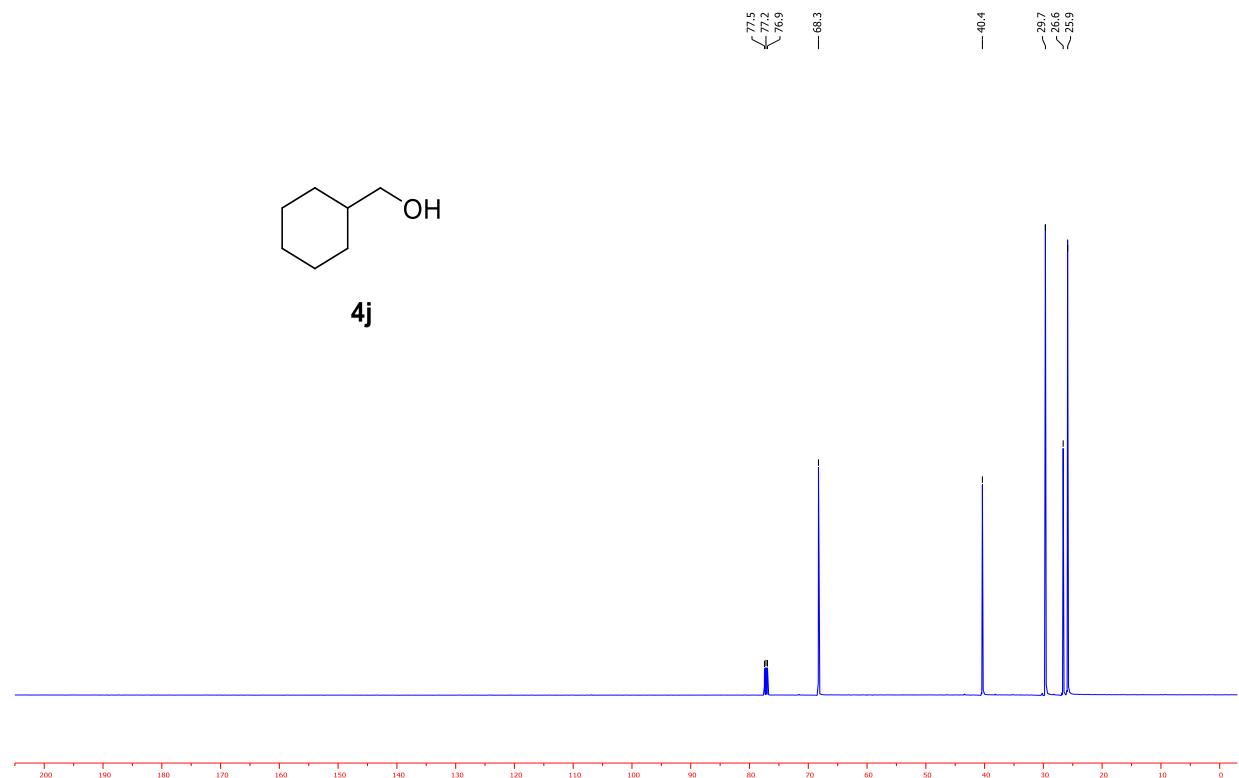




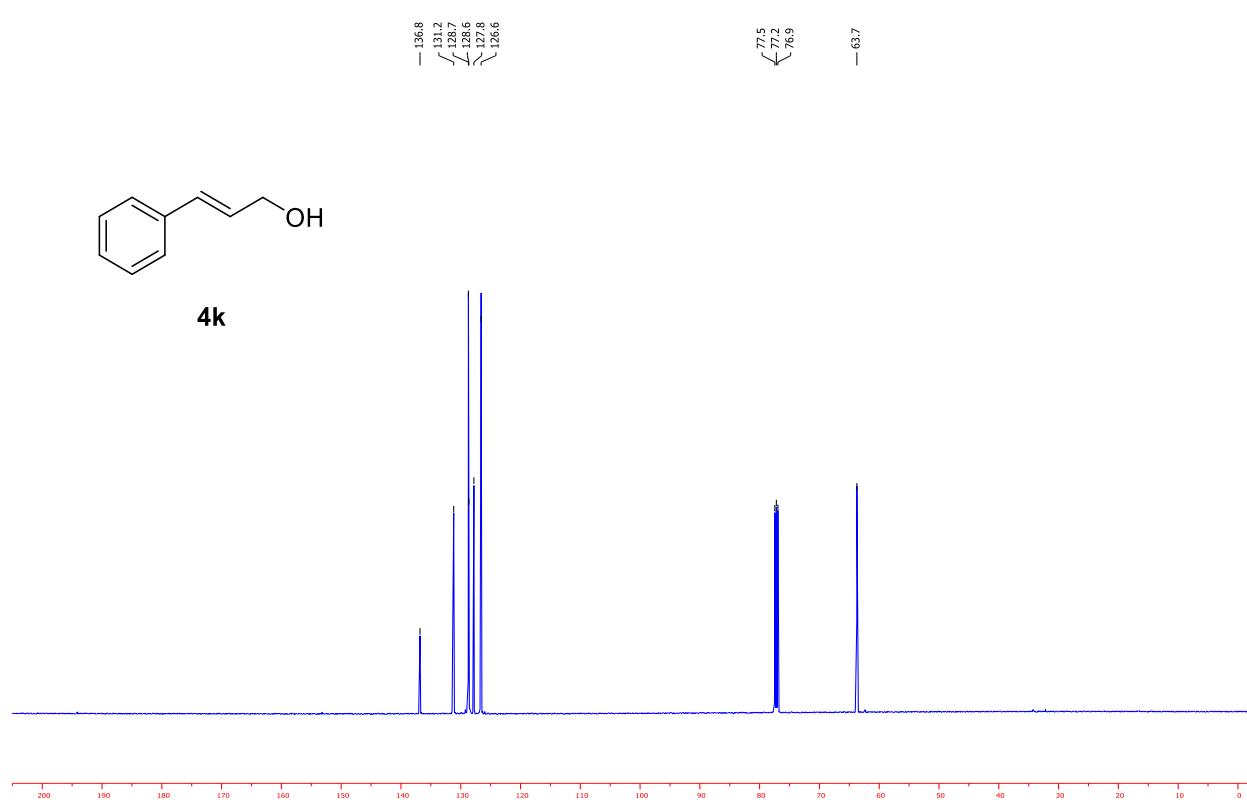
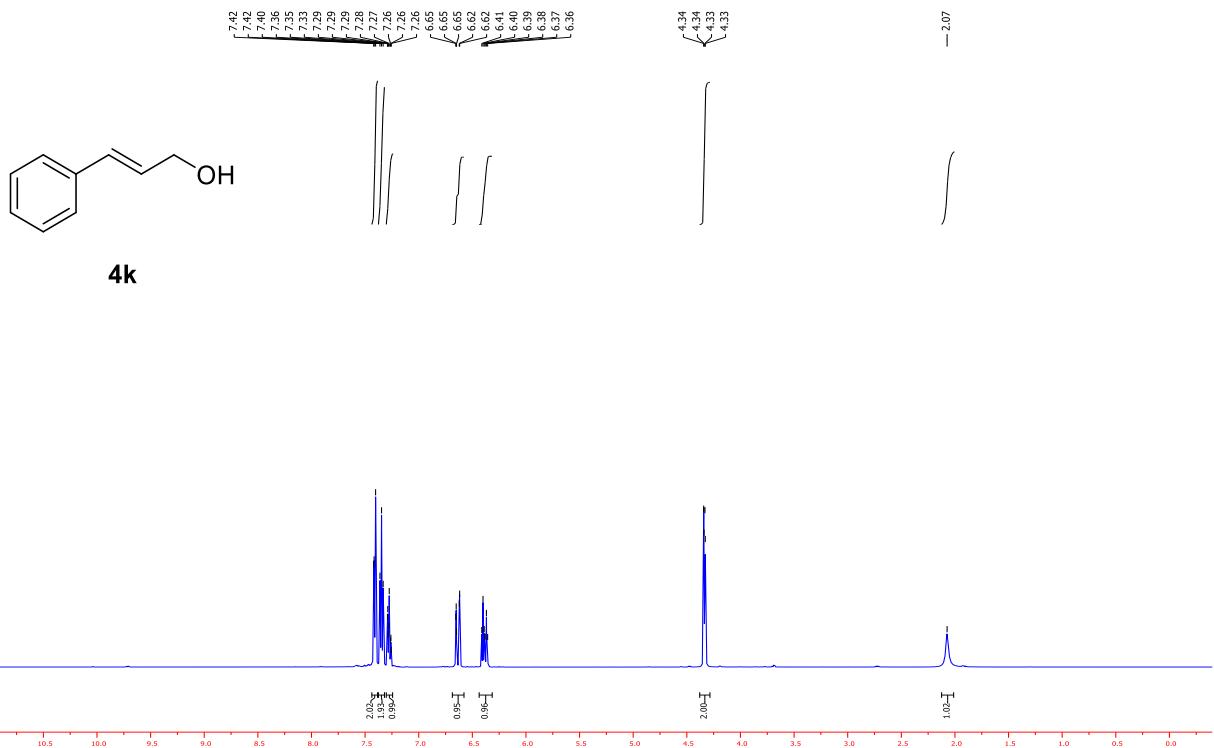


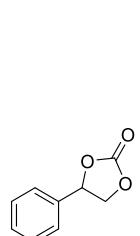
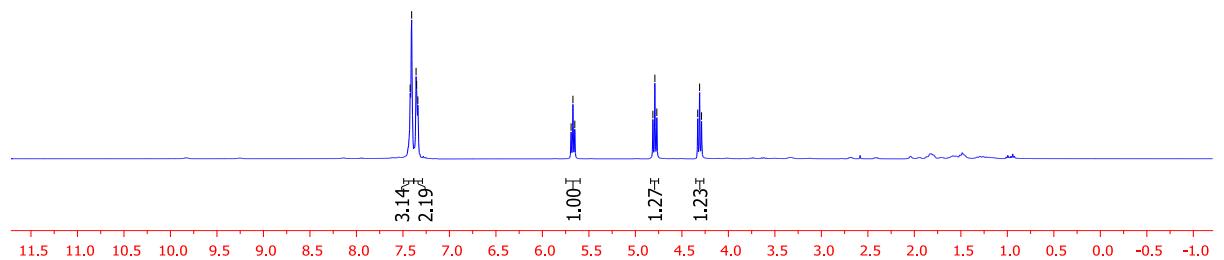
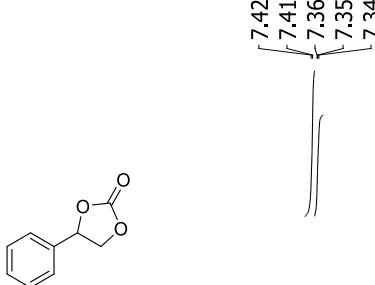


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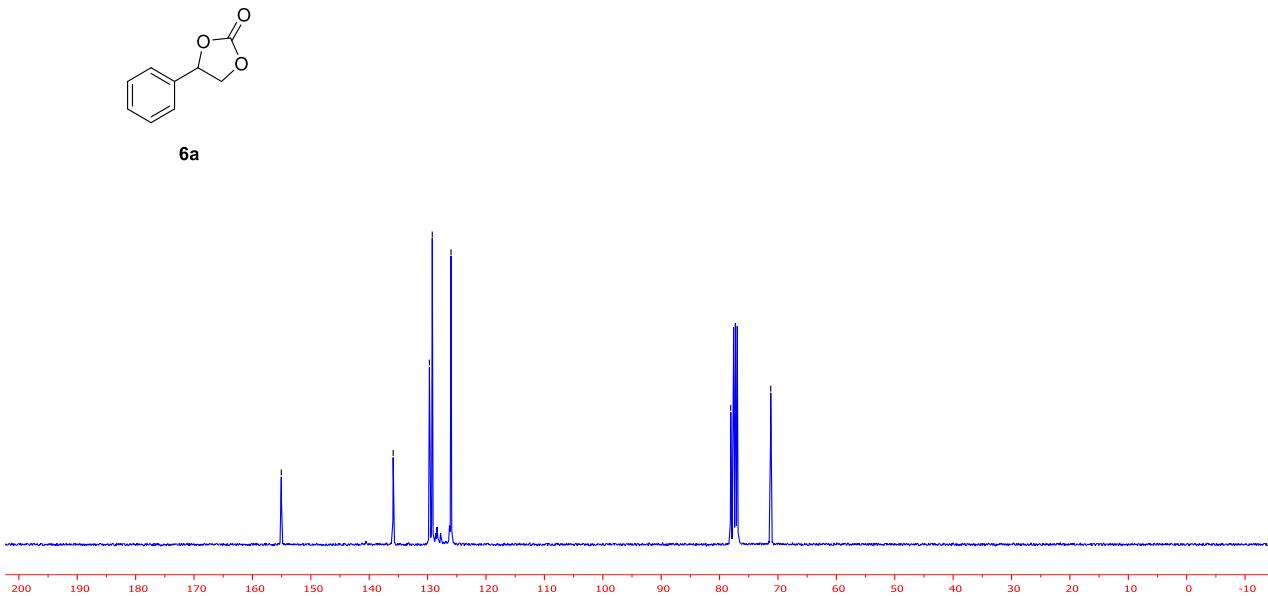


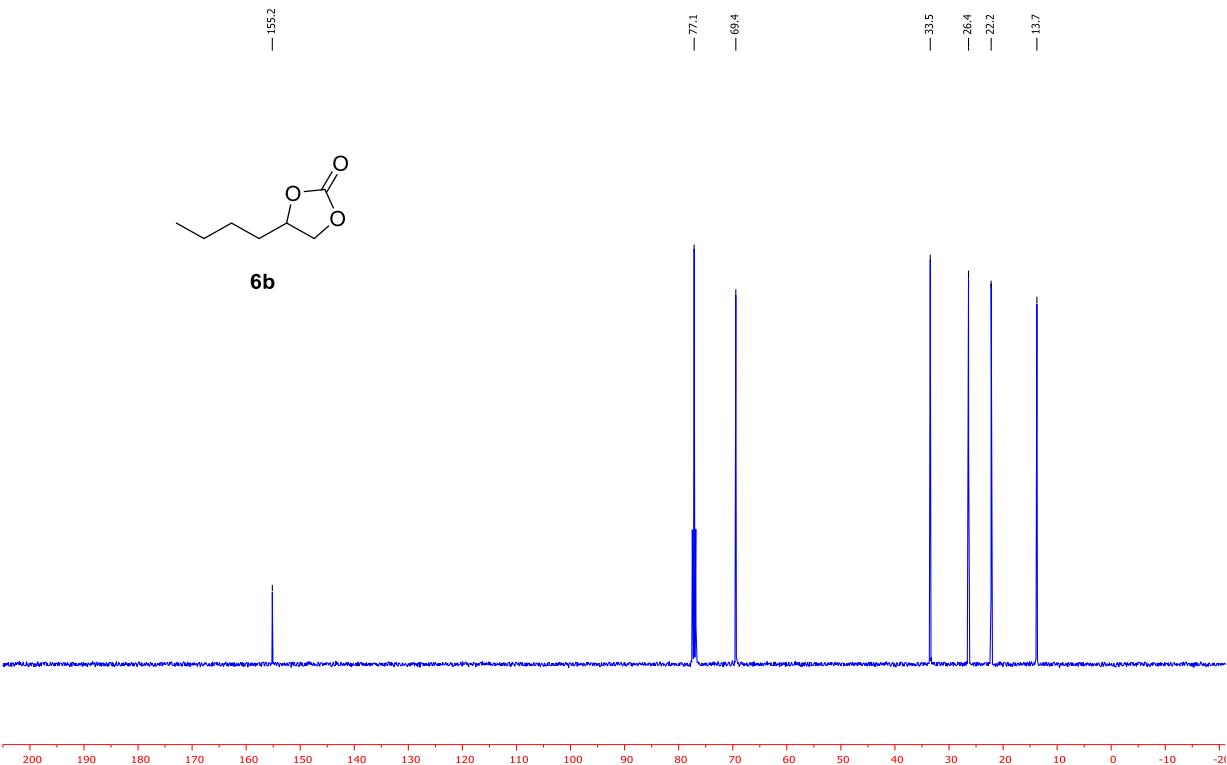
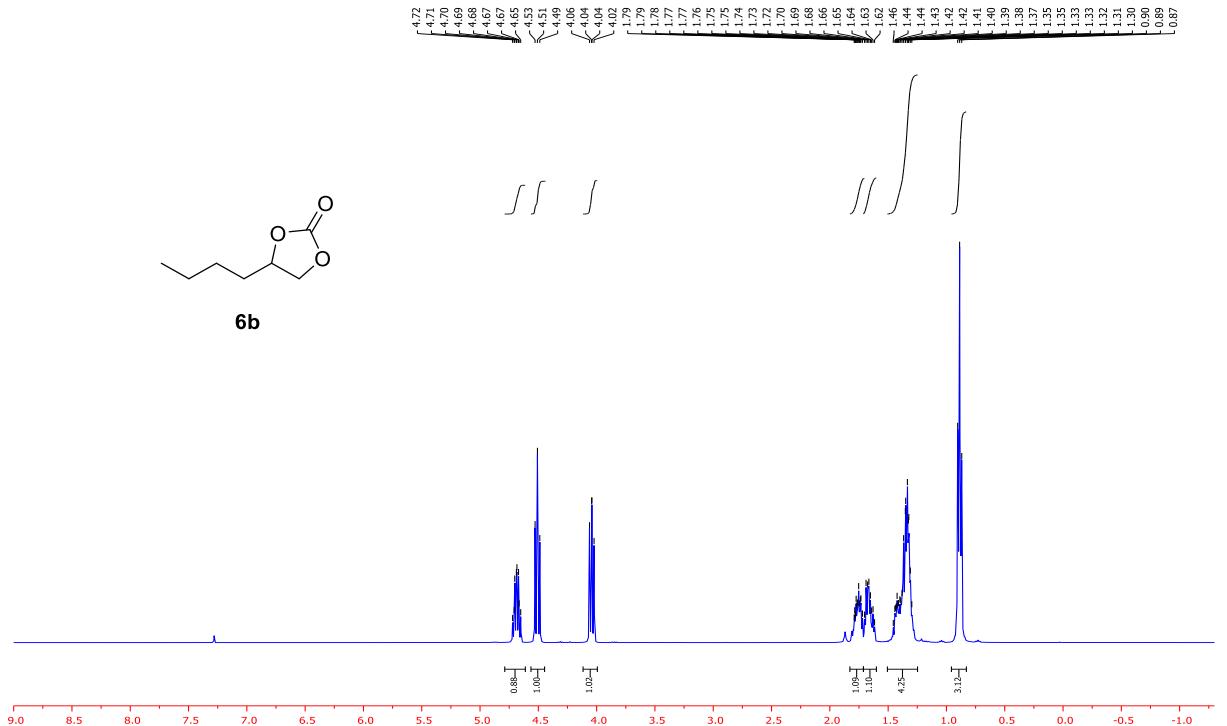
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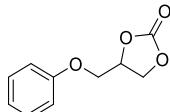




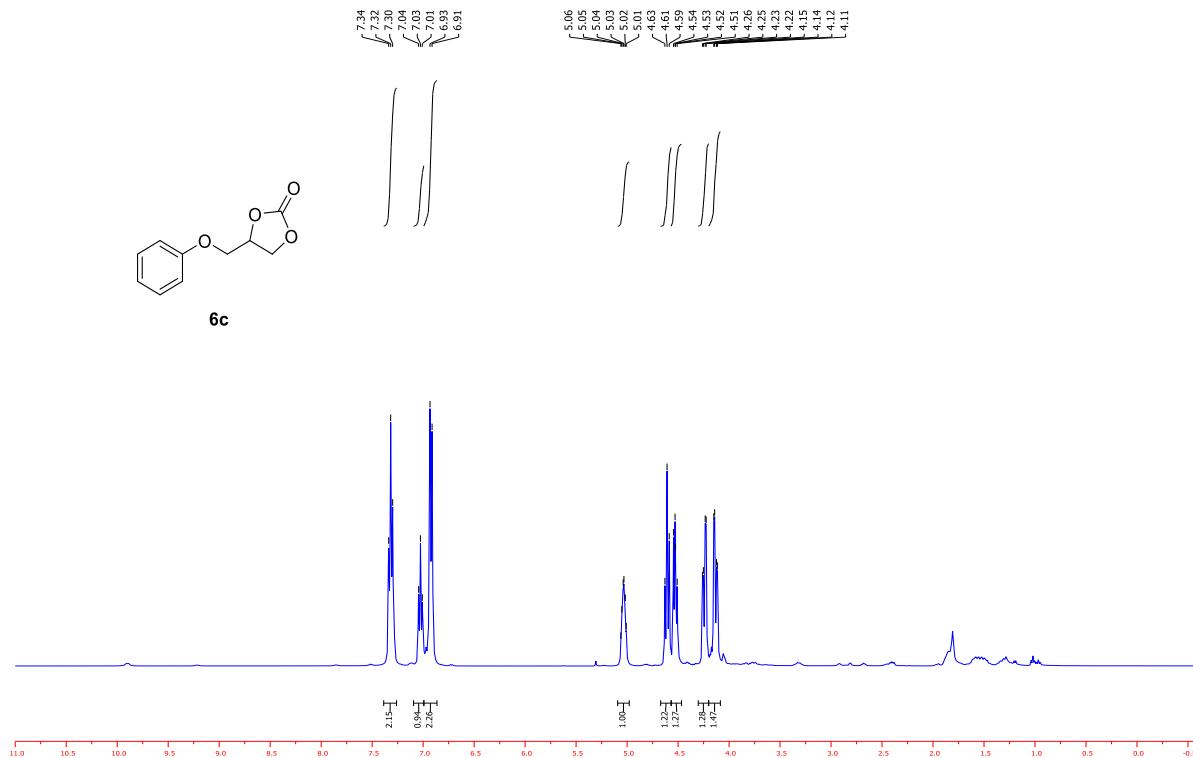
—155.1      —159.7      ~129.2      ~126.0      —78.1      —71.2







**6c**



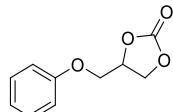
— 157.8  
— 154.8

— 129.7

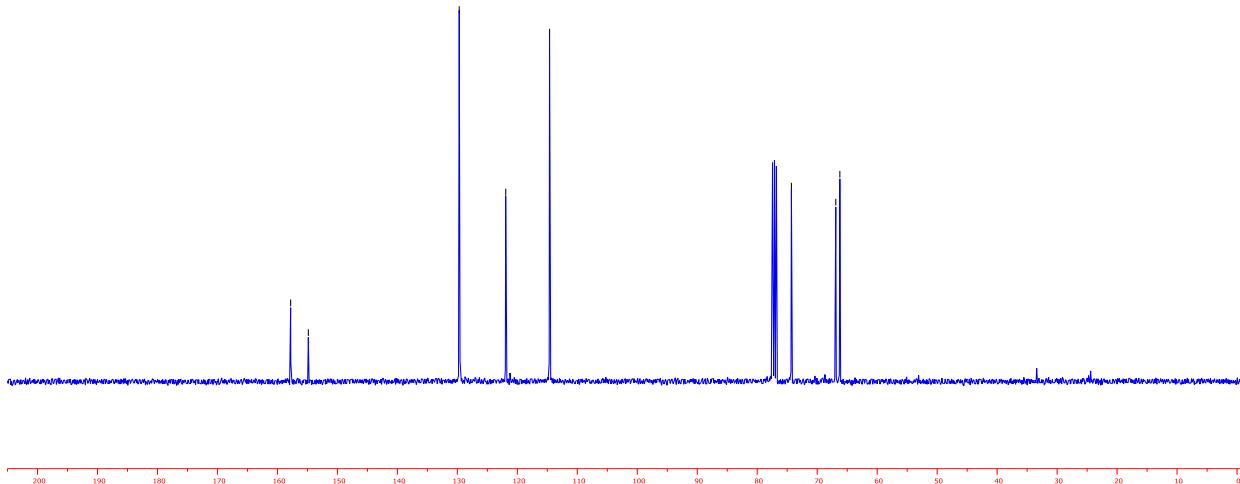
— 121.9

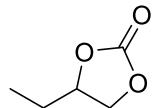
— 114.6

— 74.3  
— 66.9  
— < 66.2

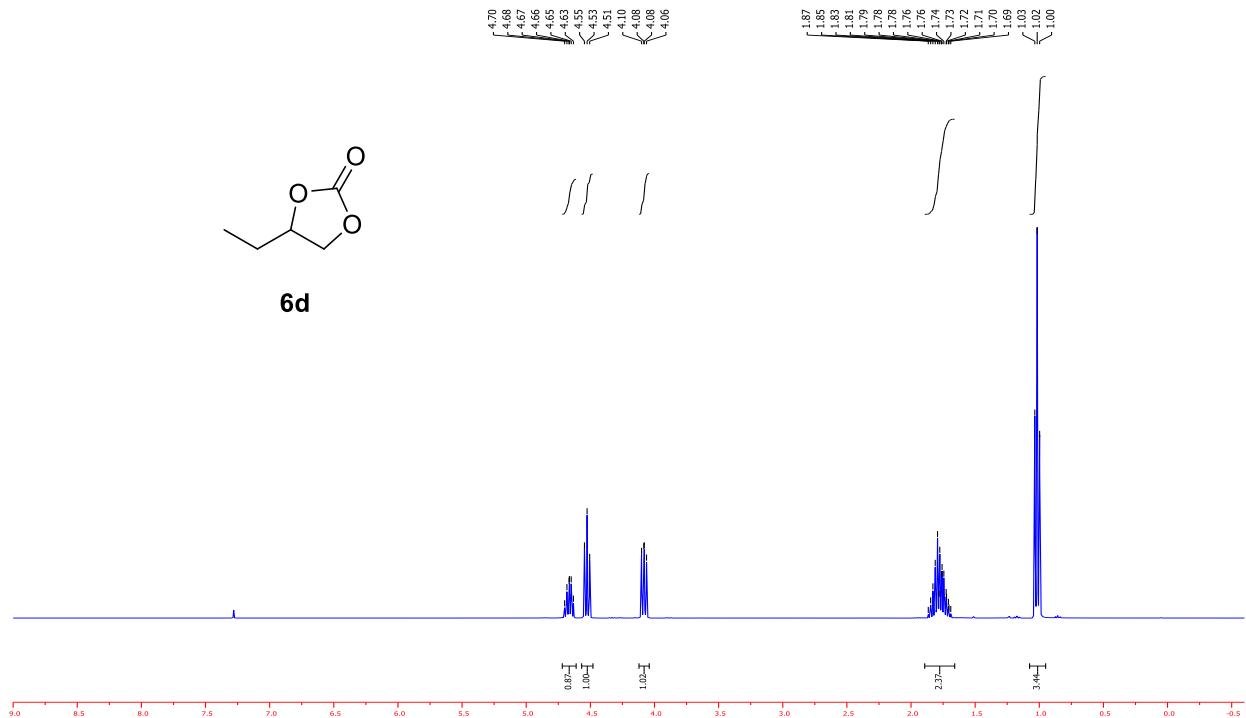


**6c**





**6d**



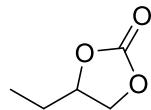
— 155.2

— 78.1

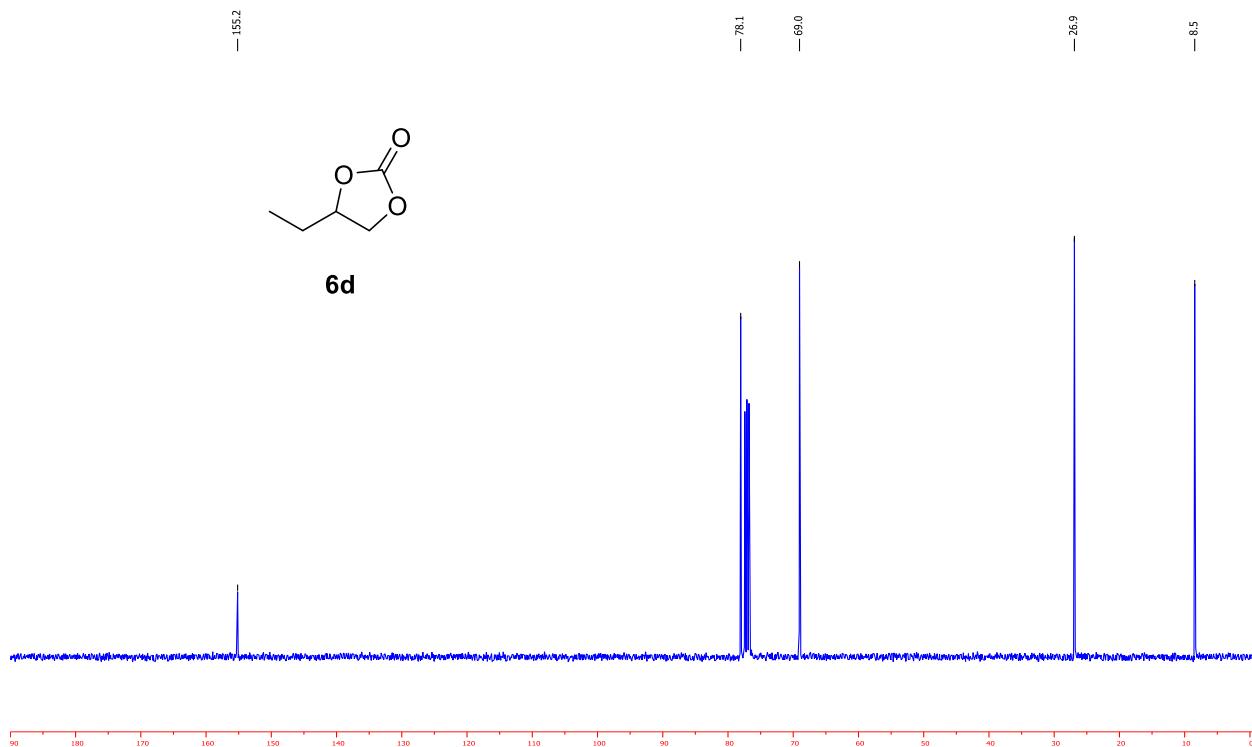
— 69.0

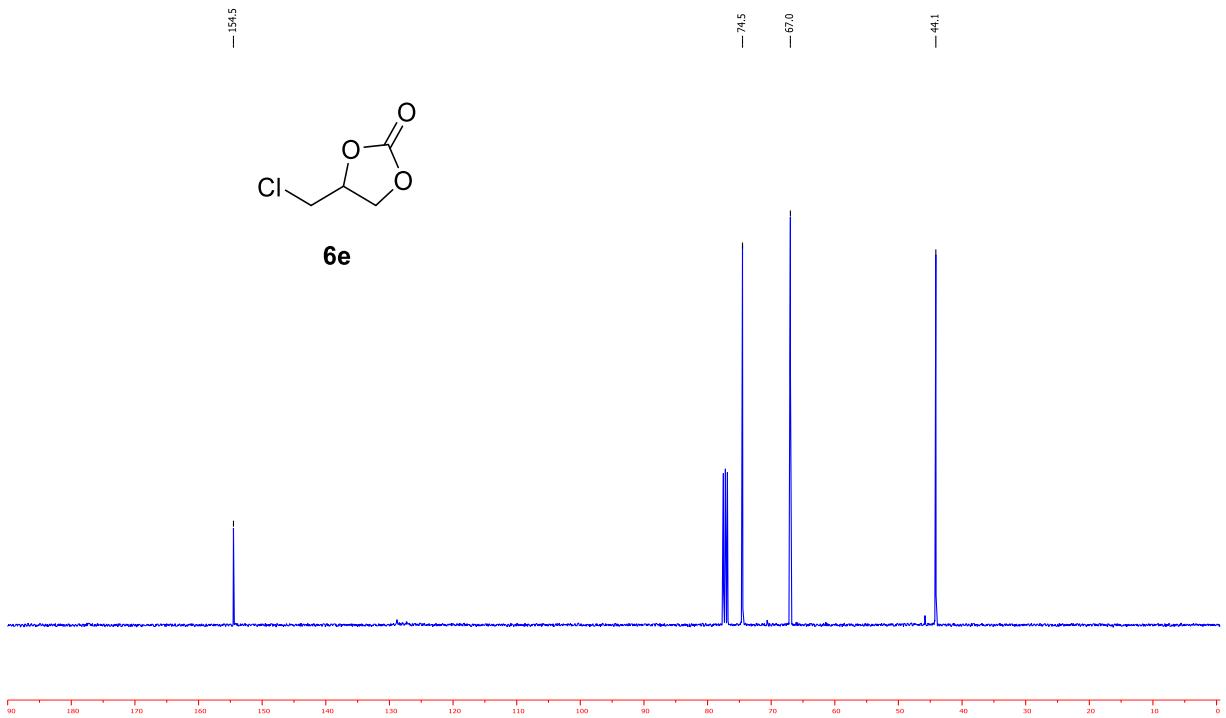
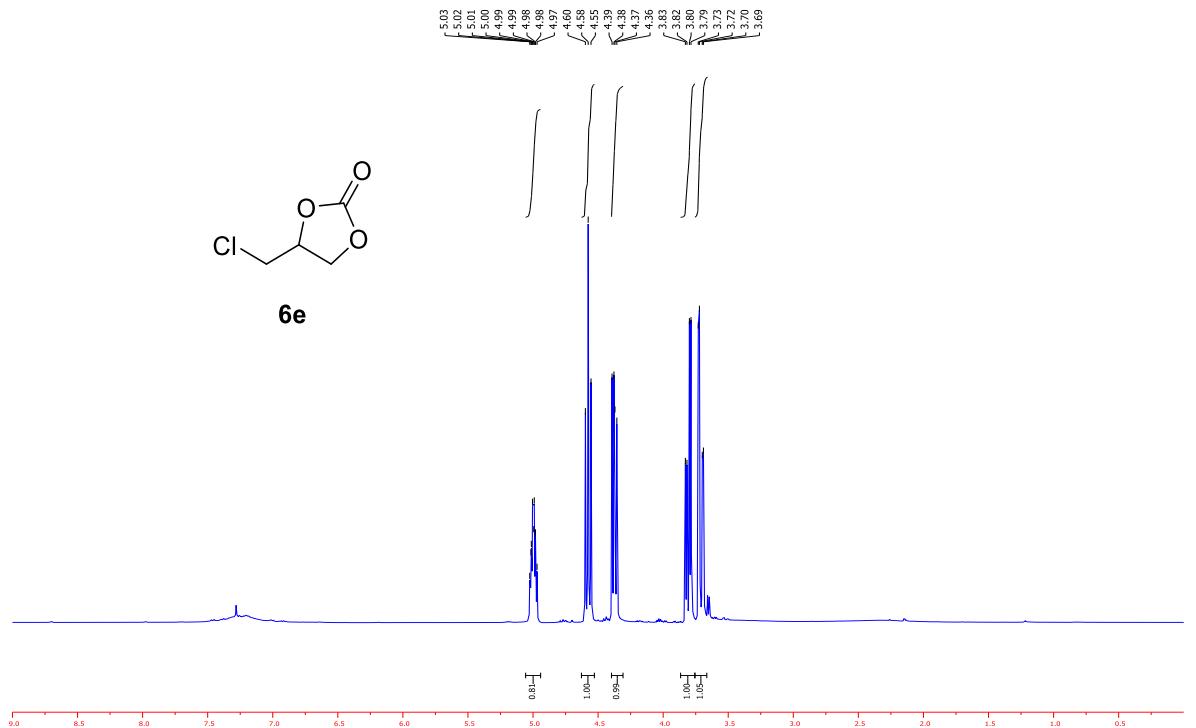
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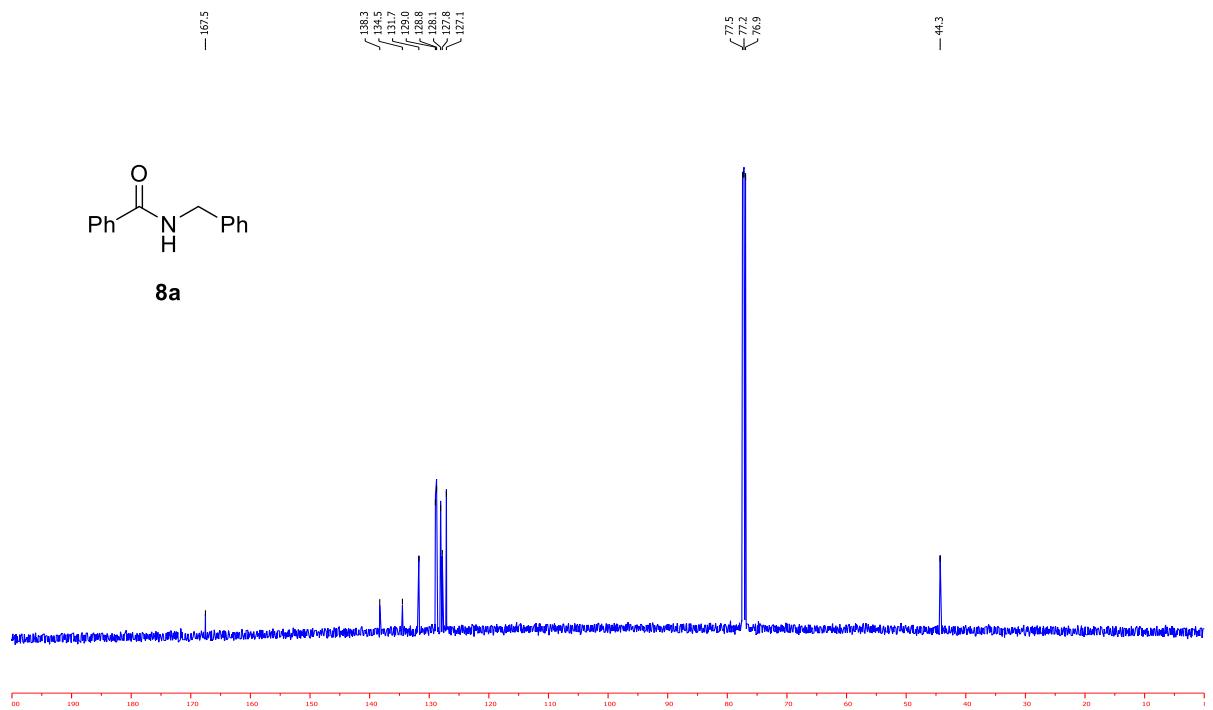
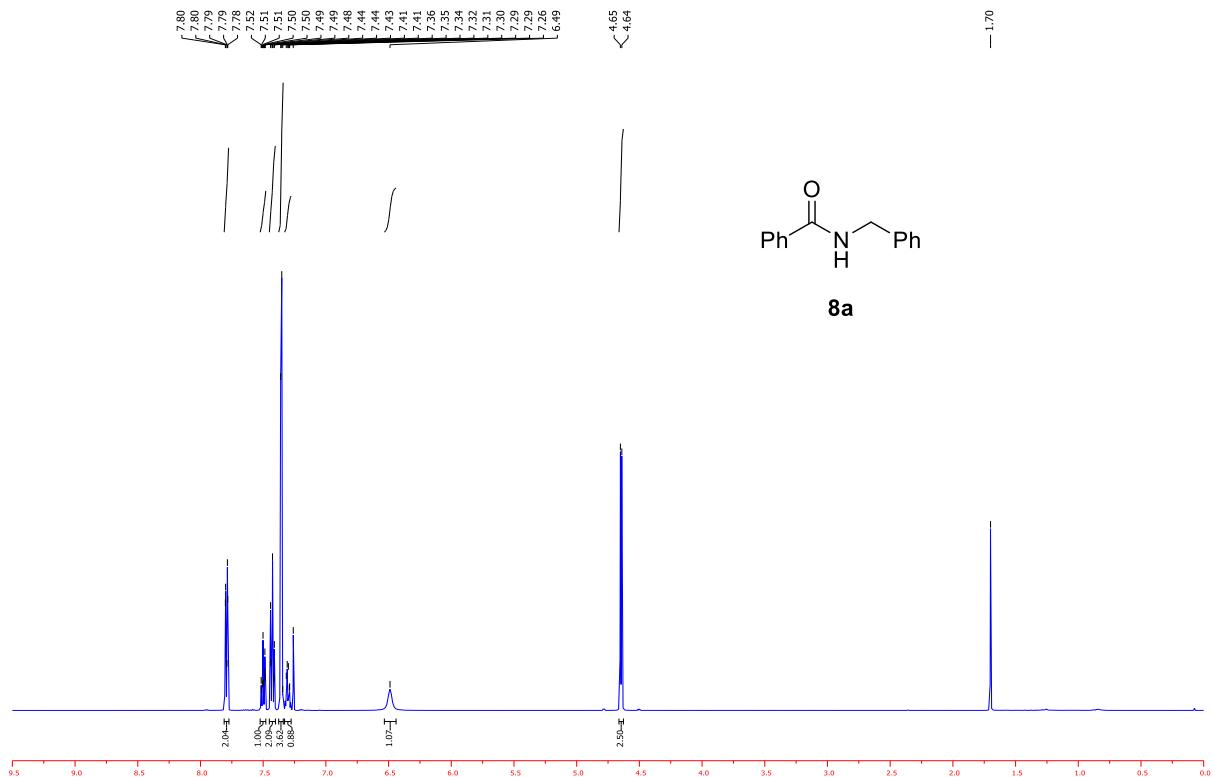
— 8.5

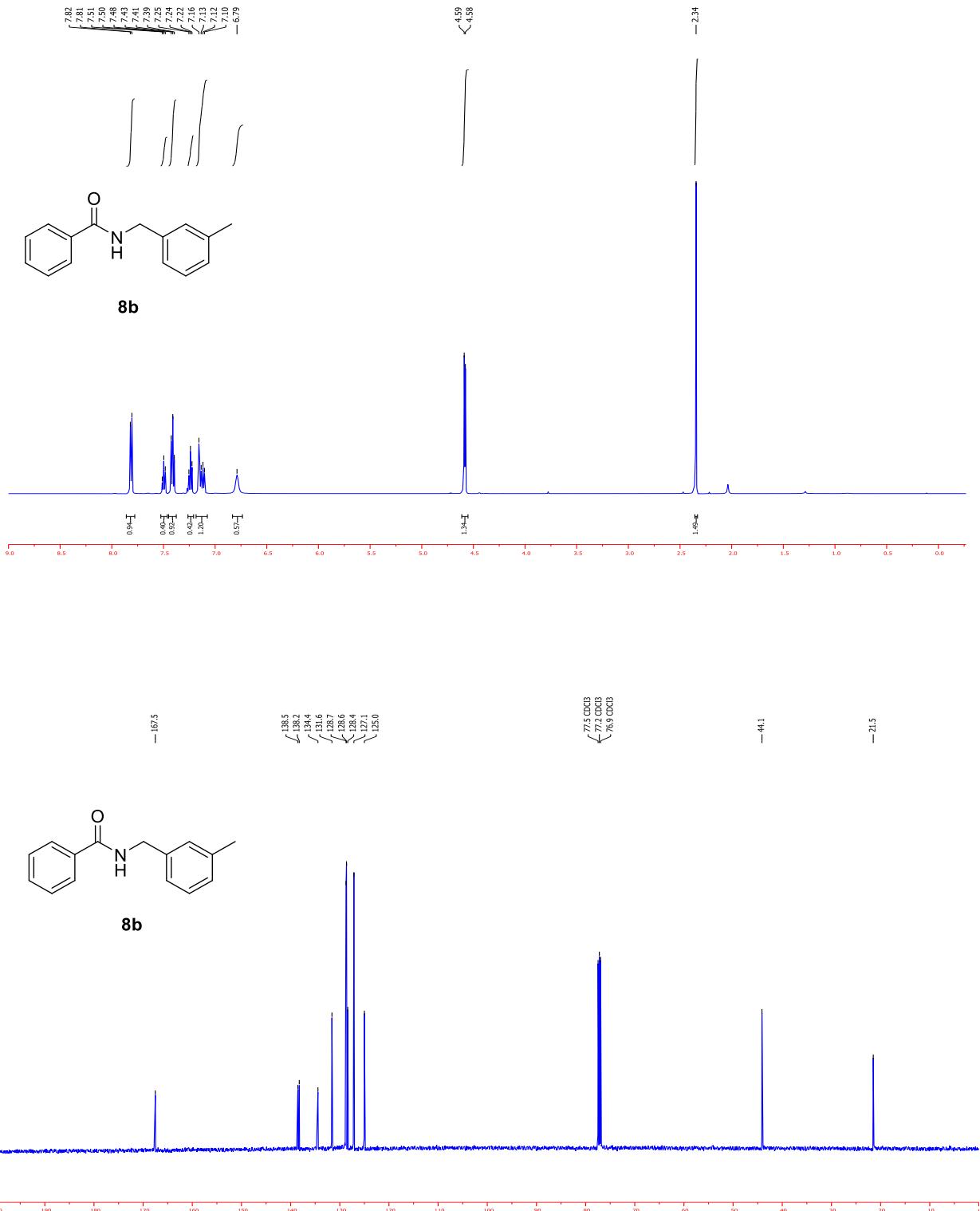


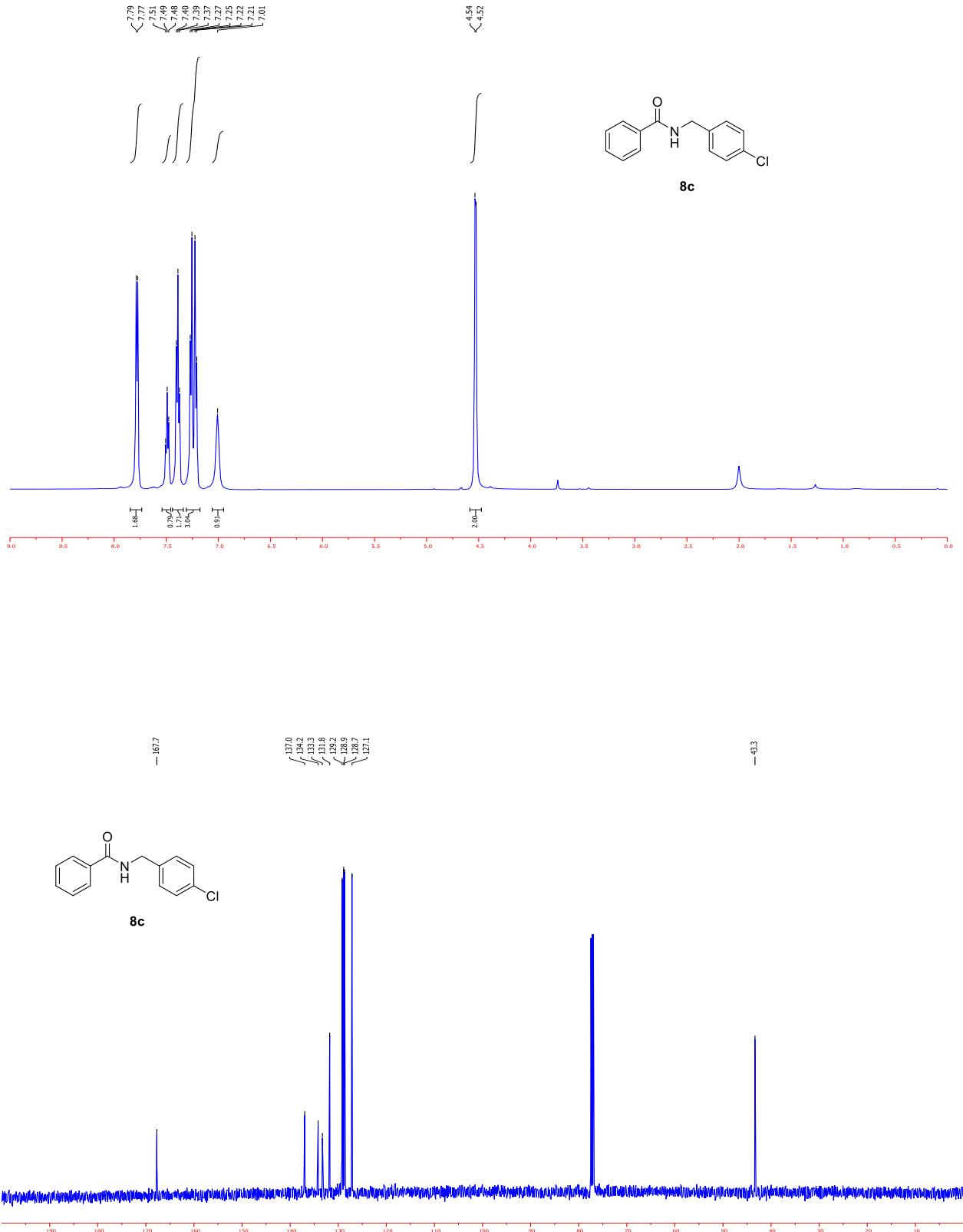
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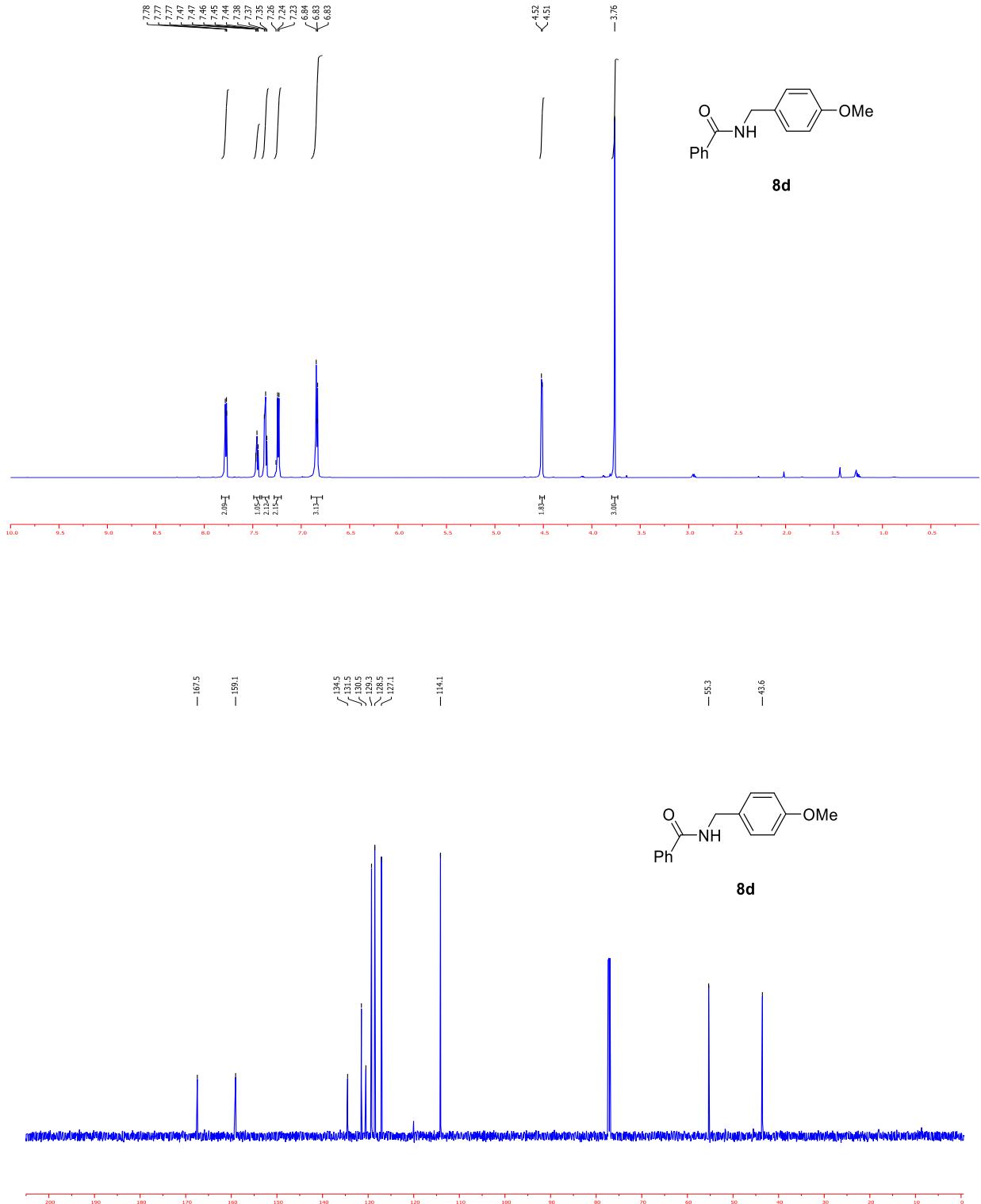


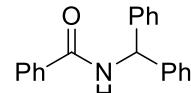
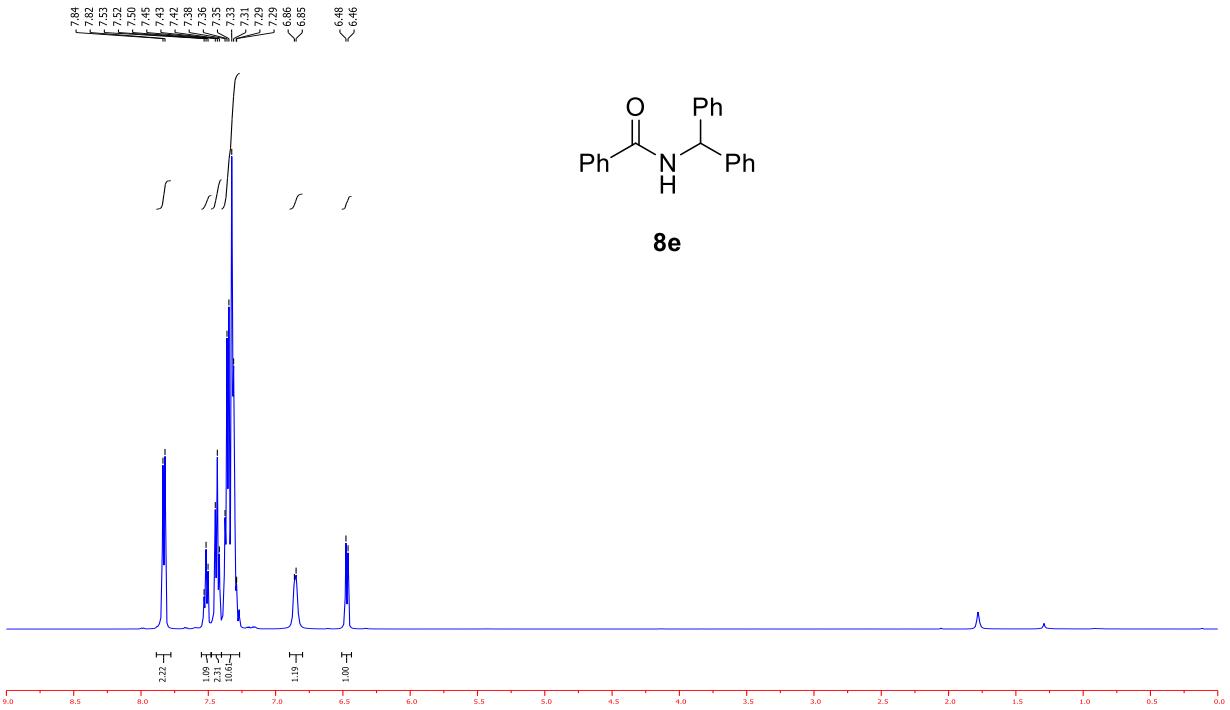




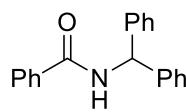
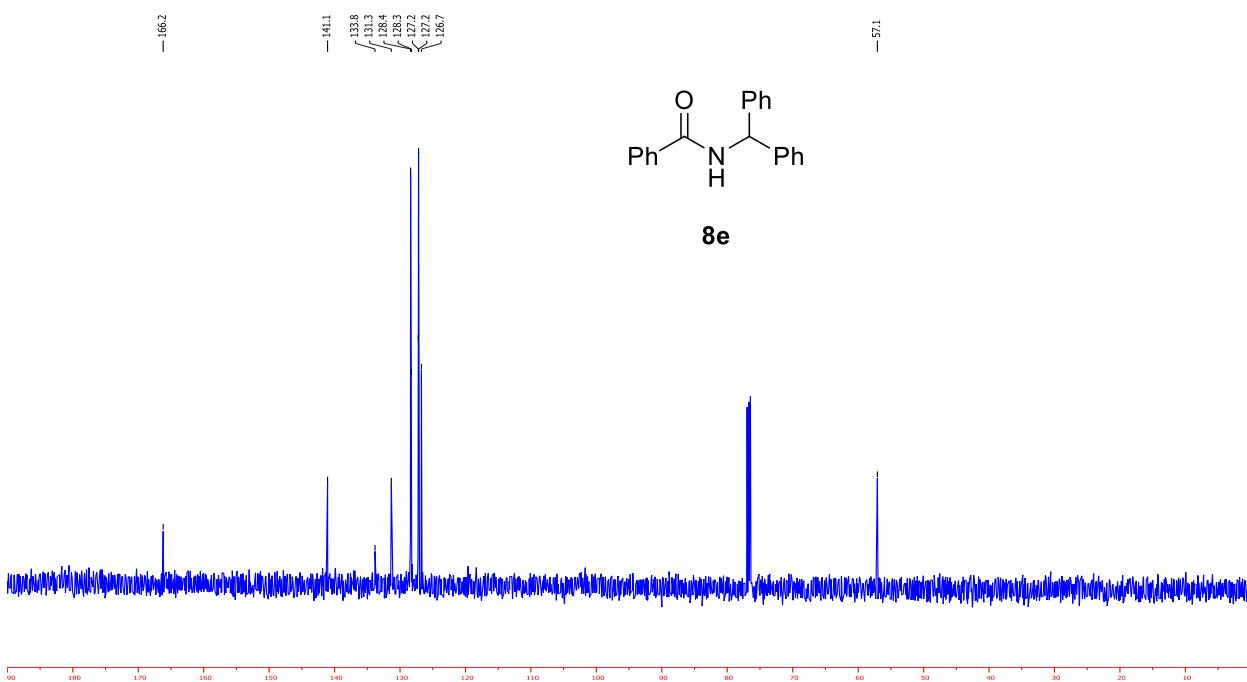




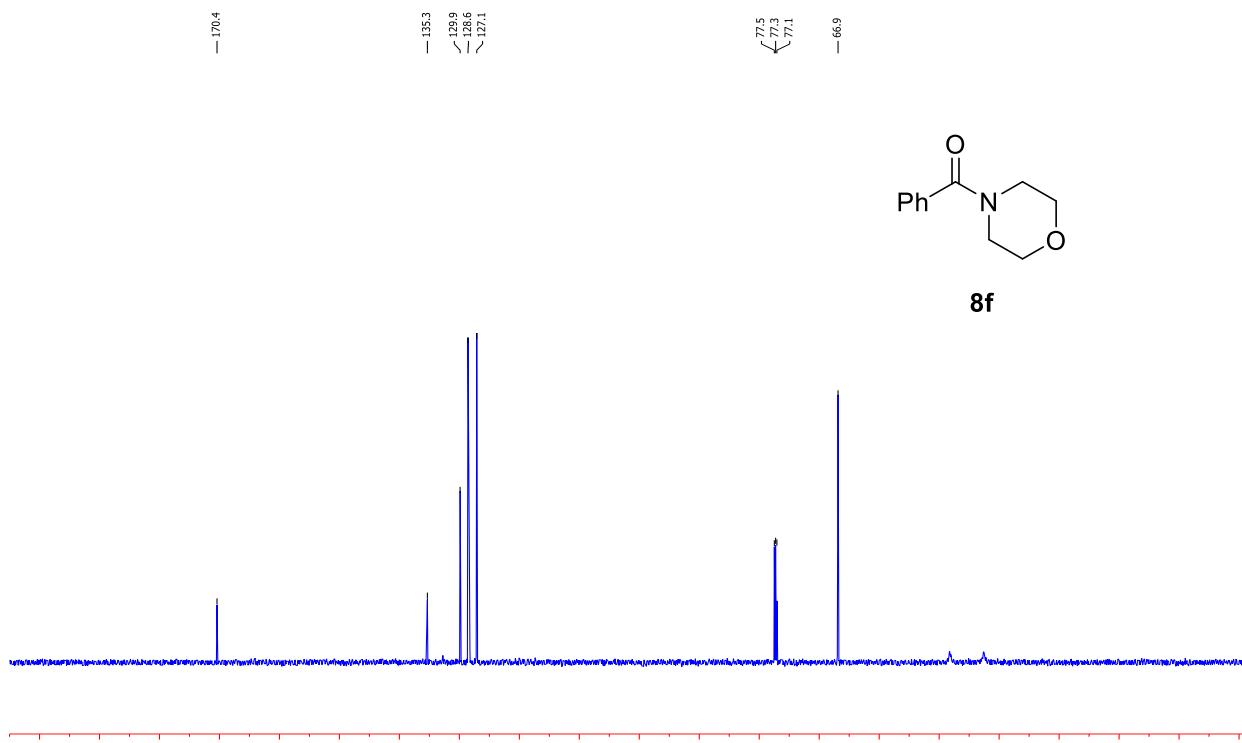
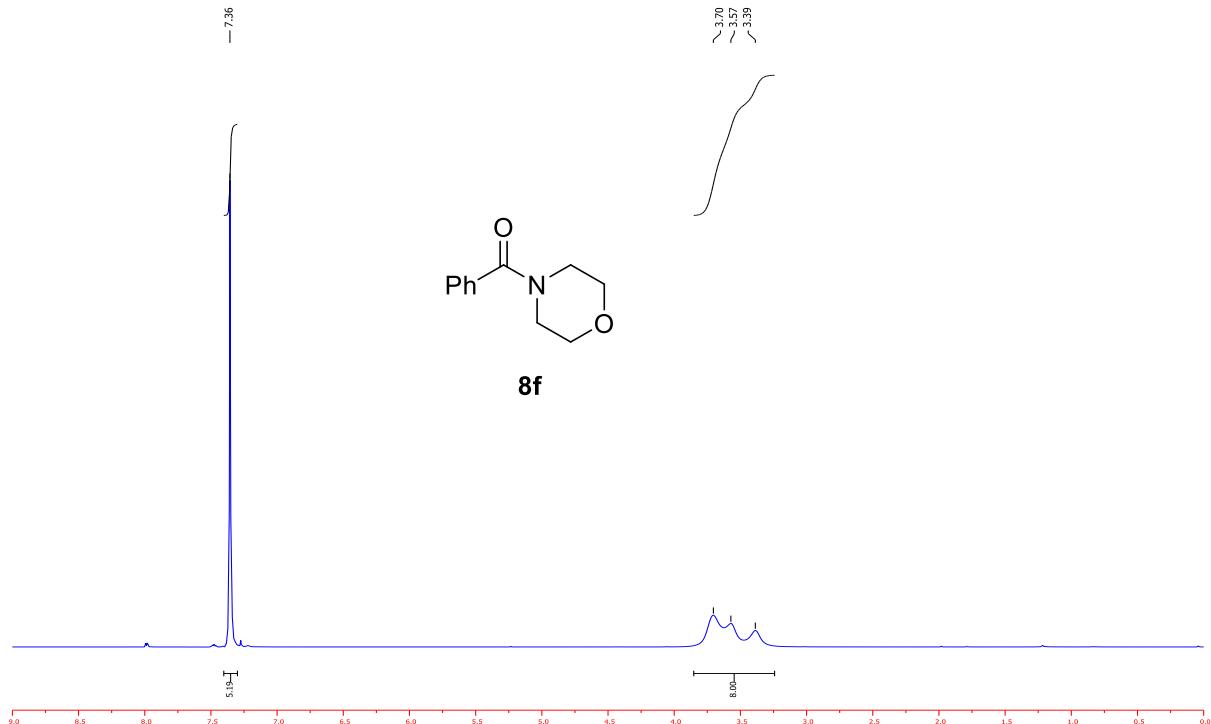




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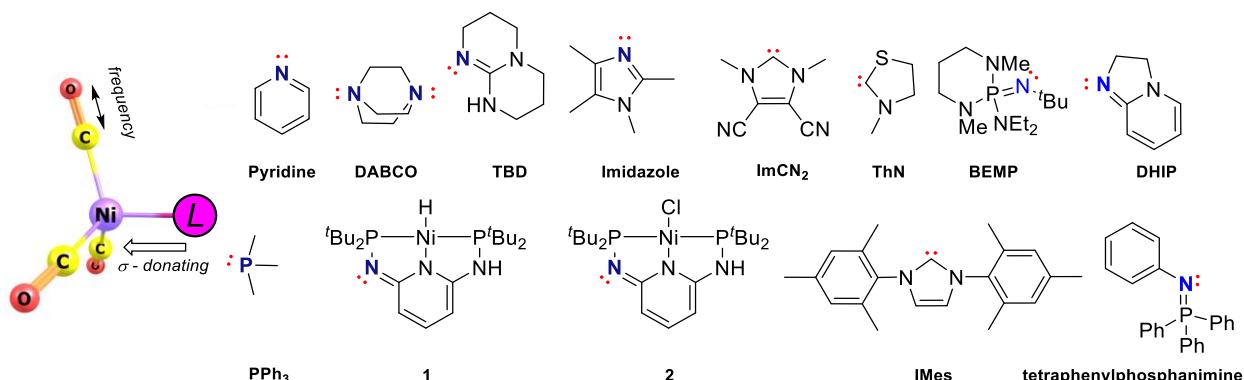
8e



## Computational Details

### Computational methods

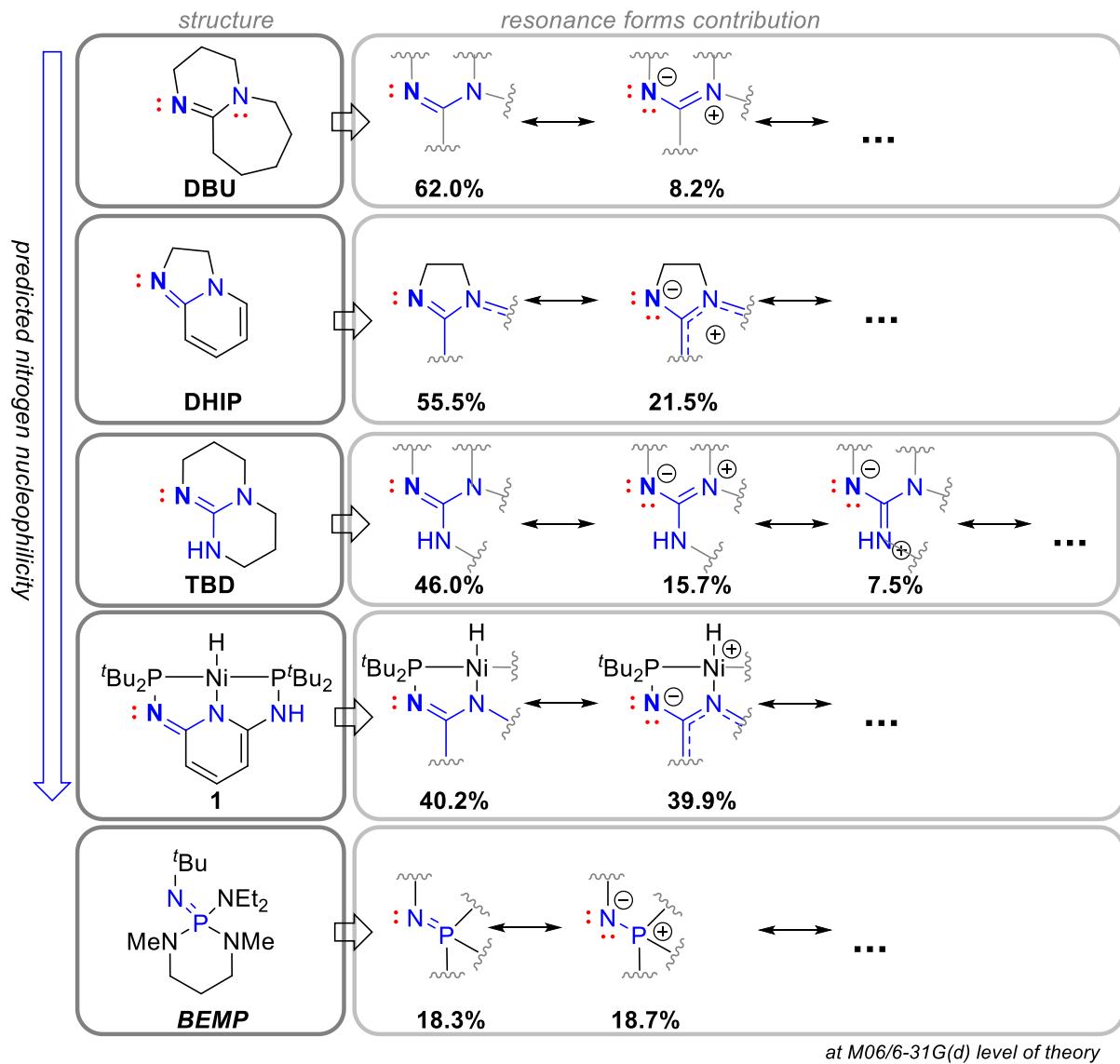
All geometry optimizations were carried with Gaussian 09 program at M06/6-31G(d,p) method level applying *UltraFine* integration grid.<sup>1</sup> For transition metals, the SDD pseudo potential was applied with the corresponding basis set.<sup>2</sup> The frequency calculations required for the Tolman analysis were scaled by 0.955. The Natural Population Analysis and The Natural Resonance Theory (NBO-NRT) calculations were performed with the NBO6 program at M06/6-31G(d) method level.<sup>3,4</sup> The obtained resonance structures from NRT analysis which have the larger contribution than 1% were summed to obtain more general representation of the zwitterionic resonance forms.



Ligand ( <i>L</i> )	$\nu(\text{CO})^a$	NPA <sup>c</sup>	$\nu(\text{CO})^b$
Pyridine	2075.0	-0.47	2070.5
DABCO	2071.6	-0.51	
TBD	2067.3	-0.62	
Imidazole	2066.8	-0.53	2051.7
ImCN <sub>2</sub>	2066.6	0.20	2066.2
DHIP	2066.8	-0.56	
PMe <sub>3</sub>	2065.9	0.87	2065.2
ThN	2063.0	-0.19	2061.0
<b>2</b>	2064.0	-0.99	
<b>1</b>	2060.7	-1.00	
IMes	2051.4	0.15	2050.5
BEMP	2060.7	-1.18	

tetraphenylphosphanimine	2062.4	-1.09
<sup>a</sup> Frequencies are in [cm <sup>-1</sup> ] at M06/6-31G(d,p)/SDD scaled by 0.955. <sup>b</sup> Values taken from the reference <sup>5</sup> . <sup>c</sup> Natural Population Analysis charge on the nucleophilic atom.		

**Figure S2.** Calculated Tolman Electronic Parameters for sigma donating ligands.



**Figure S3.** The contribution of resonance forms in DBU, TBD, **1** and BEMP from NBO analysis.

## Geometries

TBD



(Ground state)

E(M06/6-31G(d,p)) = -438.614928884 after 1 cycles  
Conv=0.86D-08 -V/T = 2.0037

Temp. 298.150 K Press. 1.00000 Atm.

E + zero-point Energies = -438.411029

E + thermal Energies = -438.402259

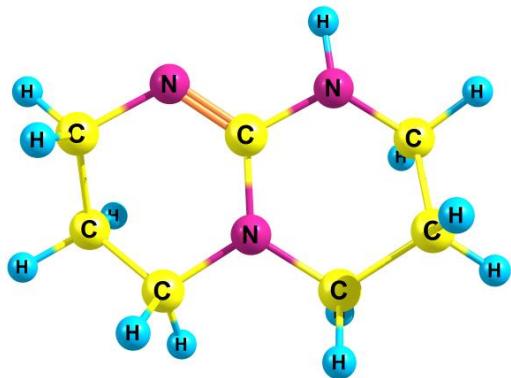
E + thermal Enthalpies = -438.401315

E + thermal Free Energies = -438.444759

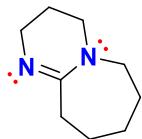
Geometry at E(M06/6-31G(d,p))

Charge: 0 multiplicity: 1

H -0.3933743333 -1.5572405129 -1.3086324780  
H -0.4992457321 -1.9560241525 0.4093353897  
H 0.8379609090 -0.0512214345 1.0480889753  
H 1.6792914159 -0.8094024231 -0.3133741947  
H 0.6527919715 0.8434328211 -1.8640603201  
H 1.4960795644 1.6950786043 -0.5790183862  
H -2.9035530410 -1.9726894982 -0.5206316399  
H -2.7555651795 -1.5233460910 1.1802106975  
H -3.6913038972 0.8645255494 1.8325994363  
H -4.7770743318 1.6753967996 0.6910473419  
H -4.3674401785 -0.0939519849 -0.9855775224  
H -4.9494911165 -0.8367229596 0.5173263754  
C -0.4479426140 -1.1163954855 -0.2993133727  
C 0.7729979214 -0.2651539167 -0.0266640827  
C 0.6347513007 1.0469160757 -0.7781527353  
N -0.5704124451 1.7519331929 -0.4162406871  
C -2.8532316412 -1.1097372201 0.1594398678  
N -1.6685855438 -0.3392893900 -0.1665645826  
C -1.6057373459 1.0399036566 -0.1681693651  
N -2.7972706292 1.6936144387 0.0845952214  
C -3.8897230921 1.0386250599 0.7584459086  
C -4.1185499620 -0.2867365409 0.0644680398  
H -2.6444780369 2.6802548718 0.2351711010



**DBU**



(Ground state)

E(M06/6-31G(d,p) ) = -461.857973851 after 1 cycles  
 Conv=0.93D-08 -V/T = 2.0040

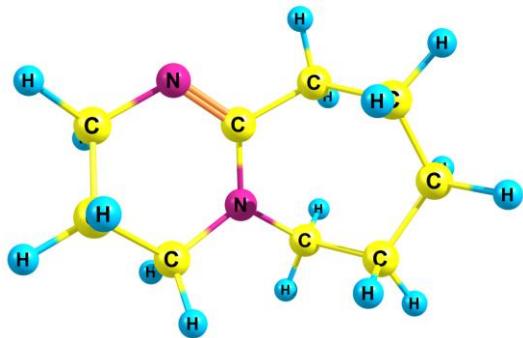
Temp. 298.150 K Press. 1.00000 Atm.  
 E + zero-point Energies = -461.614147  
 E + thermal Energies = -461.604408  
 E + thermal Enthalpies = -461.603464  
 E + thermal Free Energies = -461.649039

Geometry at E(M06/6-31G(d,p) )

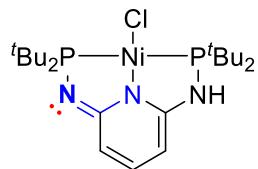
Charge: 0 multiplicity: 1

```
C 3.9995983207 0.8263089064 -0.3839798577
C 4.5356547364 -0.3267395458 0.4536212074
C 3.4947062224 -1.0496463941 1.2950767806
C 2.3399604923 -1.6097437141 0.4729613640
N 1.3465695207 -0.6206646144 0.0956905156
C 1.5619061511 0.3276718755 -0.8821894670
C 2.9576477920 0.4298127587 -1.4330876314
C 0.1498023588 -0.5728019573 0.9245855410
C -0.5838596366 0.7354995706 0.7313860667
C -0.6384425077 1.0483142246 -0.7535244500
N 0.6879151841 1.1516780144 -1.3238427602
H 4.8441895986 1.3033555653 -0.8949699042
H 3.5658046709 1.5973194738 0.2698479963
H 5.3362616302 0.0421643455 1.1066107419
H 5.0079465690 -1.0583020637 -0.2208192971
H 3.9806714747 -1.8709678687 1.8374999685
```

H 3.0816117031 -0.3716699801 2.0568976420  
 H 2.7279331736 -2.1192142325 -0.4198323456  
 H 1.8116702404 -2.3805756492 1.0458609871  
 H 3.2578702246 -0.5082738287 -1.9222275331  
 H 2.8957266233 1.1903830920 -2.2142044349  
 H -0.5088170999 -1.4221413190 0.6793500427  
 H 0.4470256449 -0.6948595535 1.9769543895  
 H -0.0406468893 1.5434647401 1.2388989792  
 H -1.5815764704 0.6759835448 1.1785014157  
 H -1.2075567281 0.2575628215 -1.2717612301  
 H -1.1755729998 1.9850817879 -0.9373047266



## 2, PN<sup>3</sup>PNi-Cl



(Ground state)

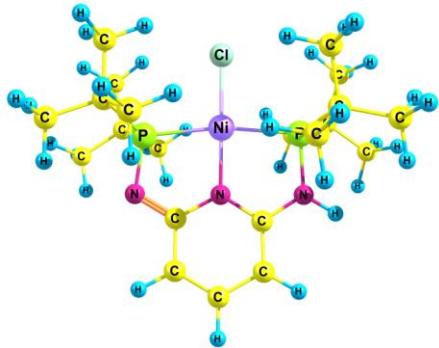
E(M06/6-31G(d,p)/SDD) = -2301.81607111 after 1 cycles  
 Conv=0.30D-08 -V/T = 2.0323 <S\*\*2> = RHF/RKS

Temp. 298.150 K Press. 1.00000 Atm.  
 E + zero-point Energies = -2301.232183  
 E + thermal Energies = -2301.197186  
 E + thermal Enthalpies = -2301.196241  
 E + thermal Free Energies = -2301.295201

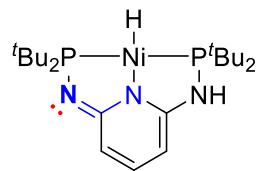
Geometry at E(M06/6-31G(d,p)/SDD)  
 Charge: 0 multiplicity: 1  
 H 1.3795816673 0.5838137666 -5.0388863507  
 C 1.1959541756 0.3901727424 -3.9836955625

C 0.5440277458 -0.7523107514 -3.6068457269  
 C 1.6308575004 1.3221297552 -3.0289192802  
 C 1.3790403123 1.0385219674 -1.7000706806  
 C 0.2940054848 -1.0216545569 -2.2295856280  
 H 0.1919701616 -1.4863839138 -4.3236903922  
 H 2.1364869145 2.2421303141 -3.3069664474  
 P -0.5339094627 -2.2610035296 -0.2059981683  
 P 1.6406359135 1.3896152565 0.9308899247  
 Ni 0.4693043790 -0.4574546781 0.5663667626  
 Cl 0.0377966024 -0.8307885578 2.6801640537  
 C 0.8030254076 2.8338461521 1.7869944654  
 C 3.4249604863 1.1299752156 1.4697837588  
 C -0.6808968761 2.6843303794 1.4333508310  
 H -0.8404445008 2.6436168649 0.3473024808  
 H -1.1032097090 1.7764055970 1.8798193284  
 H -1.2334629724 3.5506886918 1.8229132081  
 C 1.2983250425 4.1905720925 1.2881519930  
 H 0.7505238688 4.9815450115 1.8187037654  
 H 2.3654611083 4.3532606022 1.4751759885  
 H 1.1014460966 4.3261175709 0.2181085394  
 C 0.9687452182 2.7330696277 3.3024306799  
 H 0.3199030742 3.4811985032 3.7784285478  
 H 0.6741127203 1.7451100909 3.6774271343  
 H 1.9964830436 2.9440692750 3.6227802058  
 C 4.2423243765 2.4163416898 1.5436290564  
 H 3.9087357297 3.0766203208 2.3526990299  
 H 5.2934166539 2.1636713078 1.7421722048  
 H 4.2204942649 2.9809628641 0.6015861504  
 C 3.4522493338 0.4039589568 2.8157927533  
 H 2.8731085745 -0.5268937304 2.7850074114  
 H 4.4941453749 0.1572748329 3.0632543067  
 H 3.0532404213 1.0132169305 3.6334059027  
 C 4.0337511442 0.2068450137 0.4087756895  
 H 3.4554256259 -0.7193835321 0.2939162541  
 H 4.0995560996 0.6865122248 -0.5749798002  
 H 5.0506295299 -0.0683481445 0.7194973767  
 C -2.3942748295 -2.3164538213 0.0594509279  
 C -2.8362824859 -0.8537371484 -0.0630007465  
 H -3.9334678865 -0.8028015089 -0.0193537469  
 H -2.4344836175 -0.2448981118 0.7569312337  
 H -2.5178020104 -0.4115571814 -1.0162000492  
 C -2.7875770523 -2.8459975301 1.4353131765  
 H -3.8586535190 -2.6551352051 1.5942550367  
 H -2.6399328259 -3.9298690053 1.5102554190  
 H -2.2312181149 -2.3563890474 2.2437753134  
 C -3.0794858241 -3.1332890943 -1.0356487158  
 H -2.8414335193 -4.2004947058 -0.9667155180  
 H -4.1683253921 -3.0303700848 -0.9227619991  
 H -2.7935030478 -2.7856795904 -2.0333161997  
 C 0.3533864694 -3.8661110698 0.2166319013  
 C -0.1676672159 -5.0113449165 -0.6499217180  
 H 0.4967009403 -5.8799180916 -0.5351128276  
 H -1.1710301491 -5.3286857771 -0.3404260488  
 H -0.1980267904 -4.7346977723 -1.7098202499  
 C 0.2742343015 -4.2417006508 1.6940080530  
 H -0.7351769260 -4.5333748694 2.0002493843

H 0.9308048741 -5.1064203891 1.8682905287  
 H 0.6020848767 -3.4231694002 2.3443753688  
 C 1.8195950576 -3.5886090902 -0.1313687191  
 H 1.9433970828 -3.2786488448 -1.1759131697  
 H 2.2373574428 -2.8085528027 0.5212393050  
 H 2.4067250782 -4.5041852497 0.0258498962  
 N 0.7533500240 -0.0955680030 -1.2857648758  
 N -0.3513965083 -2.1118606681 -1.8586471525  
 N 1.7560593212 1.9192048671 -0.6950611766  
 H 2.2992697147 2.7214815396 -0.9889733977



**1, PN<sup>3</sup>PNi-H**



(Ground state)

E(M06/6-31G(d,p)/SDD ) = -1842.45322525 after 1 cycles  
 Conv=0.35D-09 -V/T = 2.0382

Temp. 298.150 K Press. 1.00000 Atm.  
 E + zero-point Energies = -1841.866939  
 E + thermal Energies = -1841.833166  
 E + thermal Enthalpies = -1841.832221  
 E + thermal Free Energies = -1841.928266

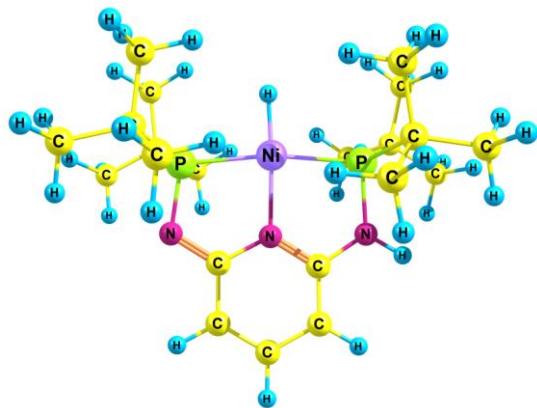
Geometry at E(M06/6-31G(d,p)/SDD )

Charge: 0 multiplicity: 1

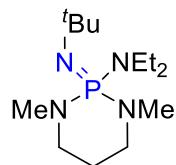
H 1.3449564845 0.6268749819 -5.0628988847  
 C 1.1730002020 0.4274025343 -4.0082338920  
 C 0.5139560650 -0.7116829947 -3.6393046037  
 C 1.6333944276 1.3497020912 -3.0577833366  
 C 1.3913682472 1.0541697996 -1.7321935076  
 C 0.2812732422 -0.9901179537 -2.2630646652

H 0.1514069156 -1.4304410961 -4.3639915522  
 H 2.1463354868 2.2617845224 -3.3406799763  
 P -0.5067510809 -2.2204136287 -0.2094790916  
 P 1.6260794434 1.3461935328 0.9200318993  
 Ni 0.4919201679 -0.4524324148 0.5358104918  
 H 0.2242491145 -0.8174777106 1.9397716390  
 C 0.7725332400 2.7824113593 1.7704761070  
 C 3.3958552338 1.0866449915 1.5045574836  
 C -0.6869394942 2.6671493159 1.3243617796  
 H -0.7834920306 2.6894097270 0.2326540860  
 H -1.1379200283 1.7372154634 1.6872773070  
 H -1.2592482604 3.5102317667 1.7327215217  
 C 1.3061217373 4.1524641860 1.3673221722  
 H 0.7221491420 4.9270377354 1.8811844000  
 H 2.3543262867 4.3019748942 1.6397705545  
 H 1.1925808407 4.3282116214 0.2925089600  
 C 0.8403153273 2.6059745574 3.2836154788  
 H 0.1609678389 3.3249257261 3.7589391150  
 H 0.5248133288 1.6008867158 3.5870994597  
 H 1.8429630899 2.7931399310 3.6822374224  
 C 4.2078317851 2.3635373223 1.6756628260  
 H 3.8468250379 2.9809328187 2.5042280232  
 H 5.2506759376 2.1006132518 1.8970460187  
 H 4.2183225008 2.9754856741 0.7656198361  
 C 3.3656526397 0.2962723064 2.8118492656  
 H 2.8034514873 -0.6373403268 2.6967581677  
 H 4.3937742651 0.0443754813 3.1024045420  
 H 2.9191673447 0.8589991320 3.6365816212  
 C 4.0498866182 0.2150055494 0.4306604356  
 H 3.4733130690 -0.6980309083 0.2426107484  
 H 4.1603364434 0.7423139560 -0.5221592991  
 H 5.0492502043 -0.0817079833 0.7728095256  
 C -2.3589595569 -2.2846499602 0.0853990668  
 C -2.8153961160 -0.8388356629 -0.1257392710  
 H -3.9067112722 -0.7828136589 -0.0183108017  
 H -2.3639708868 -0.1659791338 0.6130740784  
 H -2.5556078269 -0.4768665680 -1.1267957126  
 C -2.6958973482 -2.7077403585 1.5087208336  
 H -3.7609997319 -2.5193729644 1.6988107331  
 H -2.5230244166 -3.7765041209 1.6715260191  
 H -2.1172199703 -2.1439086404 2.2500035790  
 C -3.0727495623 -3.1753953500 -0.9257674019  
 H -2.8604475044 -4.2365576718 -0.7689572214  
 H -4.1574769093 -3.0374427156 -0.8212849219  
 H -2.7843857926 -2.9167123944 -1.9486250390  
 C 0.3766437638 -3.8229106071 0.2139197652  
 C -0.2356645172 -5.0256567598 -0.4934248113  
 H 0.4326454939 -5.8905340103 -0.3839221164  
 H -1.2015493684 -5.3065421738 -0.0608605578  
 H -0.3720872375 -4.8327721125 -1.5625923460  
 C 0.4328455656 -4.0539893049 1.7197204984  
 H -0.5489783459 -4.2650193757 2.1517283208  
 H 1.0743776600 -4.9217066577 1.9244520433  
 H 0.8540809246 -3.1873287855 2.2413805573  
 C 1.8037674364 -3.6143467057 -0.2953928029  
 H 1.8265596806 -3.4462779121 -1.3764254749

H 2.2788799770 -2.7573451882 0.1996985347  
 H 2.4021498789 -4.5065495290 -0.0694566724  
 N 0.7571241555 -0.0684951336 -1.3364363860  
 N -0.3598795667 -2.0776583825 -1.8717872968  
 N 1.7848275875 1.9019303947 -0.6999423481  
 H 2.3334295053 2.7088275156 -0.9679819269



BEMP



(Ground state)

E(RM06/6-31G(d,p)) = -1073.86048876 after 1 cycles  
 Conv=0.33D-08 -V/T = 2.0057 <S\*\*2> = RHF/RKS

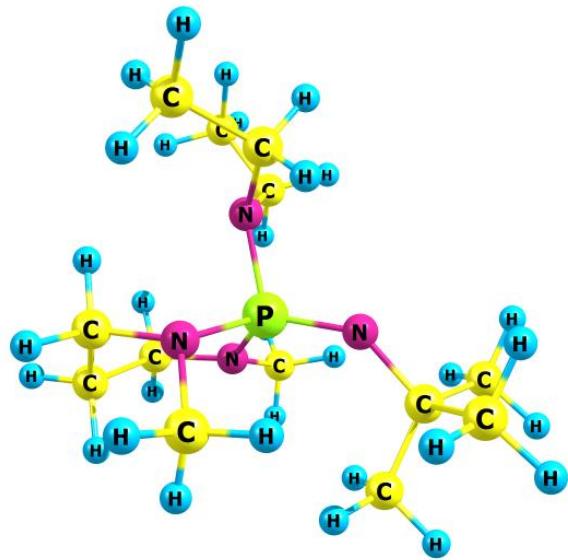
Temp. 298.150 K Press. 1.00000 Atm.  
 E + zero-point Energies = -1073.418471  
 E + thermal Energies = -1073.395933  
 E + thermal Enthalpies = -1073.394989  
 E + thermal Free Energies = -1073.468151

Geometry at E(RM06/6-31G(d,p))

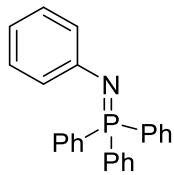
Charge: 0 multiplicity: 1

C	-1.919474000	-3.195723000	-1.439815000
C	-1.726268000	-1.704979000	-1.678506000
N	-2.394084000	-0.886061000	-0.663411000
P	-1.883048000	-1.156445000	0.938923000
N	-1.802303000	-2.854006000	1.012536000
C	-1.297851000	-3.624178000	-0.121312000
H	-1.464556000	-3.771749000	-2.256276000
H	-2.991778000	-3.438014000	-1.429916000
H	-2.111552000	-1.406748000	-2.663864000

H	-0.652155000	-1.469817000	-1.662335000
N	-2.615216000	-0.449556000	2.089212000
N	-0.286714000	-0.608416000	0.784450000
C	-3.811632000	-0.691550000	-0.898806000
H	-3.955643000	-0.214770000	-1.877081000
H	-4.400733000	-1.626023000	-0.886054000
H	-4.218499000	-0.021558000	-0.135589000
C	-3.858220000	-0.502195000	2.831801000
C	-4.769049000	-1.671710000	2.451184000
H	-5.070557000	-1.615652000	1.397922000
H	-4.266385000	-2.633760000	2.608094000
H	-5.682226000	-1.664780000	3.061549000
C	-4.612563000	0.813288000	2.622911000
H	-5.513098000	0.858417000	3.250293000
H	-3.963773000	1.658757000	2.879040000
H	-4.923108000	0.933012000	1.577381000
C	-3.509589000	-0.611972000	4.319081000
H	-4.411782000	-0.568206000	4.944096000
H	-2.993741000	-1.556829000	4.532657000
H	-2.842146000	0.208225000	4.606821000
C	0.710252000	-1.155734000	1.698578000
H	0.701104000	-0.608535000	2.659125000
H	0.435826000	-2.191620000	1.929096000
C	2.102772000	-1.145220000	1.094773000
H	2.824663000	-1.616154000	1.771284000
H	2.106281000	-1.692478000	0.143467000
H	2.453976000	-0.125604000	0.896603000
C	-0.148124000	0.836586000	0.532024000
H	-1.106114000	1.335953000	0.729137000
H	0.550850000	1.246391000	1.277132000
C	0.327766000	1.158873000	-0.872412000
H	1.261534000	0.634613000	-1.109439000
H	-0.427652000	0.858374000	-1.606739000
H	0.501449000	2.235497000	-0.987440000
C	-1.685708000	-3.537223000	2.285204000
H	-1.893094000	-2.840746000	3.103872000
H	-2.403064000	-4.369497000	2.345652000
H	-0.676247000	-3.955723000	2.441826000
H	-1.529488000	-4.682480000	0.068251000
H	-0.192881000	-3.551397000	-0.185741000



Tetraphenylphosphanimine



(Ground state)

E(RM06/6-31G(d,p)) = -1321.90025603 after 1 cycles  
 Conv=0.36D-08 -V/T = 2.0056 <S\*\*2> = RHF/RKS

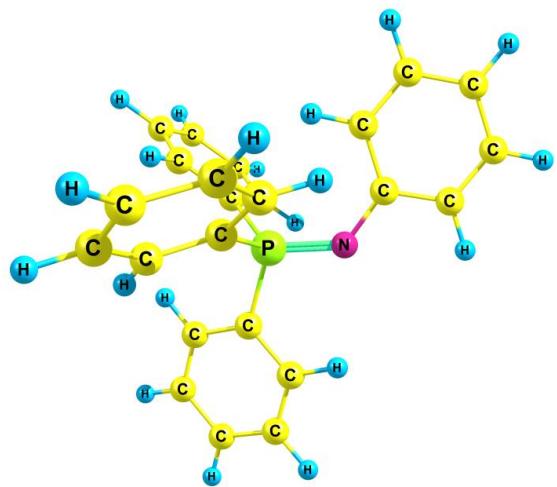
Temp. 298.150 K Press. 1.00000 Atm.  
 E + zero-point Energies = -1321.531120  
 E + thermal Energies = -1321.509199  
 E + thermal Enthalpies = -1321.508254

Geometry at E(RM06/6-31G(d,p))

Charge: 0 multiplicity: 1

N -2.6916772110 -0.3462886280 -4.0070171497  
 C -2.4814231122 -1.1866312579 -2.9263413275  
 C -2.2559727042 -2.5493434186 -3.1981653082  
 C -2.4718245853 -0.7898803226 -1.5745350620  
 C -2.0346750030 -3.4610861318 -2.1779899122  
 C -2.2450233314 -1.7098493550 -0.5570832966  
 C -2.0252752723 -3.0523306080 -0.8450154185  
 H -2.2614399437 -2.8624224291 -4.2401924331

H -2.6401395986 0.2570093422 -1.3181124937  
H -1.8657686100 -4.5076579694 -2.4264635106  
H -2.2428689923 -1.3672364636 0.4765009208  
H -1.8511421916 -3.7690961600 -0.0461662768  
P -2.9137696924 1.2134993898 -4.0088579912  
C -4.5745813844 1.7671329185 -3.4863614704  
C -5.0879224251 3.0259419162 -3.8152671241  
C -5.3636195083 0.8690719407 -2.7638676308  
C -6.3650447766 3.3895023445 -3.4052316652  
C -6.6416967040 1.2360141932 -2.3550393319  
C -7.1406894092 2.4950298400 -2.6718564130  
H -4.4920256156 3.7211588934 -4.4060921428  
H -4.9727598216 -0.1194475997 -2.5285494847  
H -6.7596872557 4.3689673529 -3.6653642528  
H -7.2507370145 0.5332253732 -1.7915881318  
H -8.1413011051 2.7792452088 -2.3539904254  
C -1.7261418313 2.2099718176 -3.0415290325  
C -2.0920150860 3.2398299741 -2.1732588735  
C -0.3769871552 1.8626525447 -3.1721813150  
C -1.1160088243 3.9263763504 -1.4559797738  
C 0.5936407498 2.5489841164 -2.4548639384  
C 0.2240777700 3.5832191523 -1.5979561131  
H -3.1414153584 3.5028668960 -2.0506010678  
H -0.0979909243 1.0403351943 -3.8307209962  
H -1.4054250772 4.7281046751 -0.7804776936  
H 1.6404303152 2.2735083042 -2.5582248207  
H 0.9843679891 4.1185922871 -1.0337433129  
C -2.7181969161 1.7751712965 -5.7206213324  
C -2.3474763368 3.0880794730 -6.0219430141  
C -2.9657626018 0.8680726154 -6.7527026529  
C -2.2412855746 3.4945264319 -7.3478364278  
C -2.8560304406 1.2784267946 -8.0760571189  
C -2.4987370810 2.5907389296 -8.3739428614  
H -2.1197872556 3.7898980953 -5.2196544188  
H -3.2212756088 -0.1578072833 -6.4961532863  
H -1.9470377384 4.5154646796 -7.5796260556  
H -3.0453614483 0.5699756314 -8.8791288941  
H -2.4118589018 2.9082511820 -9.4106523190



**DHIP**

File: 2\_SP\_M06\_HighBasis.log

(Ground state)

E(RM06/Gen) = -380.758537271 after 1 cycles  
Conv=0.34D-08 -V/T = 2.0066 <S\*\*2> = RHF/RKS

Temp. 298.150 K Press. 1.00000 Atm.  
E + zero-point Energies = -380.618573  
E + thermal Energies = -380.611510  
E + thermal Enthalpies = -380.610566  
E + thermal Free Energies = -380.651014

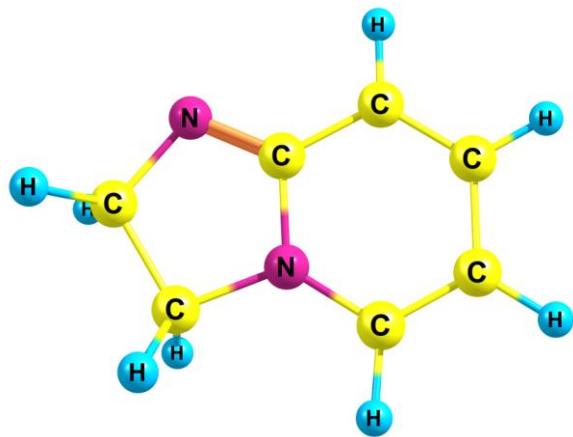
Single Point Energies:

E1(RM06/Gen) = -380.747810771 after 10 cycles  
Conv=0.48D-08 -V/T = 2.0062 <S\*\*2> = RHF/RKS  
E2(RM06/Gen) = -380.850027996 after 14 cycles  
Conv=0.94D-08 -V/T = 2.0039 <S\*\*2> = RHF/RKS

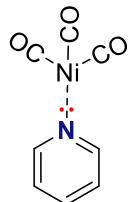
Geometry at E(RM06/Gen)

Charge: 0 multiplicity: 1

C -2.4415472924 -1.0859684296 0.5331045190  
C -1.6766267656 -0.0805644188 1.0382782743  
N -0.5364566457 0.2971532957 0.4078247093  
C -0.0569885892 -0.2880156041 -0.7796355175  
C -0.8691899708 -1.3505972689 -1.3111952604  
C -2.0089874296 -1.7232383831 -0.6723747358  
C 0.3911125885 1.3520721917 0.8026914834  
C 1.4570937513 1.2535796794 -0.3211054262  
N 1.0424471224 0.1981538733 -1.2380912031  
H -3.3517932011 -1.3879037963 1.0379683485  
H -1.9241467278 0.4626598480 1.9476637033  
H -0.5303768390 -1.8260633521 -2.2260007311  
H -2.6126895331 -2.5285747647 -1.0858676433  
H -0.1220516072 2.3219469431 0.8290658787  
H 0.7951925771 1.1527405537 1.8032832090  
H 2.4494255431 1.0270383444 0.0927395736  
H 1.5565830190 2.2065812882 -0.8583491816



## Py-NiCO<sub>3</sub>



(CO) A1 frequency: 2172.8200

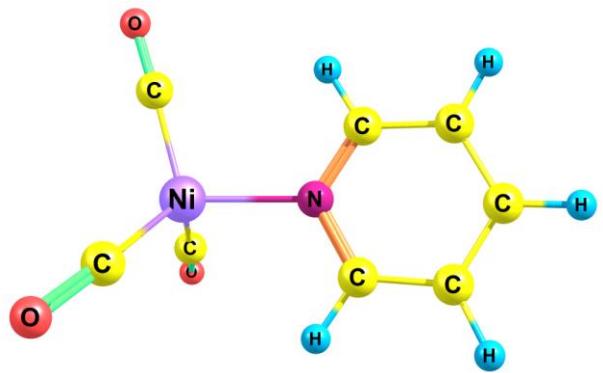
E(M06/6-31G(d,p)/SDD) = -758.952122268 after 1 cycles  
0.4860D-08

Temp. 298.150 K Press. 1.00000 Atm.  
E + zero-point Energies = -758.838602  
E + thermal Energies = -758.824595  
E + thermal Enthalpies = -758.823651  
E + thermal Free Energies = -758.882720

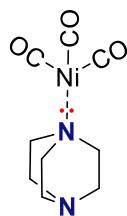
Geometry at E(M06/6-31G(d,p)/SDD)

Charge: 0 multiplicity: 1

Ni 1.0669170769 4.4332059864 -2.2717690416  
C -0.5068159833 5.3097066465 -2.0971506092  
O -1.4833751955 5.9101089731 -2.0053478891  
C 1.6235898390 4.2861588332 -3.9815901217  
O 1.9843013587 4.2254381786 -5.0727762317  
C 2.3609466276 5.0340677094 -1.1602139705  
O 3.1891108739 5.4653476910 -0.4885562789  
N 0.6499716994 2.4518559113 -1.6240427473  
C 0.6776225011 1.4038292131 -2.4578605095  
C 0.3453982487 2.2210063874 -0.3395290996  
C 0.4085717442 0.1047102927 -2.0499525614  
H 0.9270881062 1.6224596286 -3.4946112064  
C 0.0636096257 0.9559992751 0.1559969495  
H 0.3298556975 3.0947528685 0.3099298631  
C 0.0960414141 -0.1251301694 -0.7162719625  
H 0.4465647295 -0.7062392735 -2.7712509753  
H -0.1758668985 0.8286513548 1.2075986460  
H -0.1192541553 -1.1300376866 -0.3620242940



## DABCO-NiCO<sub>3</sub>



(CO) A1 frequency: 2169.2273

E(M06/6-31G(d,p)/SDD) = -855.945460935 after 1 cycles  
0.5074D-08

Temp. 298.150 K Press. 1.00000 Atm.  
E + zero-point Energies = -855.737364  
E + thermal Energies = -855.721412  
E + thermal Enthalpies = -855.720468  
E + thermal Free Energies = -855.783388

Geometry at E(M06/6-31G(d,p)/SDD)

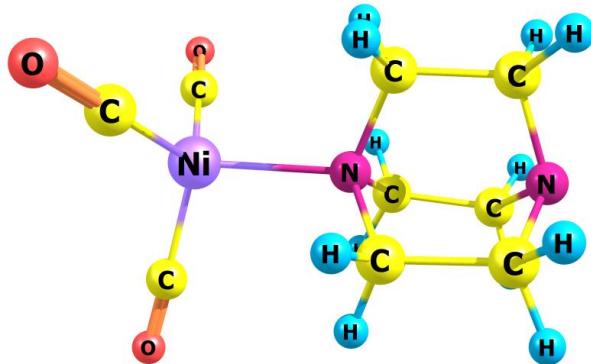
Charge: 0 multiplicity: 1

Ni 1.0762858558 4.4658363307 -2.2842078961  
C -0.5415112433 5.1546599302 -2.6921465802  
O -1.5622171378 5.6146027940 -2.9589020684  
C 2.1549517164 4.2250619997 -3.7116725037  
O 2.8417804684 4.0925615363 -4.6255839587  
C 1.8796901147 5.2572216609 -0.8748180824  
O 2.3933398019 5.7819458029 0.0114746984  
C -0.3492301494 2.4760372558 -0.5009062341  
C 1.8767959977 1.7997958860 -1.0941974991  
C 0.1005020811 1.6312021563 -2.7035355593  
C -0.5569303653 1.0453688854 0.0504038898  
H 0.0111340150 3.1697936148 0.2689402981  
H -1.2763993500 2.8975154245 -0.9105358585  
H 2.6471577318 1.8826022681 -1.8709899294  
H 2.2224089321 2.3810405389 -0.2294198056  
C 1.5760420515 0.3294050027 -0.7199961813  
C -0.3042696754 0.2358074307 -2.1704472404  
H 0.8771440021 1.5657640144 -3.4768336559  
H -0.7483272106 2.1719645099 -3.1404983175  
H -0.1680888976 0.9518838447 1.0729869756  
H -1.6222342956 0.7830463588 0.0828719313  
H 2.0775921619 -0.3662378846 -1.4054714287  
H 1.9279780238 0.0979415763 0.2935012388

```

H 0.1367520469 -0.5644601638 -2.7785418073
H -1.3935060354 0.1006016163 -2.1964316139
N 0.6463567626 2.4525140046 -1.5974740665
N 0.1391627068 0.0708896157 -0.7876249251

```



### DHIP--NiCO<sub>3</sub>

(CO) A1 frequency: 2164.1930

(Ground state)

E(RM06/Gen) = -891.626064087 after 1 cycles  
 Conv=0.42D-08 -V/T = 2.0818 <S\*\*2> = RHF/RKS

Temp. 298.150 K Press. 1.00000 Atm.  
 E + zero-point Energies = -891.460926  
 E + thermal Energies = -891.444092  
 E + thermal Enthalpies = -891.443148  
 E + thermal Free Energies = -891.510062

Single Point Energies:

E1(RM06/Gen) = -891.615353709 after 11 cycles  
 Conv=0.50D-08 -V/T = 2.0816 <S\*\*2> = RHF/RKS  
 E2(RM06/Gen) = -891.810602347 after 19 cycles  
 Conv=0.47D-08 -V/T = 2.0788 <S\*\*2> = RHF/RKS

Geometry at E(RM06/Gen)

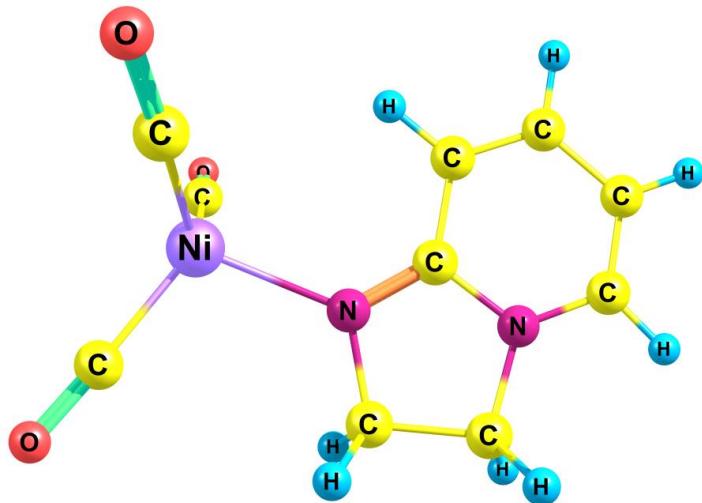
Charge: 0 multiplicity: 1

```

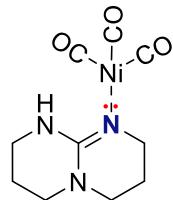
C -2.7401908944 -0.4287997669 30.1939621733
C -1.7583220263 0.0553908909 31.0022855152
N -0.5013031325 0.2311893842 30.5200761746
C -0.1215682921 -0.0738329529 29.2166239817
C -1.1457893861 -0.5858630951 28.3587225189
C -2.4070284550 -0.7510041999 28.8450786458
C 0.6768107404 0.6763608011 31.2652367633
C 1.7465610676 0.7269181626 30.1529698523

```

H -3.7457010006 -0.5618955403 30.5753045313  
H -1.9117869217 0.3263511222 32.0437538441  
H -0.8743707349 -0.8269207686 27.3354094322  
H -3.1824567163 -1.1389087243 28.1886445576  
H 0.4886609969 1.6483286092 31.7344083360  
H 0.9130283132 -0.0490737336 32.0538648200  
H 2.6462691513 0.1614148602 30.4243033348  
H 2.0673104601 1.7571185663 29.9435743855  
N 1.1299952562 0.1543852458 28.9582890205  
Ni 2.1505938616 -0.0647100684 27.1679424437  
C 2.0485651051 -1.8165243906 26.7308855360  
O 2.0121413676 -2.9237021307 26.4167246282  
C 3.8406123773 0.4619213400 27.5230716076  
O 4.9300504113 0.7880809817 27.7056829986  
C 1.3213039818 1.0136801263 25.9765044685  
O 0.8261270665 1.6899956339 25.1869558862



## TBD-NiCO<sub>3</sub>



(CO) A1 frequency: 2164.7610

(Ground state)

E(M06/6-31G(d,p)/SDD) = -949.386675583 after 1 cycles  
0.2758D-08

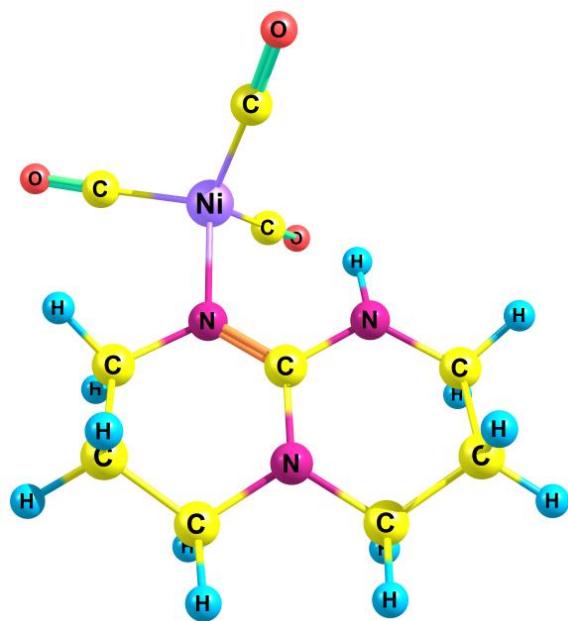
Temp. 298.150 K Press. 1.00000 Atm.  
E + zero-point Energies = -949.156519  
E + thermal Energies = -949.138013  
E + thermal Enthalpies = -949.137068  
E + thermal Free Energies = -949.206277

Geometry at E(M06/6-31G(d,p)/SDD)

Charge: 0 multiplicity: 1

Ni 1.0093102543 4.4983792494 -2.1976771857  
C -0.5648469812 4.8229398439 -3.0288536781  
O -1.5354420618 5.0555594240 -3.6025588771  
C 2.3424677962 4.2341458052 -3.3908034794  
O 3.1903987692 4.1055960400 -4.1580330049  
C 1.5076097088 5.7202648625 -0.9675258482  
O 1.8636488558 6.5373303158 -0.2370743815  
C 1.6526837142 1.5576973757 -1.7266771200  
C 0.0301428184 2.4384164502 -0.2145404502  
C 1.2062454493 0.1835826509 -1.2656676279  
H 2.6911803451 1.7452582466 -1.4050535806  
H 1.6638840684 1.5983032273 -2.8233116041  
C 0.9332625144 0.2296862781 0.2205790842  
H 1.9698217902 -0.5681052503 -1.4951609156  
H 0.2845244815 -0.1067545173 -1.7871597600  
H 0.5325252326 -0.7254783794 0.5847683598  
H 1.8655516759 0.4262854900 0.7813104018  
C -0.6748303183 1.2115619761 1.8078071363  
H -0.9680441920 0.1711433386 2.0010801048  
H 0.0575371262 1.4876383450 2.5896882852  
C -1.8759709659 2.1298894268 1.8763654839  
H -2.6547146233 1.7698590378 1.1921566788

H -2.2877739561 2.1349772640 2.8912651683  
C -1.4445213922 3.5217751027 1.4671699023  
H -2.3047342442 4.1962804157 1.3959954508  
H -0.7636039159 3.9394218620 2.2297457412  
H -0.6289829370 4.3065231662 -0.3404517965  
N 0.8057787418 2.6369764334 -1.2411648351  
N -0.0580625011 1.2565463199 0.4908520915  
N -0.8132815333 3.4473535293 0.1669261659



## Imidazole-NiCO<sub>3</sub>



(CO) A1 frequency: 2164.1643

(Ground state)

E(M06/6-31G(d,p)/SDD) = -894.071151934

Temp. 298.150 K Press. 1.00000 Atm.

E + zero-point Energies = -893.863699

E + thermal Energies = -893.844151

E + thermal Enthalpies = -893.843207

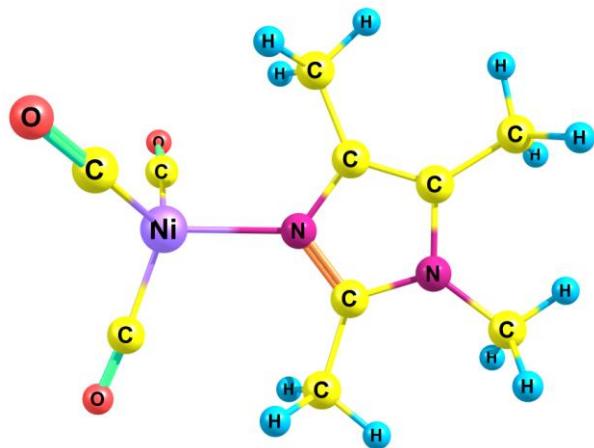
E + thermal Free Energies = -893.913453

Geometry at E(M06/6-31G(d,p)/SDD)

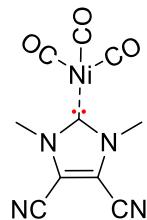
Charge: 0 multiplicity: 1

Ni 1.1008196082 4.3053044442 -2.2051400261  
C -0.4107783279 4.8984477219 -3.0036082975  
O -1.3527800644 5.3028249905 -3.5277647952  
C 2.4700134506 4.0884067415 -3.3686879985  
O 3.3362123746 3.9856384440 -4.1199072275  
C 1.5591707418 5.3185890589 -0.7881954876  
O 1.8624223136 6.0272651121 0.0688671498  
C -0.0600135114 0.2190177593 -1.6509054163  
C 1.2262311893 2.5606683796 0.8378929707  
H 2.2315081511 2.9612548348 0.6672830265  
H 0.5762084907 3.4093970229 1.0795814178  
H 1.2663292972 1.9068548316 1.7134845236  
C 0.1372121992 1.3517836948 -2.3940730083  
C 0.7375454950 1.8460915559 -0.3667406298  
N 0.6321084948 2.3542084054 -1.5813287454  
N 0.3281237939 0.5477697836 -0.3578472618  
C -0.1111684582 1.5652760522 -3.8422612705  
H 0.8056973292 1.8636621011 -4.3646949641  
H -0.4874460400 0.6543303862 -4.3187733531  
H -0.8486746498 2.3597158850 -4.0085670154  
C -0.5640891637 -1.1262009490 -2.0206011843  
H 0.1800575190 -1.9157204257 -1.8497619908  
H -1.4730847489 -1.4012500336 -1.4690128637

H -0.8162250771 -1.1472956445 -3.0842671319  
 C 0.2973708554 -0.3329540932 0.7900265803  
 H 1.2982591694 -0.4658582372 1.2143468062  
 H -0.3714171940 0.0524027474 1.5669872907  
 H -0.0714497378 -1.3119713597 0.4782372021



### ImCN<sub>2</sub>-NiCO<sub>3</sub>



(CO) A1 frequency: 2164.0202

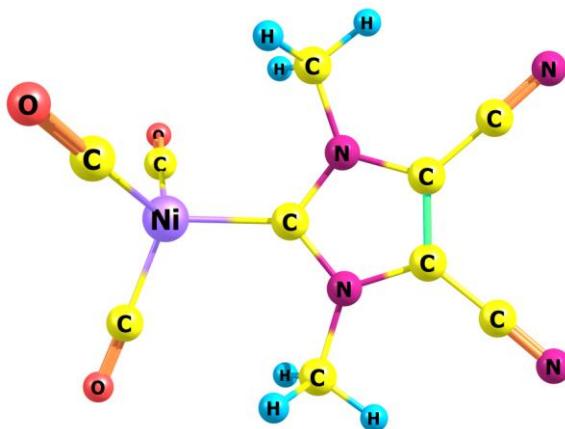
(Ground state)

E(M06/6-31G(d,p)/SDD) = -999.819035961 after 1 cycles  
0.3565D-08

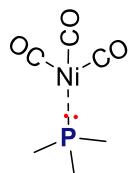
Temp. 298.150 K Press. 1.00000 Atm.  
 E + zero-point Energies = -999.669529  
 E + thermal Energies = -999.649708  
 E + thermal Enthalpies = -999.648764  
 E + thermal Free Energies = -999.720632

Geometry at E(M06/6-31G(d,p)/SDD)  
 Charge: 0 multiplicity: 1  
 Ni 1.0398336710 4.2219622960 -2.1770586175  
 C -0.4609906133 4.8461572450 -2.9831811605

O -1.4176477816 5.2170825456 -3.5032602139  
 C 2.3976604836 4.0870556518 -3.3717924270  
 O 3.2509990300 3.9852273866 -4.1360441650  
 C 1.5127007456 5.2954932703 -0.7906156031  
 O 1.8148956188 5.9941341372 0.0722342604  
 C 0.6313955290 2.3948168313 -1.5572813842  
 C -0.0255324483 0.2166408285 -1.5937249680  
 N 0.7349930784 1.8423657892 -0.3145596648  
 C 1.2042094152 2.5568963498 0.8632815556  
 H 2.2144835186 2.9341464615 0.6871816888  
 H 0.5376860054 3.3956564566 1.0790738079  
 H 1.2148670651 1.8729309516 1.7148350970  
 N 0.1615332238 1.3728260099 -2.3304106153  
 C -0.1085845690 1.4882942418 -3.7557753202  
 H -0.8764350383 2.2469665233 -3.9274321166  
 H 0.8042848303 1.7769251193 -4.2828379245  
 H -0.4583871589 0.5244186555 -4.1324700011  
 C 0.3398756140 0.5161077859 -0.3090094158  
 C 0.3427977633 -0.3060024363 0.8398667942  
 N 0.3569551214 -0.9573407744 1.8039130087  
 C -0.5020894909 -0.9986793120 -2.1340053100  
 N -0.8960555334 -1.9847113842 -2.6097616153



**PMe<sub>3</sub>-NiCO<sub>3</sub>**



(CO) A1 frequency: 2163.2079

(Ground state)

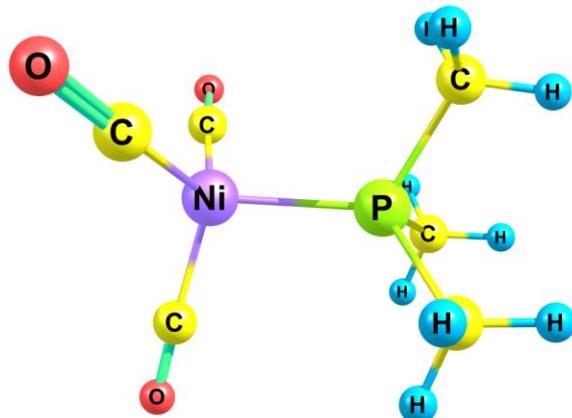
E(M06/6-31G(d,p)/SDD) = -971.839082064 after 1 cycles  
0.4955D-08

Temp. 298.150 K Press. 1.00000 Atm.  
E + zero-point Energies = -971.701605  
E + thermal Energies = -971.685422  
E + thermal Enthalpies = -971.684477  
E + thermal Free Energies = -971.747755

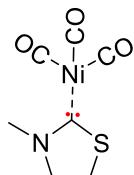
Geometry at E(M06/6-31G(d,p)/SDD)

Charge: 0 multiplicity: 1

Ni 0.9972913827 4.3152410698 -2.2870584679  
C -0.5806725829 4.9326469223 -2.9233319363  
O -1.5995961760 5.2947913026 -3.3159851431  
C 2.2481553909 4.0783047249 -3.5731380893  
O 3.0410919471 3.8848651922 -4.3840077235  
C 1.6058621008 5.2400681789 -0.8549503309  
O 1.9918227595 5.7900276746 0.0789247926  
P 0.5719571321 2.2633197277 -1.5019021737  
C 0.1429969153 0.9751352902 -2.7360079280  
H -0.0365224057 0.0022881250 -2.2614296762  
H -0.7549283121 1.2813184746 -3.2831566836  
H 0.9616860416 0.8794023515 -3.4574622191  
C -0.8137311083 2.1135256951 -0.3068895470  
H -0.9486480675 1.0783355127 0.0312114756  
H -0.6131288770 2.7528261673 0.5595799881  
H -1.7388131431 2.4634085009 -0.7777136857  
C 1.9403477492 1.4559302717 -0.5821259798  
H 2.2135033254 2.0776044127 0.2775201542  
H 1.6591726273 0.4554698564 -0.2300179031  
H 2.8172853607 1.3767575089 -1.2334627833



## ThN-NiCO<sub>3</sub>



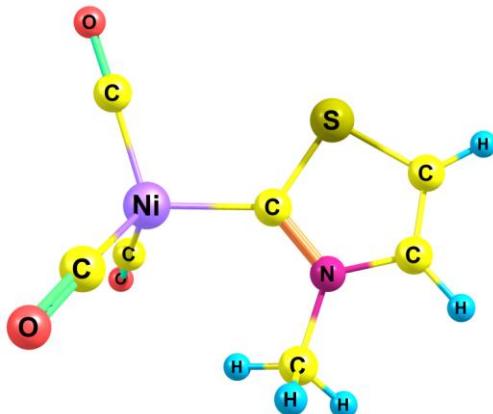
(CO) A1 frequency: 2160.1597

(Ground state)

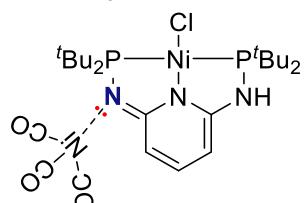
E(M06/6-31G(d,p)/SDD) = -1119.00522572 after 1 cycles  
0.4757D-08

Temp. 298.150 K Press. 1.00000 Atm.  
E + zero-point Energies = -1118.896951  
E + thermal Energies = -1118.881998  
E + thermal Enthalpies = -1118.881054  
E + thermal Free Energies = -1118.941963

Geometry at E(M06/6-31G(d,p)/SDD)  
Charge: 0 multiplicity: 1  
Ni 1.1852403208 4.2819323656 -2.1781398041  
C -0.3816783885 5.1851245462 -2.1023863600  
O -1.3835687607 5.7492477001 -2.0467749584  
C 1.8219915976 4.2425302065 -3.8854062266  
O 2.2304997381 4.2389077044 -4.9602718042  
C 2.4069188704 4.9713402914 -1.0326845504  
O 3.1697043609 5.3803900510 -0.2729805067  
C 0.8641565015 2.4240366882 -1.6193267282  
C 0.6143220810 -0.0930216658 -1.4558827789  
C 0.4146964464 0.5484629181 -0.2901514159  
H 0.5582753124 -1.1564251610 -1.6441237979  
H 0.1675682838 0.1196526081 0.6742368151  
N 0.5520541334 1.9288686725 -0.4040629194  
C 0.4105631461 2.7923945080 0.7641199125  
H 1.3842578825 2.9569365872 1.2375368975  
H 0.0046913856 3.7534907469 0.4435469111  
H -0.2704356566 2.3263380603 1.4808916446  
S 0.9823069952 1.0772727924 -2.6919703601



**2-NiCO<sub>3</sub>**



(Ground state)

E(RM06/6-31G(d,p)/SDD) = -2812.67109941 after 3 cycles

Conv=0.22D-08 -V/T = 2.0512 <S\*\*2> = RHF/RKS

Temp. 298.150 K Press. 1.00000 Atm.

E + zero-point Energies = -2812.062152

E + thermal Energies = -2812.017511

E + thermal Enthalpies = -2812.016567

E + thermal Free Energies = -2812.138044

Geometry at E(RM06/6-31G(d,p)/SDD)

Charge: 0 multiplicity: 1

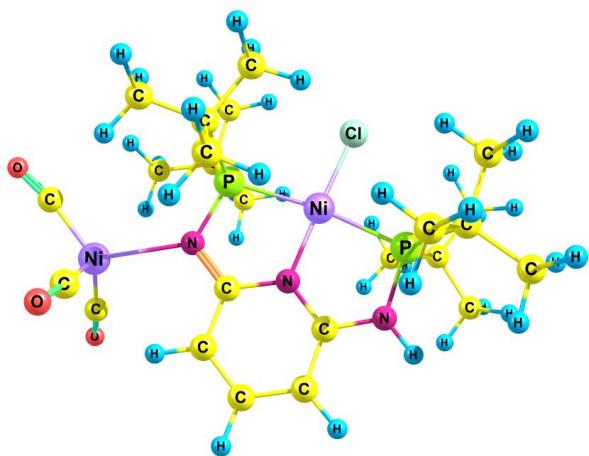
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H 16.4681290064 0.8341368550 -5.0131024055
C 16.2709959070 0.5991285020 -3.9693305151
C 15.5452583338 -0.5224473011 -3.6580384583
C 16.7570099915 1.4387455183 -2.9677726441
C 16.4759913980 1.0902663446 -1.6589706138
C 15.2687804857 -0.8632844370 -2.3078769239
H 15.1699298995 -1.1762172941 -4.4331175701
H 17.3267384909 2.3369291509 -3.1859794289
P 14.4472818866 -2.2032662861 -0.3115944150
P 16.6374035049 1.3871798058 0.9956002070
Ni 15.4436355704 -0.4111626411 0.5166390077
Cl 14.9504877762 -0.7207697033 2.6307082428
C 15.7832740312 2.8739832650 1.7636970253
C 18.3615631712 1.0611467124 1.6747228042
C 14.3231249661 2.7566271881 1.3133171697

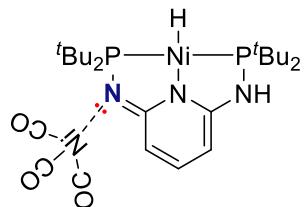
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H 14.2342411457 2.6803503380 0.2209716085  
 H 13.8419137140 1.8799988734 1.7619449379  
 H 13.7743395188 3.6533600305 1.6327037824  
 C 16.3541502425 4.1998013316 1.2603331524  
 H 15.8155604605 5.0213001413 1.7519346787  
 H 17.4180052342 4.3255673456 1.4916872700  
 H 16.2092035579 4.3233213050 0.1807737789  
 C 15.8446045286 2.8246977338 3.2892427312  
 H 15.1734889710 3.5960655920 3.6912776941  
 H 15.5146780971 1.8551116148 3.6808161726  
 H 16.8502763154 3.0406595900 3.6699011683  
 C 19.2550308333 2.2988292050 1.6634208955  
 H 18.9220341261 3.0583202371 2.3804418593  
 H 20.2745342262 2.0068565847 1.9511730383  
 H 19.3235082852 2.7613319231 0.6698029501  
 C 18.2879075312 0.4776171997 3.0866029922  
 H 17.6363134420 -0.4028863592 3.1288266836  
 H 19.2993807423 0.1750817164 3.3909743248  
 H 17.9238548695 1.1985436747 3.8251867391  
 C 18.9517800182 -0.0062460881 0.7470602834  
 H 18.3494170927 -0.9246023910 0.7636731792  
 H 19.0318910691 0.3339376732 -0.2922050058  
 H 19.9604504443 -0.2634060898 1.0972343306  
 C 12.6175962749 -2.3000633735 0.1282358944  
 C 12.1401834341 -0.8435686704 0.0916090462  
 H 11.0529869626 -0.8175839457 0.2490463197  
 H 12.6125163988 -0.2460077945 0.8803268256  
 H 12.3479688404 -0.3756342645 -0.8805016743  
 C 12.4018304850 -2.8759150728 1.5275202634  
 H 11.3365168271 -2.7767109541 1.7793362324  
 H 12.6437371703 -3.9449537031 1.5716791000  
 H 12.9804365682 -2.3476473224 2.2918016155  
 C 11.7929906122 -3.1034216463 -0.8715540771  
 H 12.0617233036 -4.1652029694 -0.8790555930  
 H 10.7358071450 -3.0354415056 -0.5777999507  
 H 11.8903233654 -2.7136864515 -1.8898491182  
 C 15.4276072790 -3.7724668117 0.0708528256  
 C 14.7377626588 -5.0530222832 -0.3903175750  
 H 15.3934572731 -5.9065685589 -0.1664415904  
 H 13.7862514082 -5.2290922737 0.1257897961  
 H 14.5581876426 -5.0480736469 -1.4693255094  
 C 15.7316464406 -3.8705247042 1.5663543194  
 H 14.8290748843 -3.9526524179 2.1809927109  
 H 16.3344204208 -4.7740033971 1.7352871699  
 H 16.2969014851 -3.0055711104 1.9312348727  
 C 16.7500795461 -3.6142960981 -0.6842694560  
 H 16.6053038214 -3.5956055917 -1.7700179951  
 H 17.2745769172 -2.6927513516 -0.3954493169

H 17.4039961655 -4.4620675187 -0.4384189381  
 N 15.7702008410 -0.0224715393 -1.3146408775  
 N 14.5526175714 -1.9531113454 -1.9849403029  
 N 16.9104149275 1.8908649814 -0.6169434547  
 H 17.4577164556 2.7011237941 -0.8777779377  
 Ni 13.9241858410 -3.3076614161 -3.6771545542  
 C 12.9884316305 -4.7938167847 -3.2754335859  
 O 12.3811050286 -5.7685597171 -3.1773381121  
 C 15.5351021883 -3.7645718556 -4.3700215364  
 O 16.5371650974 -4.1189726953 -4.8127030539  
 C 12.8573782920 -2.2110916468 -4.6510490261  
 O 12.1364218409 -1.5785230479 -5.2872352903



### 1-NiCO<sub>3</sub>



(CO) A1 frequency: 2157.8143

(Ground state)

E(M06/6-31G(d,p)/SDD) = -2353.04247931 after 1 cycles

Temp. 298.150 K Press. 1.00000 Atm.  
 E + zero-point Energies = -2352.426849  
 E + thermal Energies = -2352.384022  
 E + thermal Enthalpies = -2352.383078

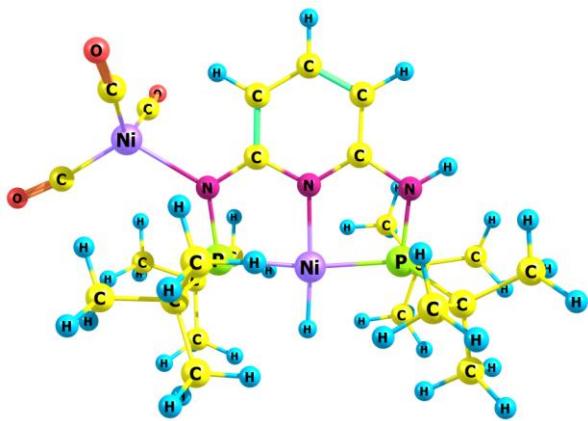
E + thermal Free Energies = -2352.500020

Geometry at E(M06/6-31G(d,p)/SDD)

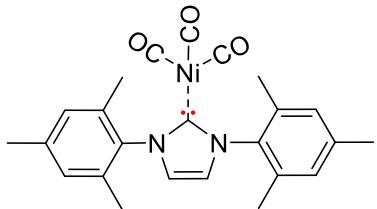
Charge: 0 multiplicity: 1

H -0.1207281948 0.4835551135 -5.6262765559  
C -0.0871854488 0.3869219630 -4.5428962803  
C -0.3642133063 -0.8497933264 -3.9562615360  
C 0.2294613485 1.4891140927 -3.7844106740  
C 0.2787263431 1.3981132357 -2.3680284884  
C -0.3038314042 -0.9081750887 -2.5744623956  
H -0.6088055004 -1.7302673030 -4.5430041014  
H 0.4441663872 2.4411726555 -4.2512662943  
P -0.6719550596 -2.0356685143 -0.1673440026  
P 0.6298458571 2.0552662135 0.0782279286  
Ni -0.0095533592 -0.0068440063 0.1064171011  
H 0.0018309218 -0.0591375358 1.5819257691  
C -0.6080103621 3.1654228941 0.9606065889  
C 2.4170740477 2.2535361789 0.6521003394  
C -1.9724152868 2.6674748942 0.4709898354  
H -2.0543116756 2.7274759179 -0.6227474955  
H -2.1548723910 1.6298716153 0.7822002887  
H -2.7637088385 3.2957762118 0.9034620361  
C -0.4970377022 4.6517643030 0.6439388745  
H -1.2960125367 5.1846182537 1.1793453377  
H 0.4573073290 5.0808017807 0.9671922626  
H -0.6176671173 4.8453389600 -0.4264410215  
C -0.5125011952 2.9638488625 2.4718668230  
H -1.3724271947 3.4544755184 2.9493266265  
H -0.5293747144 1.9027977835 2.7503070238  
H 0.3922545039 3.4232323198 2.8885563910  
C 2.9233953229 3.6907759899 0.6944026407  
H 2.3802992539 4.3070731388 1.4217490126  
H 3.9812725790 3.6880631442 0.9940140229  
H 2.8576702989 4.1663854895 -0.2888975113  
C 2.6008012294 1.6091008705 2.0270710437  
H 2.2565997093 0.5685620862 2.0372908687  
H 3.6702585884 1.6233762375 2.2803312573  
H 2.0691950387 2.1464540395 2.8199926392  
C 3.2366446427 1.4618787786 -0.3718485821  
H 2.9026960898 0.4165418119 -0.4359221359  
H 3.1683635432 1.9015026443 -1.3733630668  
H 4.2920241017 1.4620525453 -0.0662688655  
C -2.4890969504 -2.3688004827 0.1863598057  
C -3.2578728518 -1.3757255593 -0.6923099877  
H -4.3197504561 -1.3995716492 -0.4130592168  
H -2.8973566222 -0.3466507571 -0.5608415988  
H -3.1836749816 -1.6221947523 -1.7577408292  
C -2.7674306948 -2.0374352928 1.6538293269

H -3.8455410947 -2.1291835273 1.8446074440  
 H -2.2513882577 -2.7134457991 2.3437488735  
 H -2.4608277349 -1.0126734653 1.8961508512  
 C -2.9561158804 -3.7864778580 -0.1321373916  
 H -2.5282211133 -4.5317553905 0.5494084244  
 H -4.0485367279 -3.8390811511 -0.0237293809  
 H -2.7221165295 -4.0830795383 -1.1635852737  
 C 0.4602138864 -3.4234190842 0.3849924076  
 C 0.3381779074 -4.6930002599 -0.4549264327  
 H 1.0661730258 -5.4318328578 -0.0925717157  
 H -0.6525761565 -5.1541211051 -0.3916506795  
 H 0.5718643848 -4.5027138260 -1.5092706758  
 C 0.2184988880 -3.7332720013 1.8606385677  
 H -0.7373767850 -4.2449003431 2.0270995882  
 H 1.0127595388 -4.3999319270 2.2231226847  
 H 0.2411459627 -2.8243627832 2.4759157156  
 C 1.8718371821 -2.8522765003 0.2169821047  
 H 2.0617246733 -2.5379867084 -0.8175525733  
 H 2.0309542212 -1.9869649377 0.8722558802  
 H 2.6105129537 -3.6229677125 0.4777337197  
 N -0.0056465080 0.1646182771 -1.8052387645  
 N -0.5459077974 -2.0923843867 -1.8851825975  
 N 0.5822097339 2.4508155161 -1.5781030767  
 H -0.8468072661 -2.8790570235 -2.4472153620  
 Ni 1.0771860240 4.3586142459 -2.5672025149  
 C -0.4927566723 4.7185025439 -3.4006134447  
 O -1.4935248319 4.9997026360 -3.8959251221  
 C 2.5067160465 3.8935585495 -3.5815848093  
 O 3.4514897610 3.6533026283 -4.1948456286  
 C 1.5268296866 5.7687262331 -1.5434458020  
 O 1.8231889679 6.7527492899 -1.0198164104



**IMes-NiCO<sub>3</sub>**



**(CO) A1 frequency: 2148.0905**

(Ground state)

E(M06/6-31G(d,p)/SDD) = -1434.37208452 after 1 cycles  
0.7624D-08

Temp. 298.150 K Press. 1.00000 Atm.  
E + zero-point Energies = -1433.949902  
E + thermal Energies = -1433.917716  
E + thermal Enthalpies = -1433.916771  
E + thermal Free Energies = -1434.014251

Geometry at E(M06/6-31G(d,p)/SDD)

Charge: 0 multiplicity: 1

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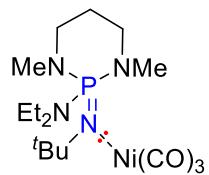
Ni 1.0410801670 4.2600358231 -2.1907056258
C -0.5106830127 4.9605224831 -2.7925278955
O -1.5074382998 5.3836198329 -3.1896807782
C 2.2403731747 4.1578468890 -3.5410317639
O 2.9971919289 4.1021752755 -4.4089577620
C 1.7351385348 5.2266266389 -0.8148936567
O 2.2047527092 5.8851799320 0.0050923660
C 0.6395002090 2.4127282626 -1.5758985613
C 0.0274067044 0.2112832929 -1.5685558342
C 0.3314507909 0.5460910513 -0.2958076260
H -0.3047202650 -0.7178679749 -2.0105498488
H 0.3250684619 -0.0241686097 0.6225956163
C 1.0690708396 2.6145384158 0.8554878700
C 2.4120612990 2.6475040893 1.2354761624
C 0.0669838240 3.2691075791 1.5785031667
C 2.7413006367 3.3581991064 2.3881246991
C 0.4433298722 3.9583973220 2.7276886304
C 1.7730377575 4.0116370874 3.1481074105
H 3.7859070993 3.4071029484 2.6965436048
H -0.3217172385 4.4803060206 3.3039001648
C -0.0061072108 1.4188373628 -3.7429269368
C 1.0533509244 1.1348987996 -4.6053195766
C -1.2785274272 1.7726586886 -4.2044732335
C 0.8208178691 1.2444404089 -5.9758284942
C -1.4622345586 1.8695727517 -5.5801555734

```

C -0.4236583259 1.6169126215 -6.4788251178  
 H 1.6383082007 1.0389479479 -6.6672994835  
 H -2.4430392621 2.1547456394 -5.9629000334  
 N 0.7010754728 1.8859840819 -0.3201749652  
 N 0.2200824765 1.3556360416 -2.3310397409  
 C 3.4627775409 1.9771151740 0.4044241146  
 H 3.2596995060 0.9072487321 0.2684665494  
 H 3.5086853305 2.4198903797 -0.6000400952  
 H 4.4495270257 2.0793625817 0.8658376577  
 C -1.3511306173 3.2642071499 1.0963943596  
 H -1.4417676593 3.8368655270 0.1629061950  
 H -1.7085573984 2.2499436620 0.8781703808  
 H -2.0201982019 3.7130789098 1.8365337306  
 C 2.1438276034 4.7531782688 4.3967582638  
 H 1.6226556305 5.7150340804 4.4583712508  
 H 1.8721123122 4.1816232393 5.2934480966  
 H 3.2199553997 4.9479965421 4.4435080984  
 C -2.4001899517 2.0248473208 -3.2440261661  
 H -3.2833902752 2.4058797062 -3.7650861711  
 H -2.6870729561 1.1067038528 -2.7145708964  
 H -2.1164482070 2.7559916326 -2.4773694264  
 C 2.3924897779 0.7309457945 -4.0684464829  
 H 2.3464767500 -0.2479629970 -3.5732078297  
 H 3.1341003968 0.6711319727 -4.8704018944  
 H 2.7545500143 1.4475842414 -3.3203167739  
 C -0.6540769526 1.7506078812 -7.9540571194  
 H -1.5114627502 1.1497552104 -8.2802216291  
 H -0.8710403544 2.7905684131 -8.2267987169  
 H 0.2206842444 1.4315064951 -8.5294258791



BEMP- $\text{Ni}(\text{CO})_3$



(Ground state)

E(RM06/6-31G(d,p)/SDD) = -1584.72095117 after 1 cycles  
Conv=0.20D-08 -V/T = 2.0468 <S\*\*2> = RHF/RKS

Temp. 298.150 K Press. 1.00000 Atm.

E + zero-point Energies = -1584.253323

E + thermal Energies = -1584.222321

E + thermal Enthalpies = -1584.221377

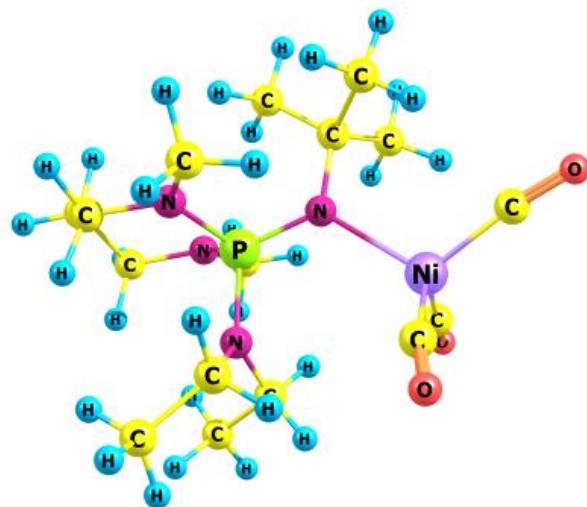
E + thermal Free Energies = -1584.313583

Geometry at E(RM06/6-31G(d,p)/SDD)

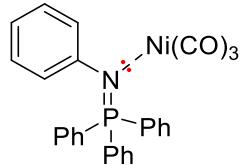
Charge: 0 multiplicity: 1

C	27.906796000	-3.390676000	-0.863782000
C	27.966662000	-1.964164000	-1.380219000
N	27.499899000	-1.017438000	-0.372885000
P	28.243177000	-1.017442000	1.140487000
N	28.429259000	-2.664566000	1.433911000
C	28.777026000	-3.592252000	0.363597000
H	28.232919000	-4.080068000	-1.652897000
H	26.866025000	-3.635132000	-0.612210000
H	27.318613000	-1.858315000	-2.260452000
H	28.996856000	-1.729473000	-1.710511000
N	27.429106000	-0.248025000	2.263154000
N	29.797610000	-0.437549000	0.847862000
C	26.810667000	0.158531000	-0.868273000
H	27.402426000	0.709554000	-1.616960000
H	25.855146000	-0.124999000	-1.333858000
H	26.594671000	0.841101000	-0.040208000
C	26.018738000	-0.598347000	2.637452000
C	25.326535000	-1.636421000	1.742960000
H	25.196259000	-1.285635000	0.714224000
H	25.876669000	-2.584079000	1.714884000
H	24.330345000	-1.840232000	2.154602000
C	25.172268000	0.674356000	2.591821000
H	24.134416000	0.451874000	2.871384000
H	25.554562000	1.435935000	3.278097000
H	25.163818000	1.105654000	1.582658000
C	26.002669000	-1.166380000	4.058733000
H	24.971145000	-1.247993000	4.425396000
H	26.443067000	-2.169951000	4.086259000
H	26.562900000	-0.533385000	4.753073000
C	30.987646000	-1.008807000	1.476583000
H	31.432138000	-0.274770000	2.163953000
H	30.679254000	-1.854848000	2.098247000
C	32.049833000	-1.471913000	0.491646000
H	32.833979000	-2.027647000	1.018008000
H	31.620542000	-2.125137000	-0.278918000
H	32.535147000	-0.628358000	-0.011605000
C	29.976210000	0.861541000	0.190983000

H	29.058633000	1.452074000	0.304659000
H	30.741728000	1.418125000	0.754844000
C	30.348843000	0.808346000	-1.283156000
H	31.264098000	0.236415000	-1.463481000
H	29.551839000	0.352937000	-1.881249000
H	30.507512000	1.824628000	-1.662391000
C	28.681110000	-3.147224000	2.779788000
H	28.600124000	-2.325016000	3.499220000
H	27.950448000	-3.922242000	3.057332000
H	29.688582000	-3.585163000	2.869958000
H	28.633808000	-4.610245000	0.751791000
H	29.848029000	-3.506587000	0.095005000
Ni	28.354790000	1.383685000	3.410224000
C	30.066065000	1.046741000	3.848742000
O	31.144600000	0.977370000	4.255726000
C	27.497612000	1.686347000	4.973046000
O	27.040571000	1.996049000	5.984415000
C	28.041030000	2.742672000	2.256978000
O	27.776160000	3.589473000	1.520610000



tetra-phe-nylphosphanimine-Ni(CO)<sub>3</sub>



(Ground state)

E(RM06/6-31G(d,p)/SDD) = -1832.76469155 after 1 cycles  
 Conv=0.43D-08 -V/T = 2.0411 <S\*\*2> = RHF/RKS

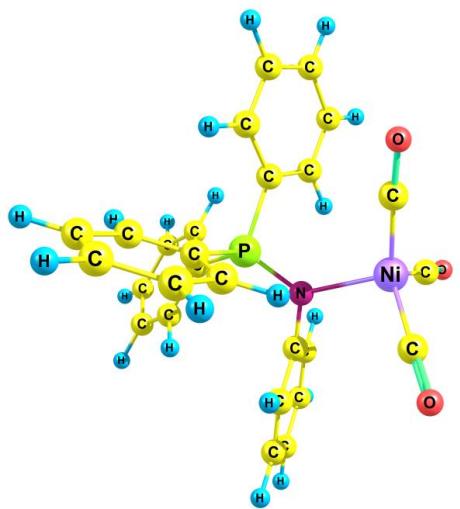
Temp. 298.150 K Press. 1.00000 Atm.  
E + zero-point Energies = -1832.370927  
E + thermal Energies = -1832.339238  
E + thermal Enthalpies = -1832.338294  
E + thermal Free Energies = -1832.439523

Geometry at E(RM06/6-31G(d,p)/SDD)

Charge: 0 multiplicity: 1

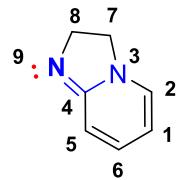
N 7.6939677587 -0.3532377813 -4.1326525517  
C 7.1957813801 -1.2505888036 -3.1606125954  
C 6.0100447276 -1.9517019655 -3.4072205329  
C 7.8647269602 -1.4692046891 -1.9494485661  
C 5.4961520150 -2.8308219043 -2.4613533447  
C 7.3478388080 -2.3495247026 -1.0052298481  
C 6.1598150989 -3.0314879404 -1.2541213612  
H 5.4953427231 -1.7771156294 -4.3524254244  
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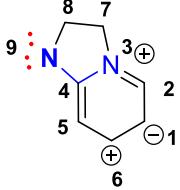
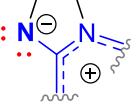
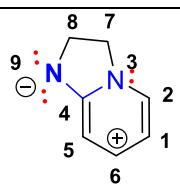
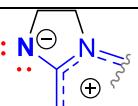
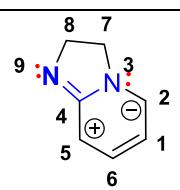
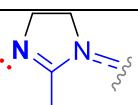
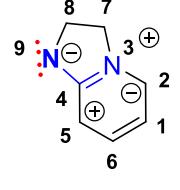
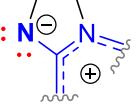
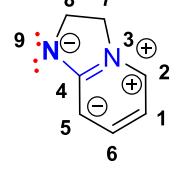
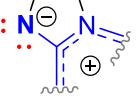
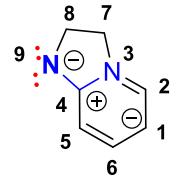
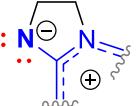


## NBO-NRT analysis

### Compound DHIP

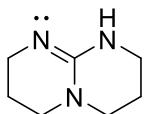


NBO bonding description	representation	Simplified representation
\$NRTSTR STR ! Wgt = 38.83% LONE 3 1 9 1 END BOND D 1 2 S 1 6 S 1 10 S 2 3 S 2 11 S 3 4 S 3 7 S 4 5 D 4 9 D 5 6 S 5 1 2 S 6 1 3 S 7 8 S 7 1 4 S 7 1 5 S 8 9 S 8 1 6 S 8 1 7 END END		
STR ! Wgt = 9.87% LONE 9 2 END BOND D 1 2 S 1 6 S 1 10 S 2 3 S 2 11 D 3 4 S 3 7 S 4 5 S 4 9 D 5 6 S 5 1 2 S 6 1 3 S 7 8 S 7 1 4 S 7 1 5 S 8 9 S 8 1 6 S 8 1 7 END END		
STR ! Wgt = 7.96% LONE 1 1 9 1 END BOND S 1 2 S 1 6 S 1 10 D 2 3 S 2 11 S 3 4 S 3 7 S 4 5 D 4 9 D 5 6 S 5 1 2 S 6 1 3 S 7 8 S 7 1 4 S 7 1 5 S 8 9 S 8 1 6 S 8 1 7 END END		
STR ! Wgt = 3.64% LONE 3 1 5 1 9 1 END BOND S 1 2 D 1 6 S 1 10 S 2 3 S 2 11 S 3 4 S 3 7 S 4 5 D 4 9 S 5 6 S 5 1 2 S 6 1 3 S 7 8 S 7 1 4 S 7 1 5 S 8 9 S 8 1 6 S 8 1 7 END END		
STR ! Wgt = 2.96% LONE 5 1 9 1 END BOND S 1 2 D 1 6 S 1 10 D 2 3 S 2 11 S 3 4 S 3 7 S 4 5 D 4 9 S 5 6 S 5 1 2 S 6 1 3 S 7 8 S 7 1 4 S 7 1 5 S 8 9 S 8 1 6 S 8 1 7 END END		

STR ! Wgt = 2.77% LONE 1 9 2 END BOND S 1 2 S 1 6 S 1 10 D 2 3 S 2 11 S 3 4 S 3 7 D 4 5 S 4 9 S 5 6 S 5 1 2 S 6 1 3 S 7 8 S 7 1 4 S 7 1 5 S 8 9 S 8 1 6 S 8 1 7 END END		
STR ! Wgt = 2.38% LONE 3 1 9 2 END BOND D 1 2 S 1 6 S 1 10 S 2 3 S 2 11 S 3 4 S 3 7 D 4 5 S 4 9 S 5 6 S 5 1 2 S 6 1 3 S 7 8 S 7 1 4 S 7 1 5 S 8 9 S 8 1 6 S 8 1 7 END END		
STR ! Wgt = 1.99% LONE 2 1 3 1 9 1 END BOND S 1 2 D 1 6 S 1 10 S 2 3 S 2 11 S 3 4 S 3 7 S 4 5 D 4 9 S 5 6 S 5 1 2 S 6 1 3 S 7 8 S 7 1 4 S 7 1 5 S 8 9 S 8 1 6 S 8 1 7 END END		
STR ! Wgt = 1.93% LONE 2 1 9 2 END BOND S 1 2 D 1 6 S 1 10 S 2 3 S 2 11 D 3 4 S 3 7 S 4 5 S 4 9 S 5 6 S 5 1 2 S 6 1 3 S 7 8 S 7 1 4 S 7 1 5 S 8 9 S 8 1 6 S 8 1 7 END END		
STR ! Wgt = 1.54% LONE 5 1 9 2 END BOND S 1 2 D 1 6 S 1 10 S 2 3 S 2 11 D 3 4 S 3 7 S 4 5 S 4 9 S 5 6 S 5 1 2 S 6 1 3 S 7 8 S 7 1 4 S 7 1 5 S 8 9 S 8 1 6 S 8 1 7 END END		
STR ! Wgt = 1.50% LONE 1 1 9 2 END BOND S 1 2 S 1 6 S 1 10 D 2 3 S 2 11 S 3 4 S 3 7 S 4 5 S 4 9 D 5 6 S 5 1 2 S 6 1 3 S 7 8 S 7 1 4 S 7 1 5 S 8 9 S 8 1 6 S 8 1 7 END END		

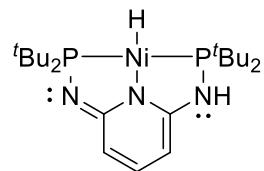
<pre> STR      ! Wgt = 1.47% LONE 1 1 9 2 END BOND S 1 2 S 1 6 S 1 10 S 2 3 S 2 11 D 3 4 S 3 7 S 4 5 S 4 9 D 5 6 S 5 12 S 6 13 S 7 8 S 7 14 S 7 15 S 8 9 S 8 16 S 8 17 END END \$END </pre>		
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## Compound TBD



NBO bonding description	representation	Simplified representation
<pre> STR      ! Wgt = 46.03% LONE 16 1 18 1 20 1 END BOND S 1 13 S 2 13 S 3 14 S 4 14 S 5 15 S 6 15 S 7 17 S 8 17 S 9 21 S 10 21 S 11 22 S 12 22 S 13 14 S 13 18 S 14 15 S 15 16 D 16 19 S 17 18 S 17 22 S 18 19 S 19 20 S 20 21 S 20 23 S 21 22 END END </pre>	<p style="text-align: center;">! Wgt = 46.03%</p>	
<pre> STR      ! Wgt = 15.72% LONE 16 2 20 1 END BOND S 1 13 S 2 13 S 3 14 S 4 14 S 5 15 S 6 15 S 7 17 S 8 17 S 9 21 S 10 21 S 11 22 S 12 22 S 13 14 S 13 18 S 14 15 S 15 16 S 16 19 S 17 18 S 17 22 D 18 19 S 19 20 S 20 21 S 20 23 S 21 22 END END </pre>	<p style="text-align: center;">! Wgt = 15.72%</p>	
<pre> STR      ! Wgt = 7.53% LONE 16 2 18 1 END BOND S 1 13 S 2 13 S 3 14 S 4 14 S 5 15 S 6 15 S 7 17 S 8 17 S 9 21 S 10 21 S 11 22 S 12 22 S 13 14 S 13 18 S 14 15 S 15 16 S 16 19 S 17 18 S 17 22 S 18 19 D 19 20 S 20 21 S 20 23 S 21 22 END END </pre>	<p style="text-align: center;">! Wgt = 7.53%</p>	
<pre> STR      ! Wgt = 1.49% LONE 18 2 20 1 END BOND S 1 13 S 2 13 S 3 14 S 4 14 S 5 15 S 6 15 S 7 17 S 8 17 S 9 21 S 10 21 S 11 22 S 12 22 S 13 14 S 13 18 S 14 15 S 15 16 T 16 19 S 17 18 S 17 22 S 19 20 S 20 21 S 20 23 S 21 22 END END </pre>	<p style="text-align: center;">! Wgt = 1.49%</p>	
<pre> STR      ! Wgt = 1.06% LONE 18 1 20 2 END BOND S 1 13 S 2 13 S 3 14 S 4 14 S 5 15 S 6 15 S 7 17 S 8 17 S 9 21 S 10 21 S 11 22 S 12 22 S 13 14 S 13 18 S 14 15 S 15 16 T 16 19 S 17 18 S 17 22 S 18 19 S 20 21 S 20 23 S 21 22 END END </pre>	<p style="text-align: center;">! Wgt = 1.06%</p>	

## Compound 1



NBO bonding description	representation	Simplified representation
<pre> STR ! Wgt = 17.56% LONE 10 1 11 4 65 2 66 1 67 1 END BOND S 1 2 D 2 3 S 2 4 S 3 6 S 3 7 D 4 5 S 4 8 S 5 65 S 5 67 S 6 65 D 6 66 S 9 11 S 9 39 S 9 52 S 9 66 S 10 13 S 10 14 S 10 67 S 11 12 S 13 15 S 13 19 S 13 23 S 14 27 S 14 31 S 14 35 S 15 16 S 15 17 S 15 18 S 19 20 S 19 21 S 19 22 S 23 24 S 23 25 S 23 26 S 27 28 S 27 29 S 27 30 S 31 32 S 31 33 S 31 34 S 35 36 S 35 37 S 35 38 S 39 40 S 39 44 S 39 48 S 40 41 S 40 42 S 40 43 S 44 45 S 44 46 S 44 47 S 48 49 S 48 50 S 48 51 S 52 53 S 52 57 S 52 61 S 53 54 S 53 55 S 53 56 S 57 58 S 57 59 S 57 60 S 61 62 S 61 63 S 61 64 S 67 68 END END </pre>	<p>Wgt = 17.56%</p>	
<pre> STR ! Wgt = 10.01% LONE 10 1 11 4 65 1 66 2 67 1 END BOND S 1 2 D 2 3 S 2 4 S 3 6 S 3 7 D 4 5 S 4 8 S 5 65 S 5 67 D 6 65 S 6 66 S 9 11 S 9 39 S 9 52 S 9 66 S 10 13 S 10 14 S 10 67 S 11 12 S 13 15 S 13 19 S 13 23 S 14 27 S 14 31 S 14 35 S 15 16 S 15 17 S 15 18 S 19 20 S 19 21 S 19 22 S 23 24 S 23 25 S 23 26 S 27 28 S 27 29 S 27 30 S 31 32 S 31 33 S 31 34 S 35 36 S 35 37 S 35 38 S 39 40 S 39 44 S 39 48 S 40 41 S 40 42 S 40 43 S 44 45 S 44 46 S 44 47 S 48 49 S 48 50 S 48 51 S 52 53 S 52 57 S 52 61 S 53 54 S 53 55 S 53 56 S 57 58 S 57 59 S 57 60 S 61 62 S 61 63 S 61 64 S 67 68 END END </pre>	<p>Wgt = 10.01%</p>	

<pre> \$NRTSTR STR ! Wgt = 9.36% LONE 4 1 10 1 11 4 65 1 66 1 67 1 END BOND S 1 2 D 2 3 S 2 4 S 3 6 S 3 7 S 4 5 S 4 8 D 5 65 S 5 67 S 6 65 D 6 66 S 9 11 S 9 39 S 9 52 S 9 66 S 10 13 S 10 14 S 10 67 S 11 12 S 13 15 S 13 19 S 13 23 S 14 27 S 14 31 S 14 35 S 15 16 S 15 17 S 15 18 S 19 20 S 19 21 S 19 22 S 23 24 S 23 25 S 23 26 S 27 28 S 27 29 S 27 30 S 31 32 S 31 33 S 31 34 S 35 36 S 35 37 S 35 38 S 39 40 S 39 44 S 39 48 S 40 41 S 40 42 S 40 43 S 44 45 S 44 46 S 44 47 S 48 49 S 48 50 S 48 51 S 52 53 S 52 57 S 52 61 S 53 54 S 53 55 S 53 56 S 57 58 S 57 59 S 57 60 S 61 62 S 61 63 S 61 64 S 67 68 END END </pre>	<p style="text-align: center;">Wgt = 9.36%</p>	<p style="text-align: center;">Wgt = 9.36%</p>
<pre> STR ! Wgt = 6.42% LONE 3 1 10 1 11 4 65 1 66 1 67 1 END BOND S 1 2 S 2 3 D 2 4 S 3 6 S 3 7 S 4 5 S 4 8 D 5 65 S 5 67 S 6 65 D 6 66 S 9 11 S 9 39 S 9 52 S 9 66 S 10 13 S 10 14 S 10 67 S 11 12 S 13 15 S 13 19 S 13 23 S 14 27 S 14 31 S 14 35 S 15 16 S 15 17 S 15 18 S 19 20 S 19 21 S 19 22 S 23 24 S 23 25 S 23 26 S 27 28 S 27 29 S 27 30 S 31 32 S 31 33 S 31 34 S 35 36 S 35 37 S 35 38 S 39 40 S 39 44 S 39 48 S 40 41 S 40 42 S 40 43 S 44 45 S 44 46 S 44 47 S 48 49 S 48 50 S 48 51 S 52 53 S 52 57 S 52 61 S 53 54 S 53 55 S 53 56 S 57 58 S 57 59 S 57 60 S 61 62 S 61 63 S 61 64 S 67 68 END END </pre>	<p style="text-align: center;">Wgt = 6.42%</p>	<p style="text-align: center;">Wgt = 6.42%</p>
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## References

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