# Supporting Information

## Half-sandwich rare-earth metal tris(alkyl) ate complexes catalyzed phosphaguanylation reaction of phosphines with carbodiimides: an efficient synthesis of phosphaguanidines

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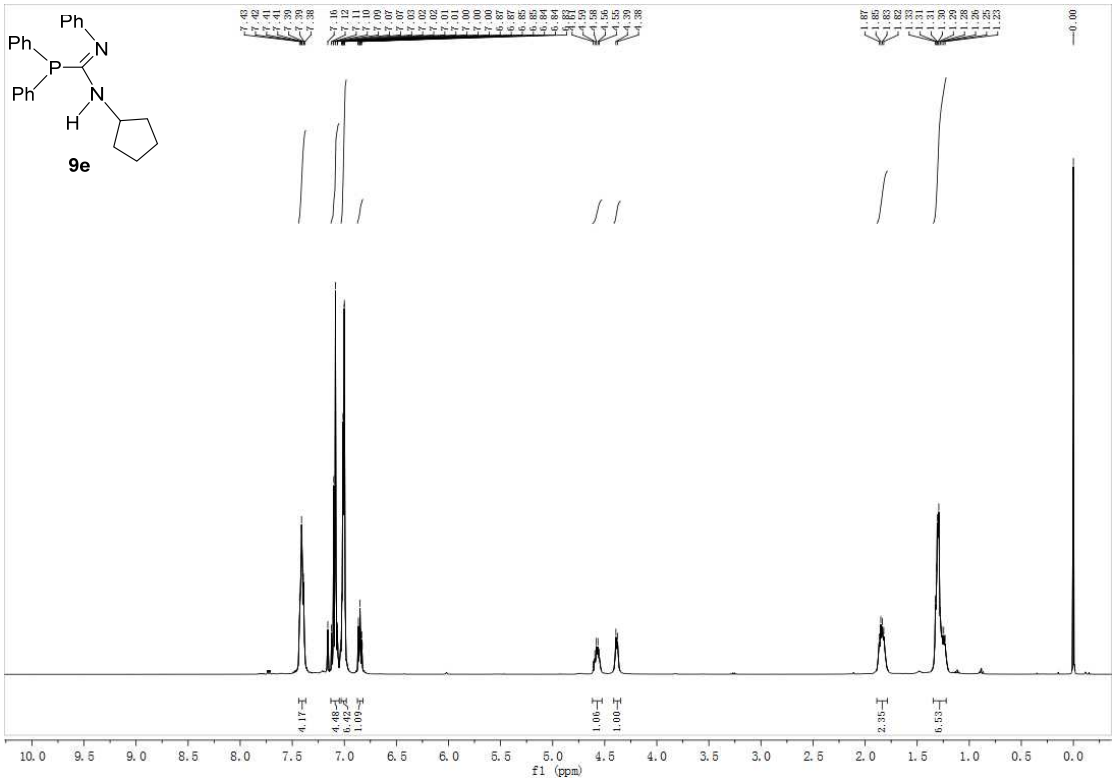
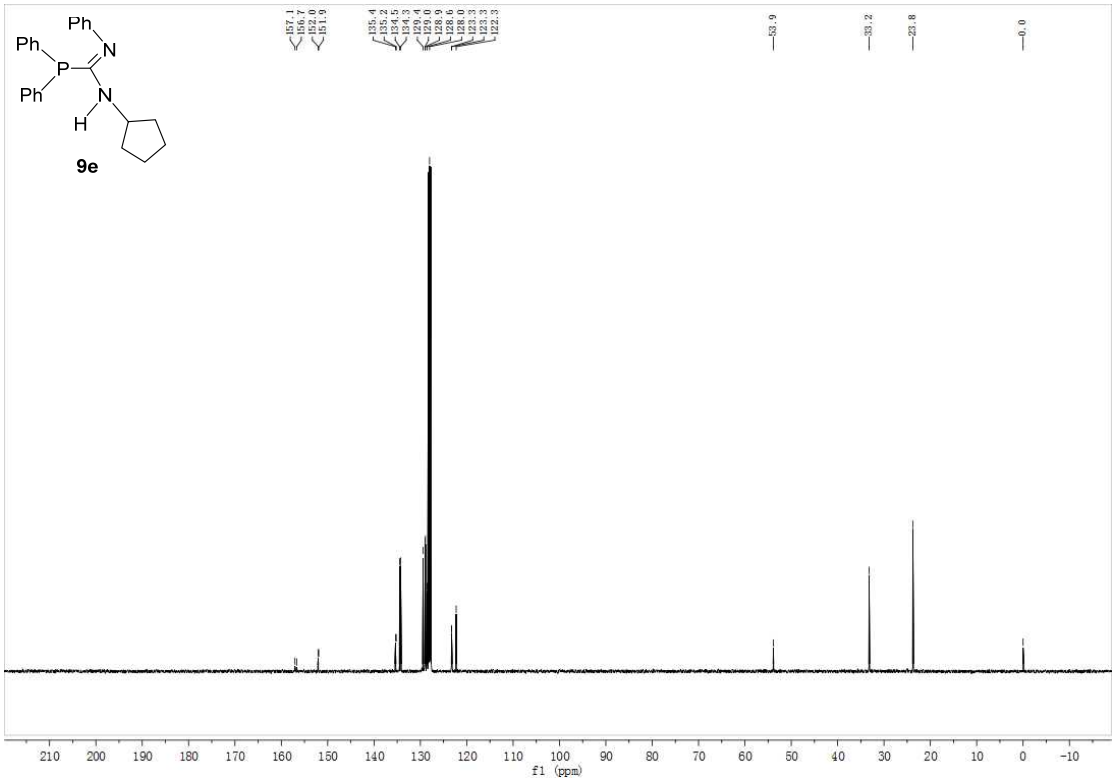
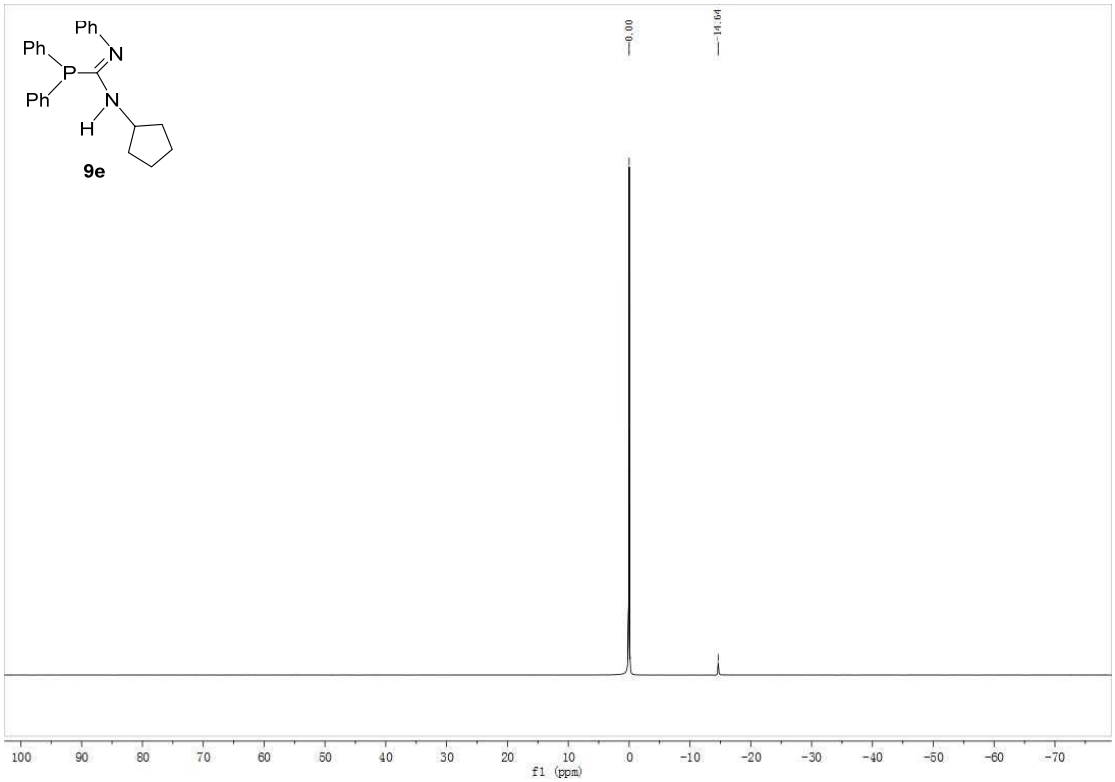
E-mail: wx_zhang@pku.edu.cn

## Contents

## 1) Copies of $^{1}H$ NMR, $^{13}C$ NMR and $^{31}P$ NMR Spectra of All New Compounds

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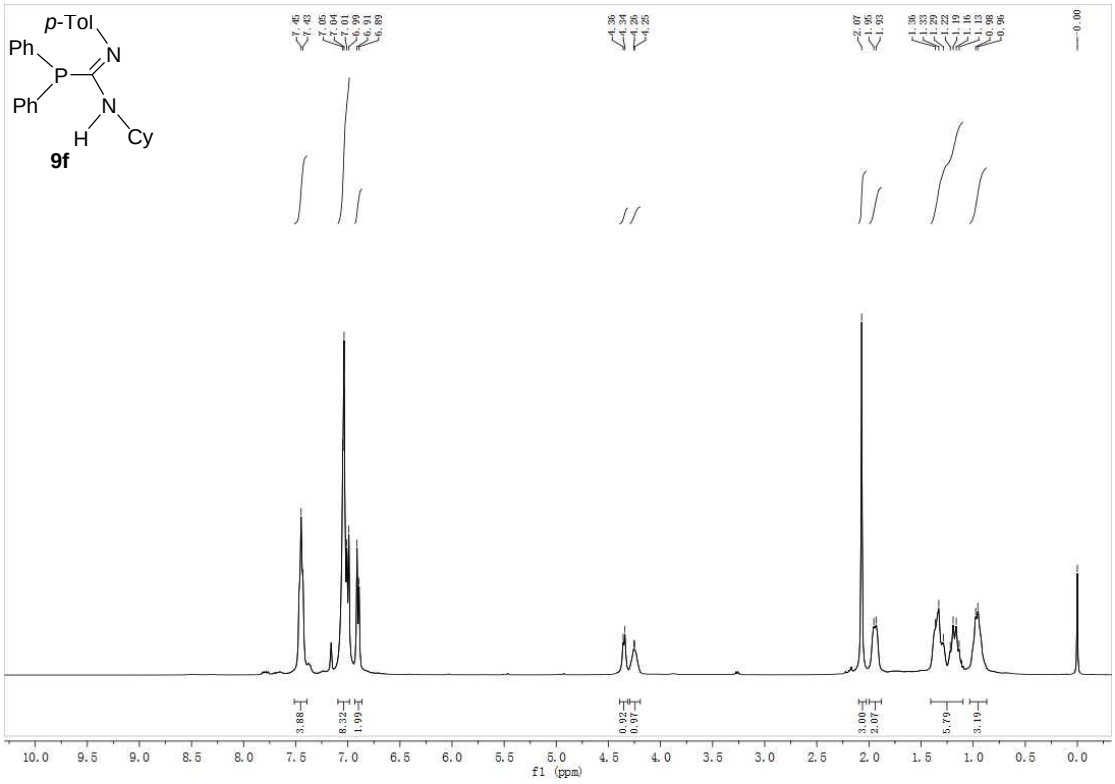
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P
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Ph
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H
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6.91
6.89
4.36
4.34
4.26
4.25
2.07
1.95
1.93
1.36
1.33
1.29
1.22
1.19
1.16
1.13
0.98
0.96
0.00
3.88
8.32
1.99
0.93
0.97
3.00
2.07
5.79
3.19
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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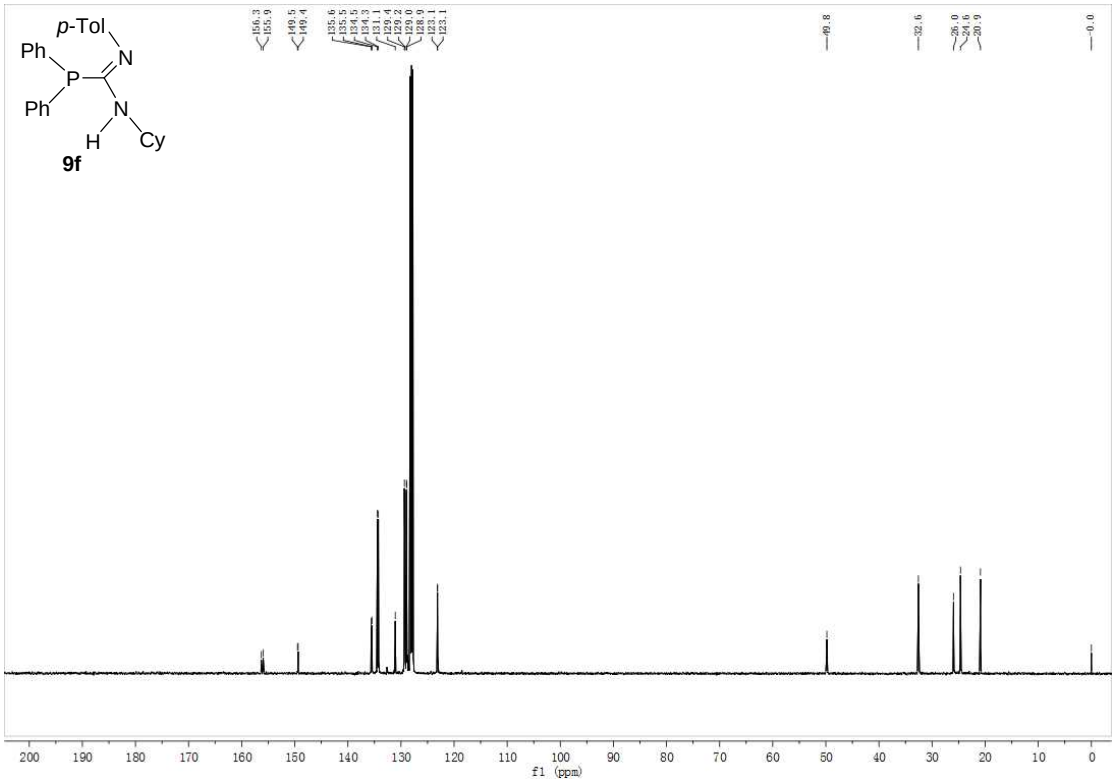
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P
Ph
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9f
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135.5
134.5
134.3
131.1
129.4
129.2
129.0
128.9
123.1
123.1
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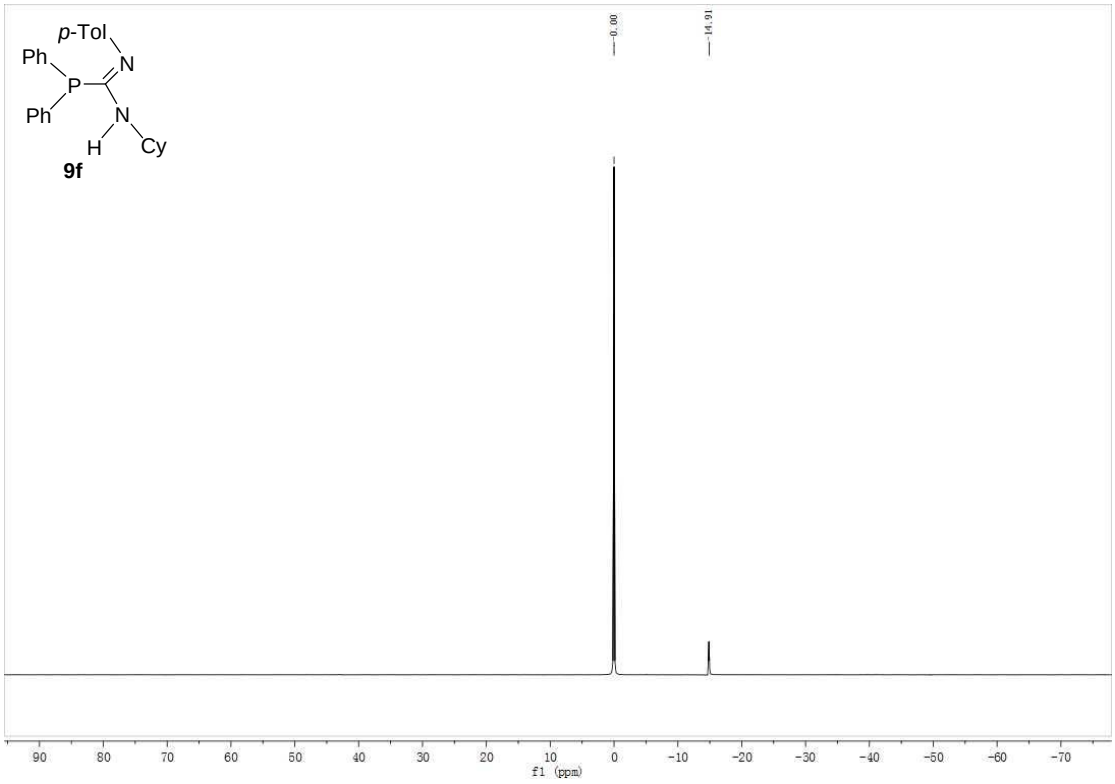
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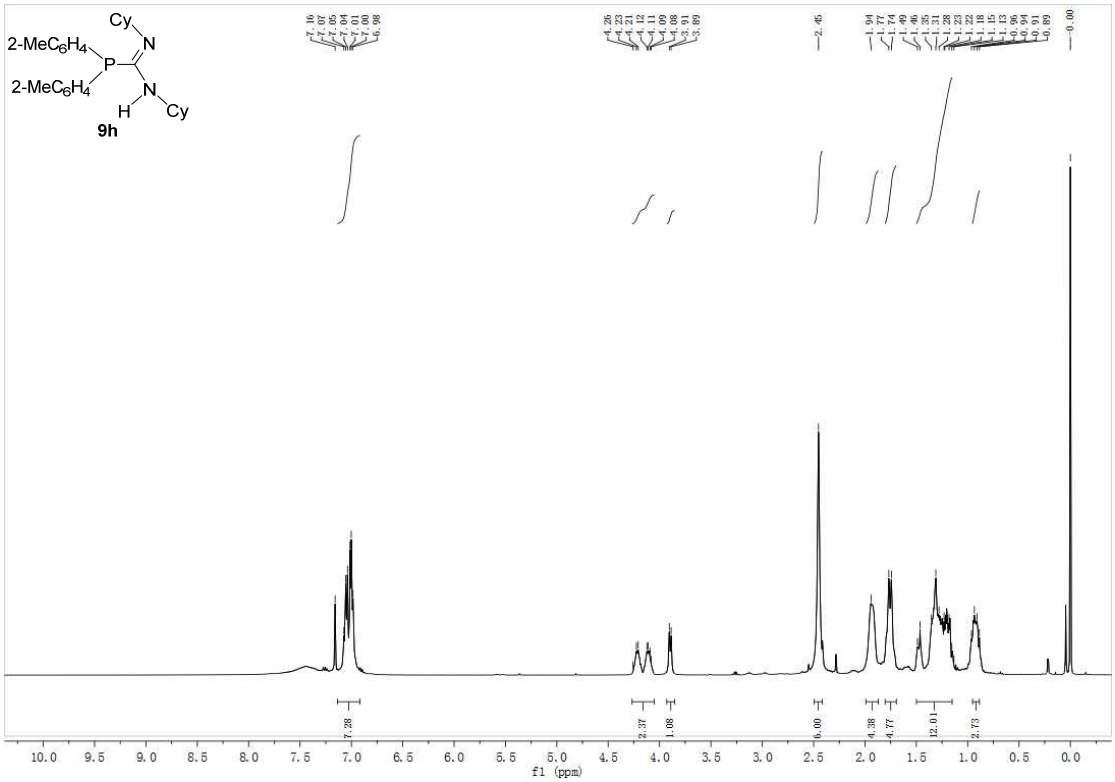
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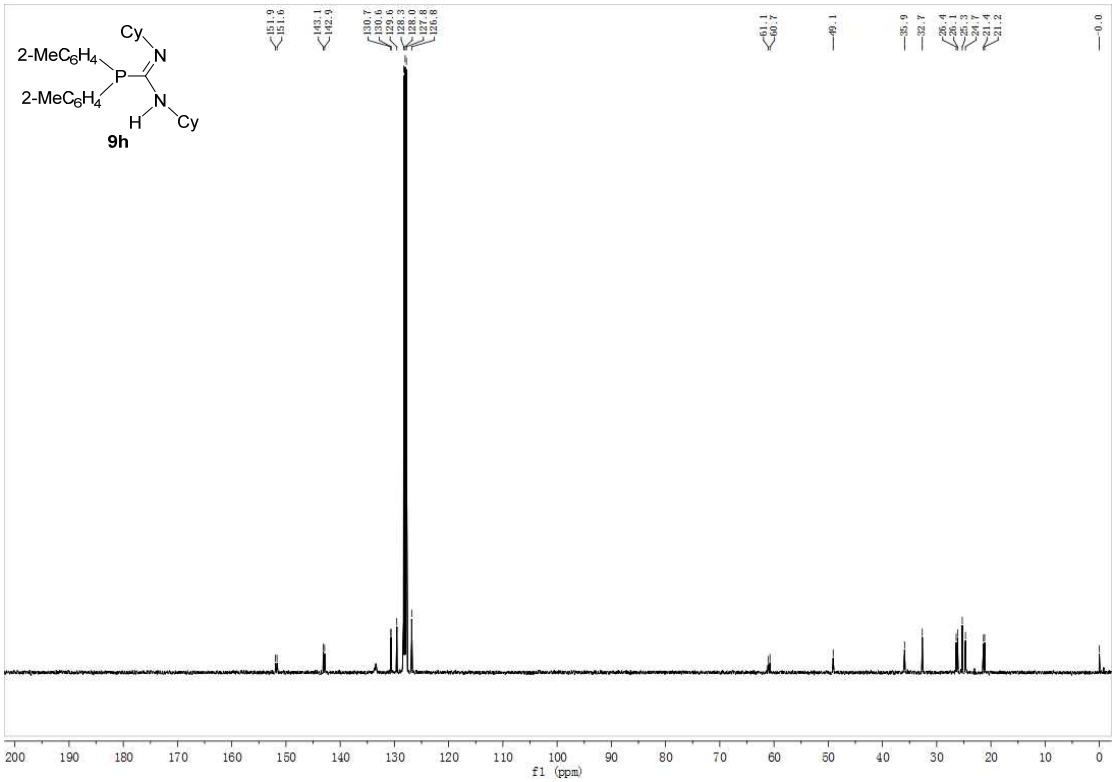
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H
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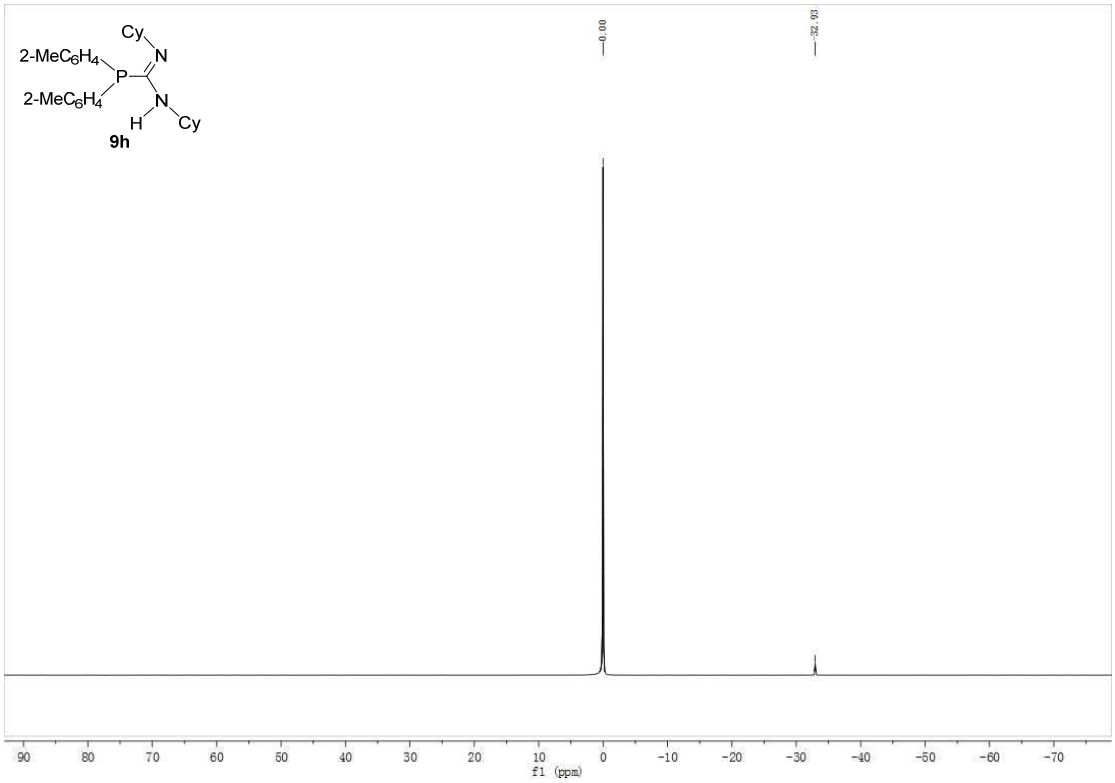
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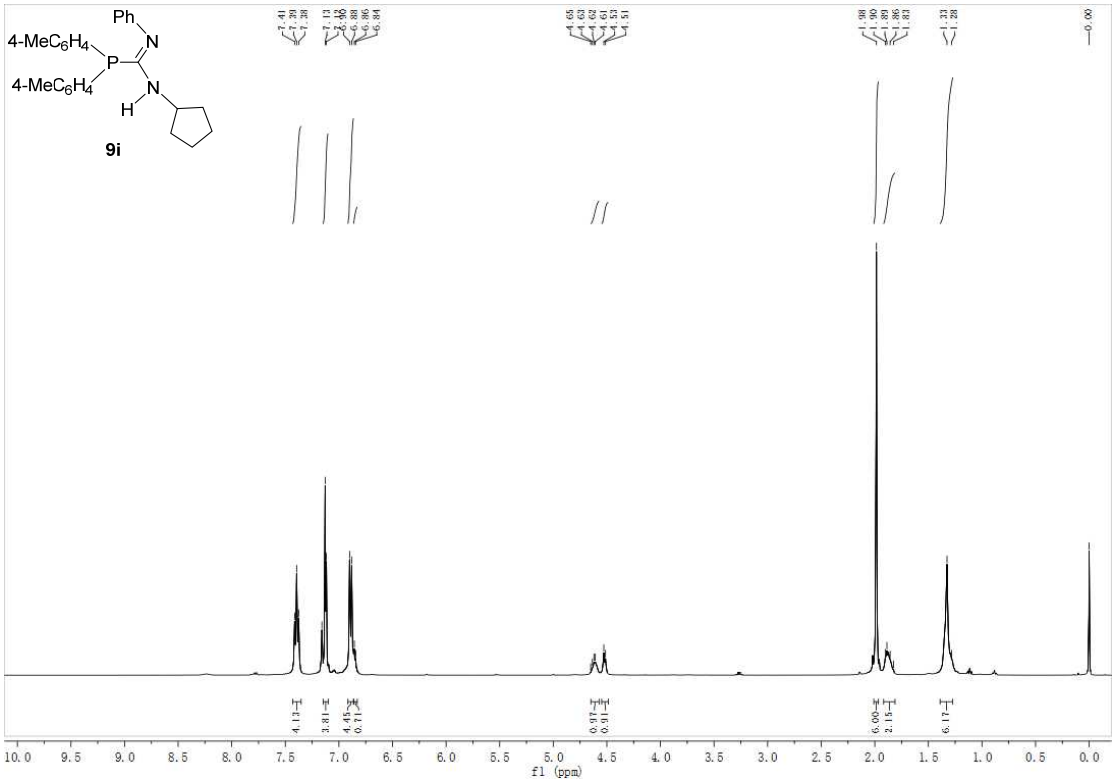
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H
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6.86
6.84
4.65
4.63
4.62
4.53
4.51
1.98
1.90
1.89
1.86
1.83
1.33
1.28
0.00
4.13
3.81
4.45
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0.91
0.91
6.00
2.15
6.17
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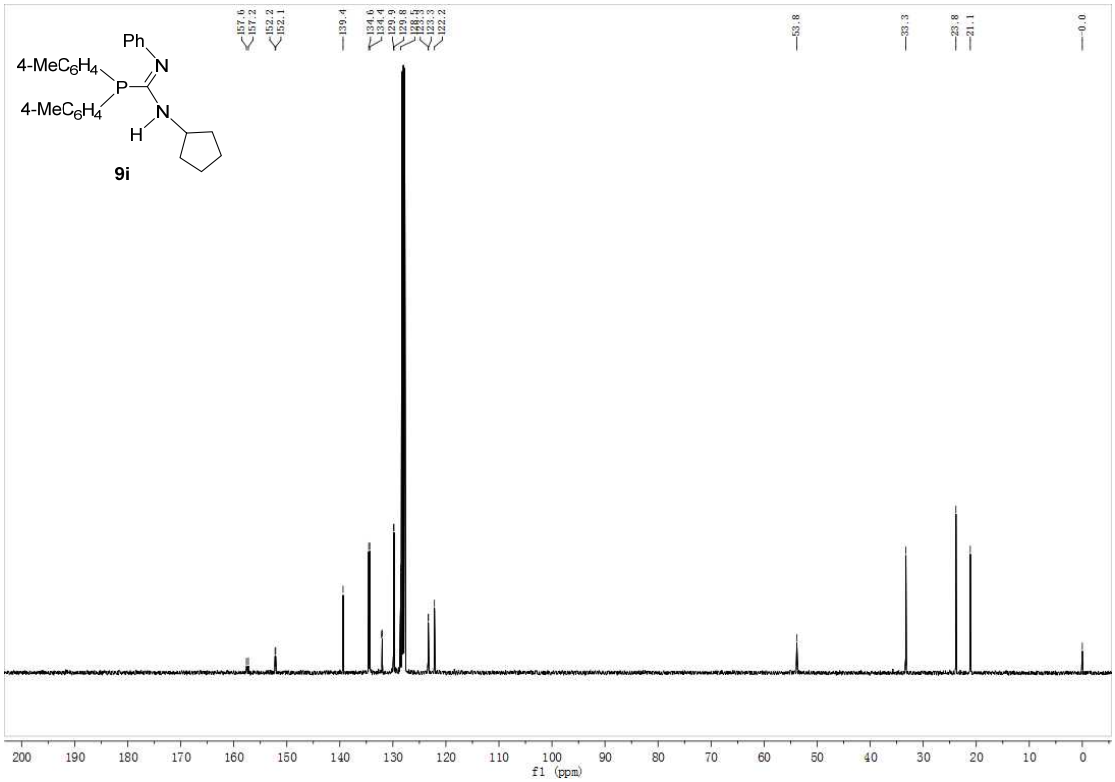
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H
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134.6
134.4
129.9
129.8
128.5
123.3
122.2
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23.8
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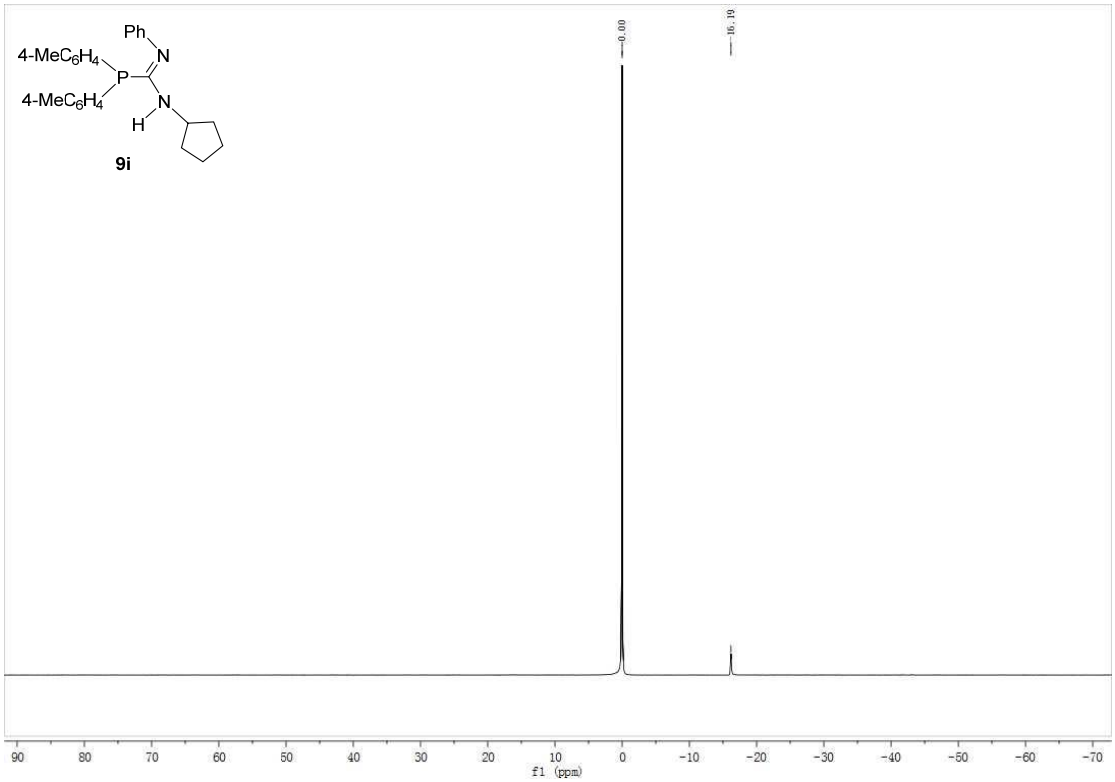
f1 (ppm)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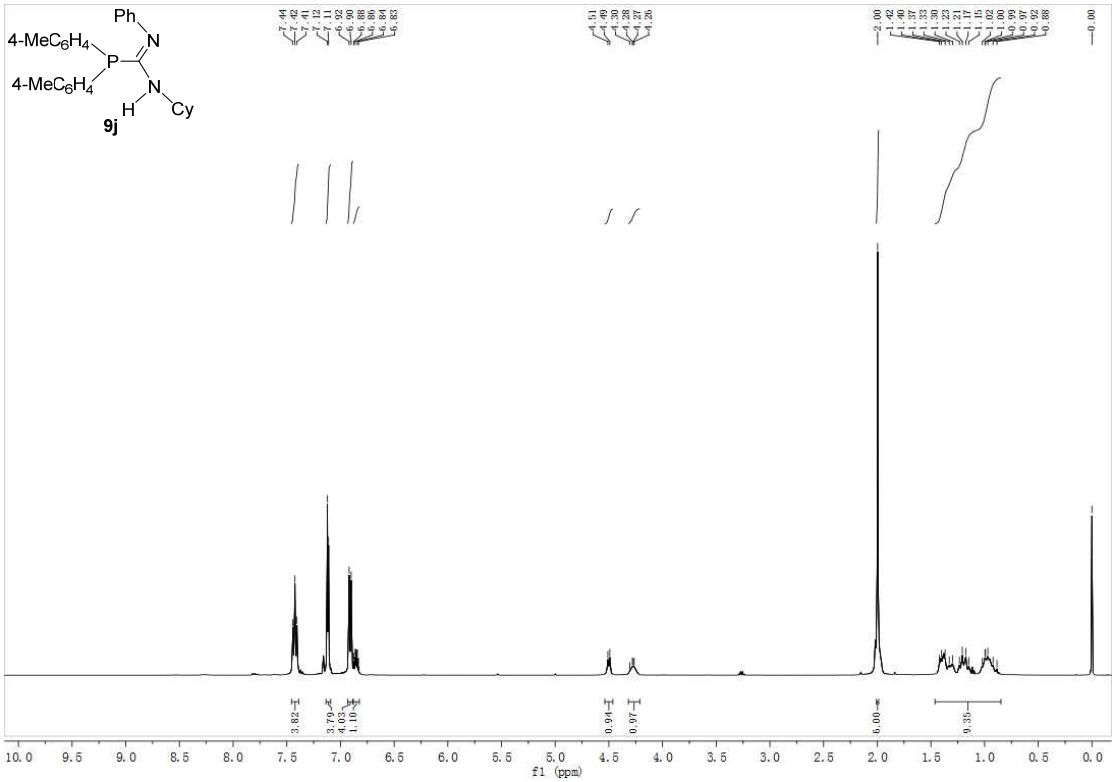
f1 (ppm)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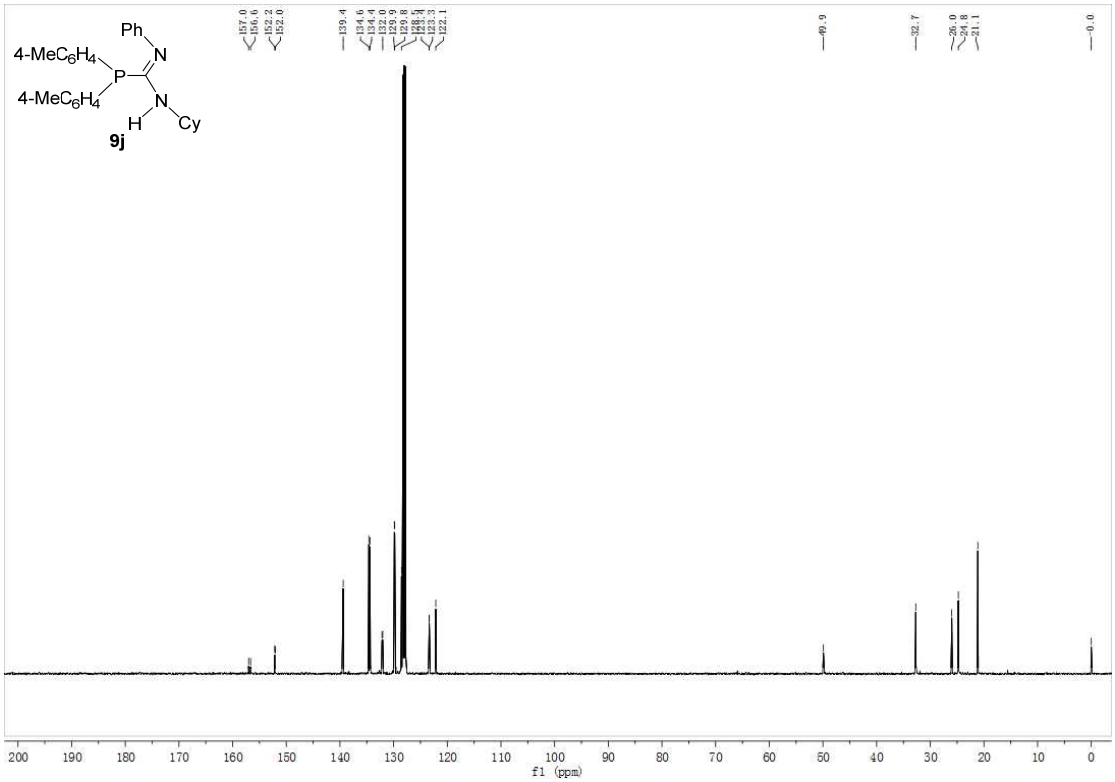
9j
f1 (ppm)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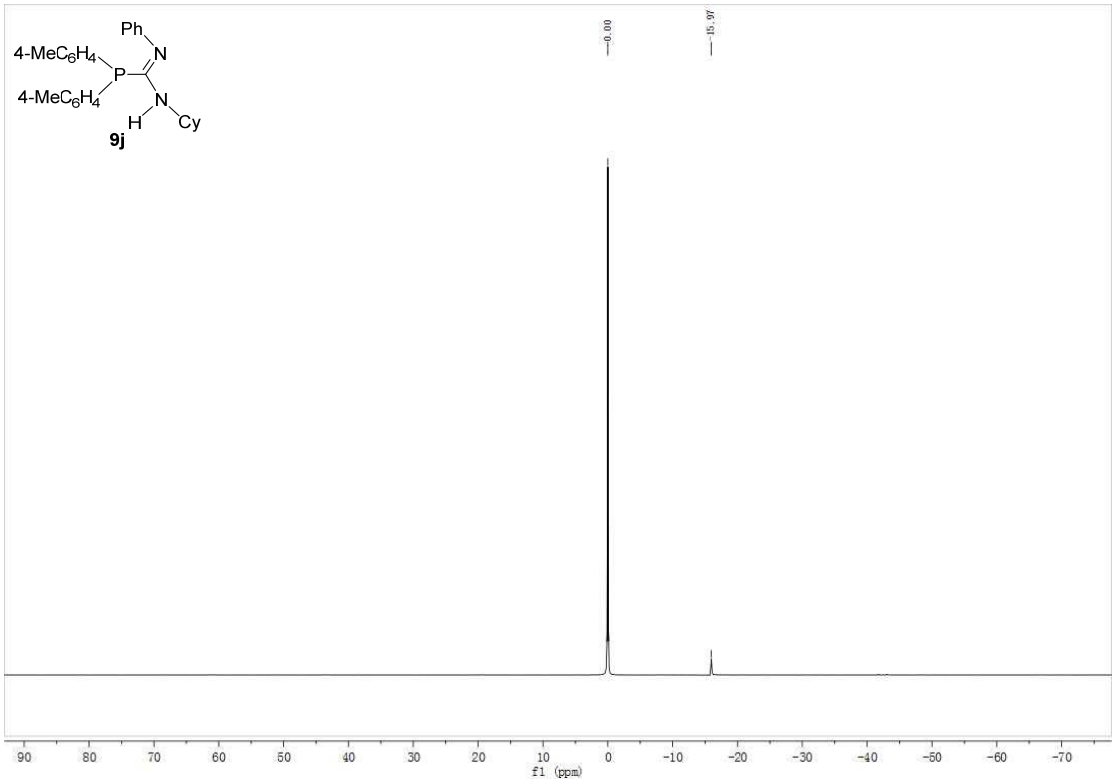
9j
f1 (ppm)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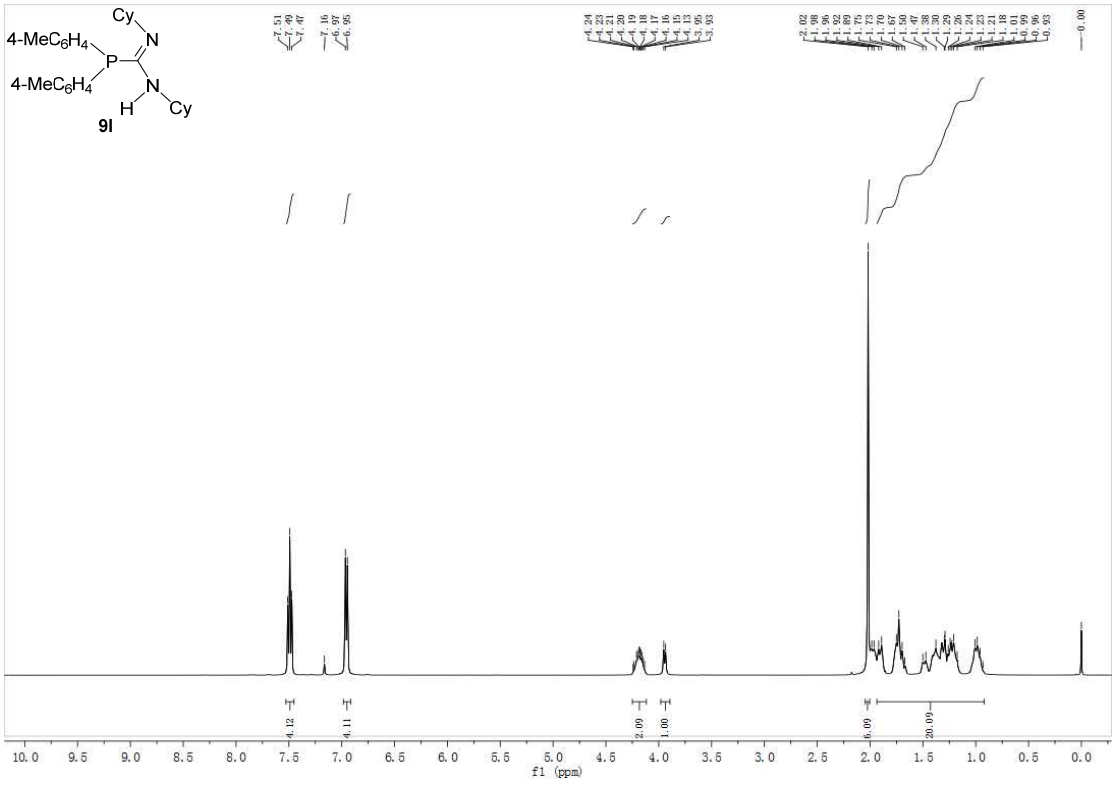
f1 (ppm)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6.95
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4.21
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4.19
4.18
4.17
4.16
4.15
4.13
3.95
3.93
2.02
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1.96
1.92
1.89
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1.67
1.50
1.47
1.38
1.30
1.29
1.26
1.24
1.23
1.21
1.18
1.01
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0.93
0.00
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4.11
2.09
1.00
6.09
20.09
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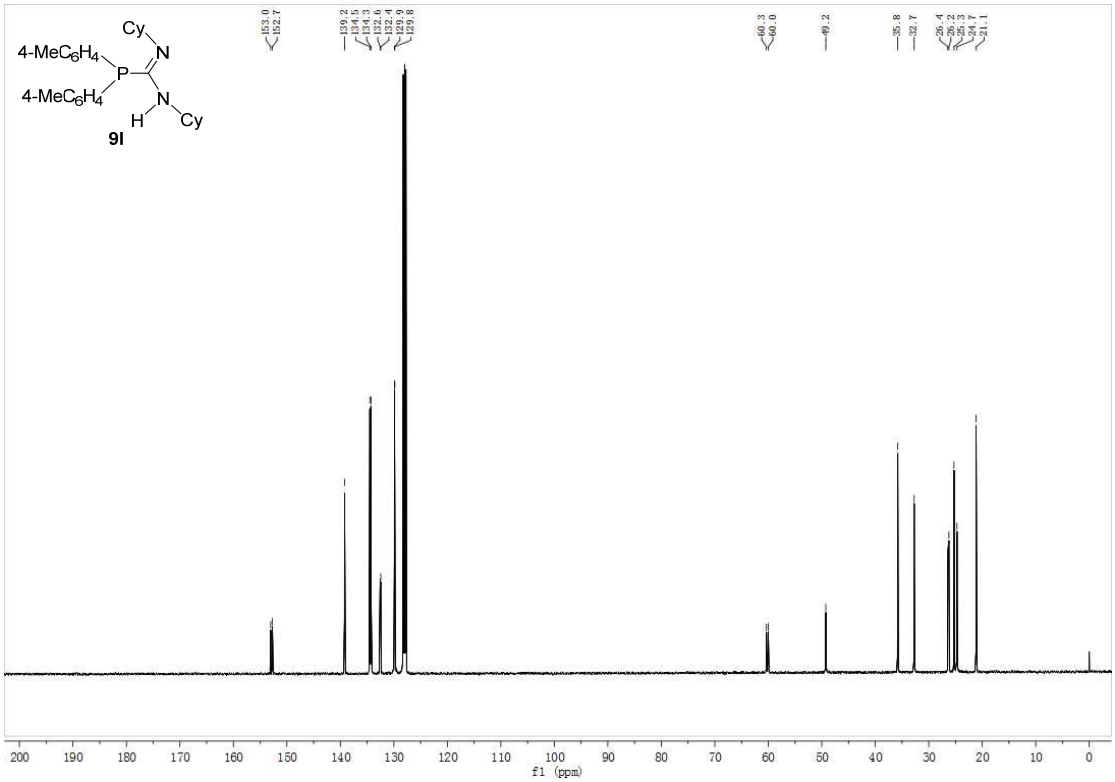
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4-MeC6H4
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H
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132.6
132.4
129.9
129.8
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49.2
35.8
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25.3
24.7
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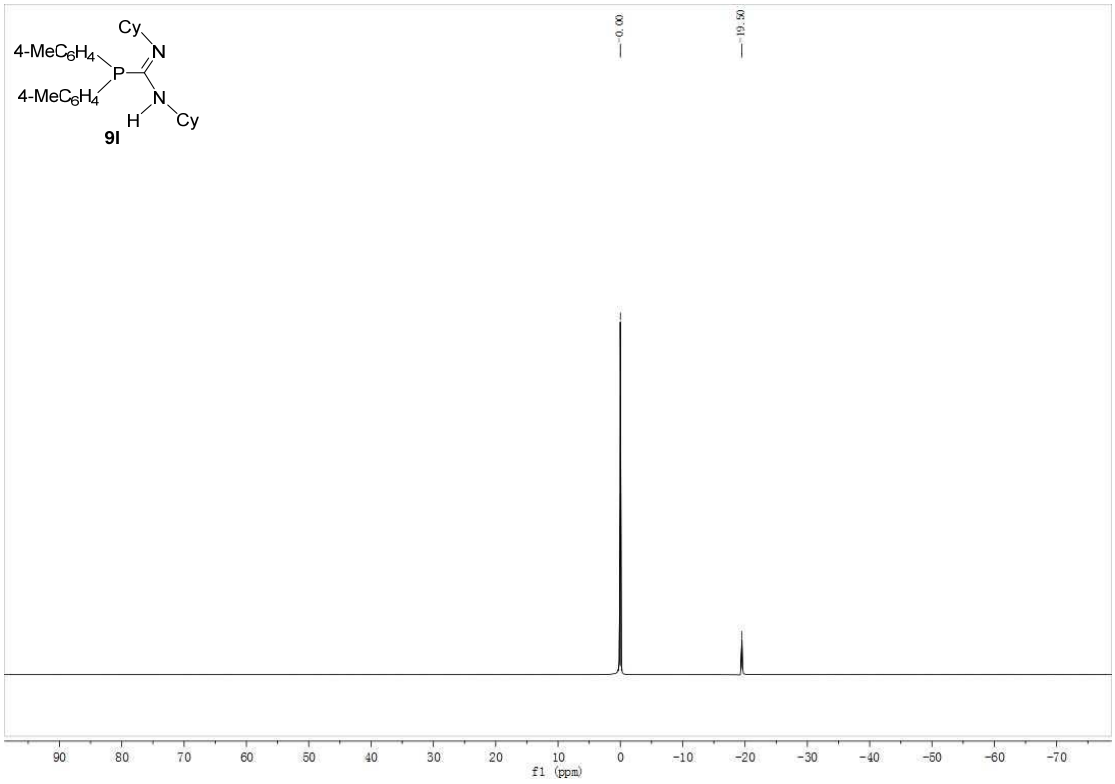
f1 (ppm)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P
4-MeC6H4
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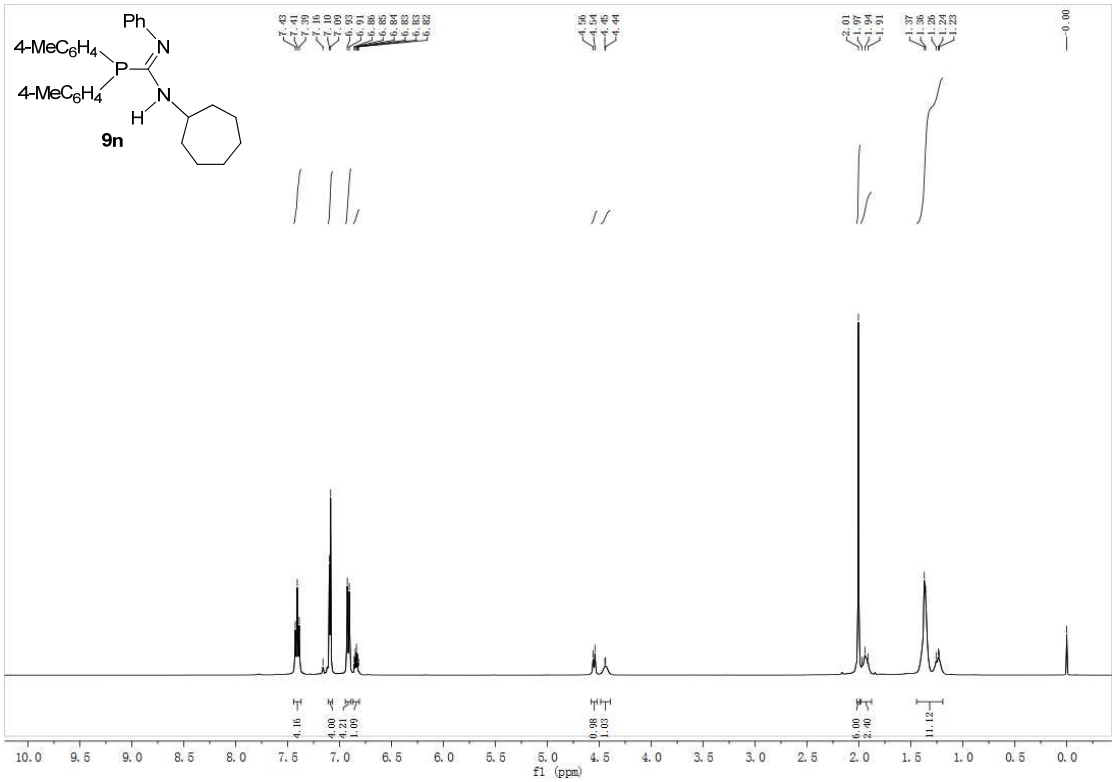
f1 (ppm)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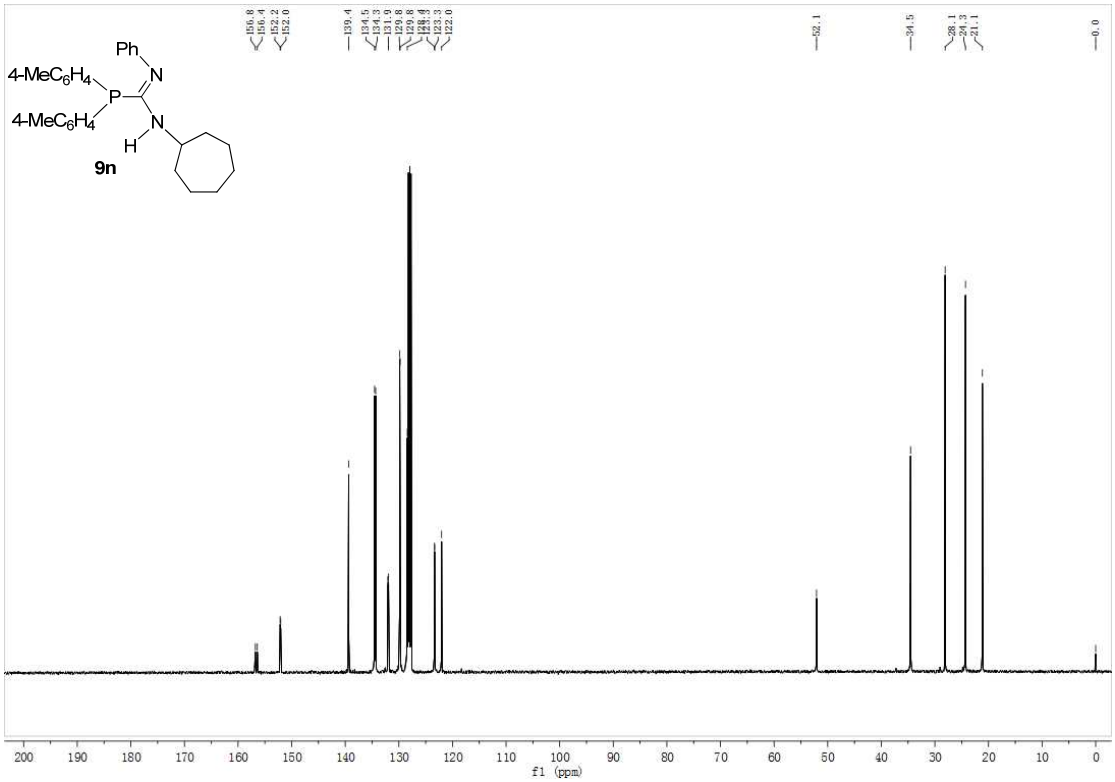
P
4-MeC6H4
N
H
9n
f1 (ppm)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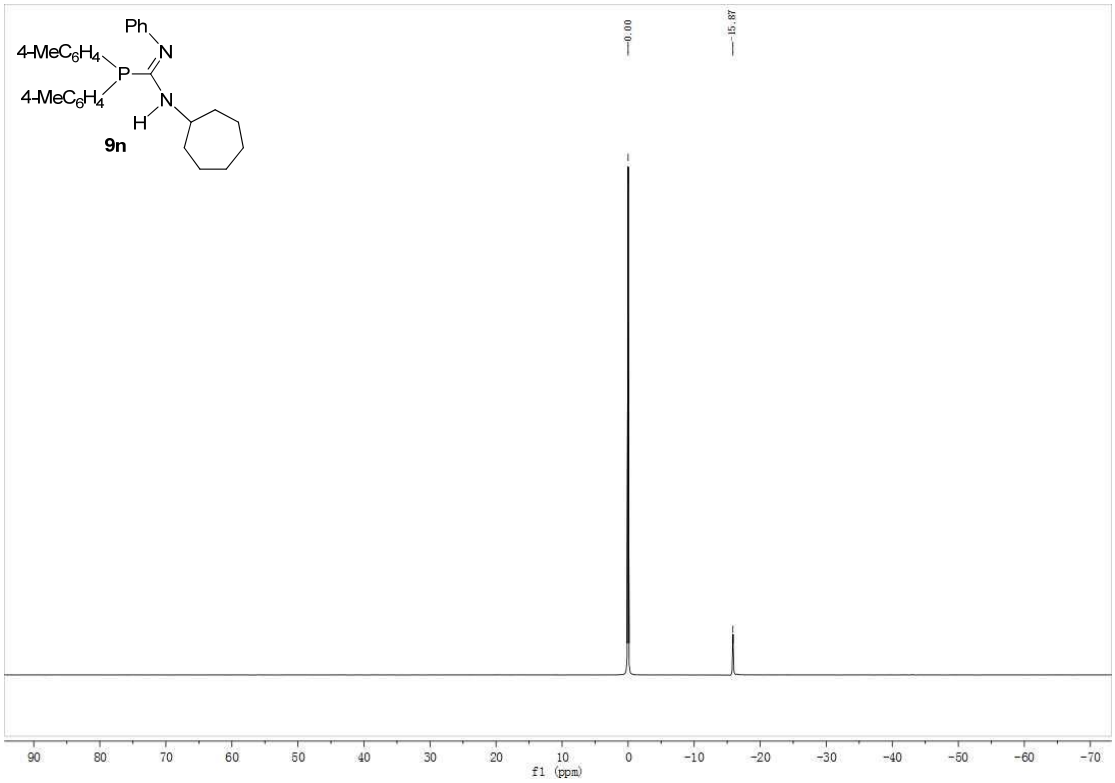
N
H
9n
f1 (ppm)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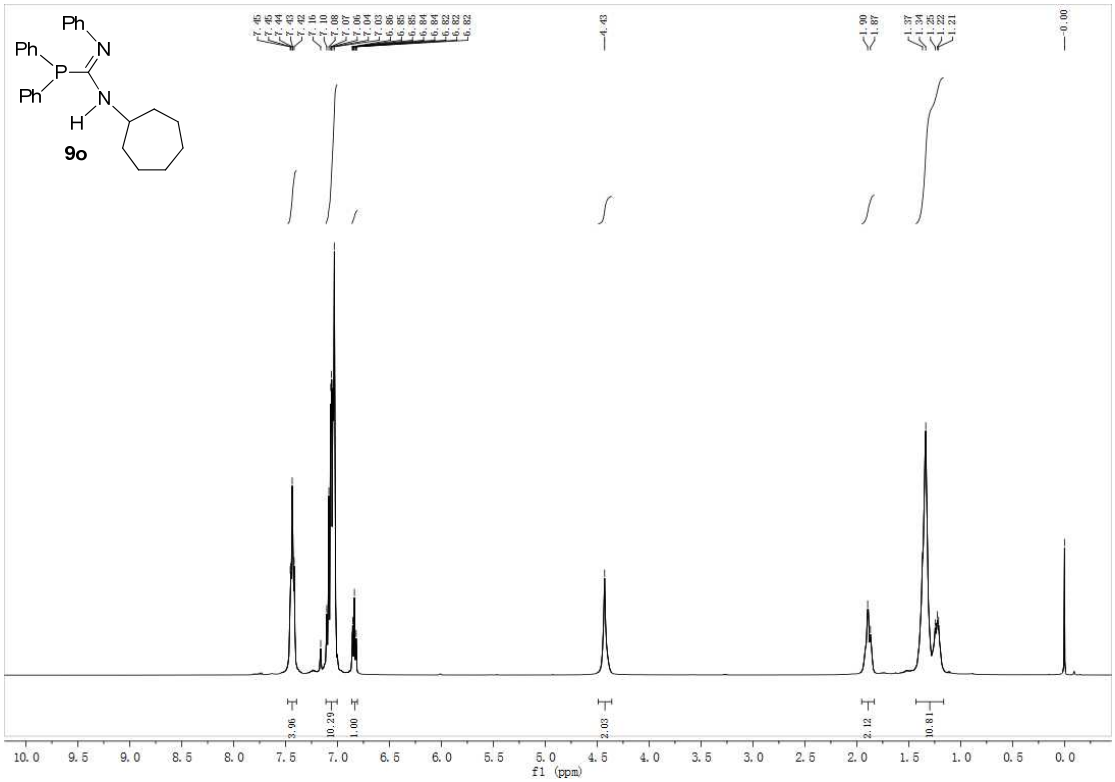
f1 (ppm)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Ph
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1.25
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1.21
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10.29
1.00
2.03
2.12
10.81
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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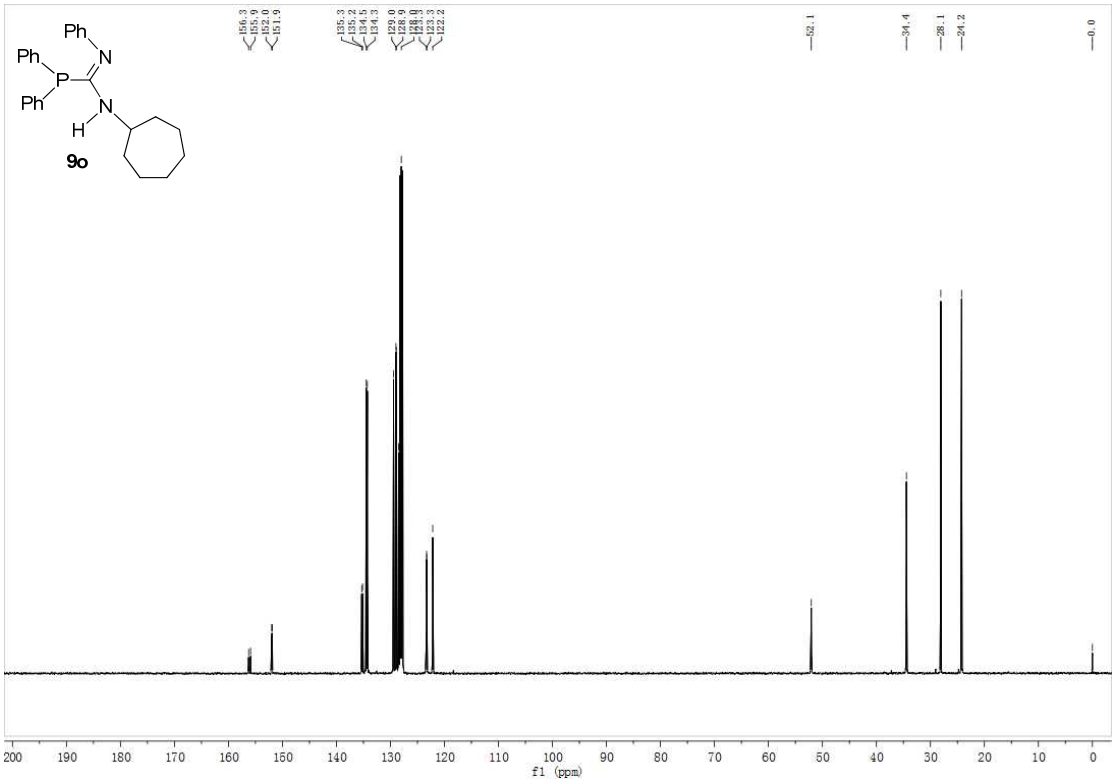
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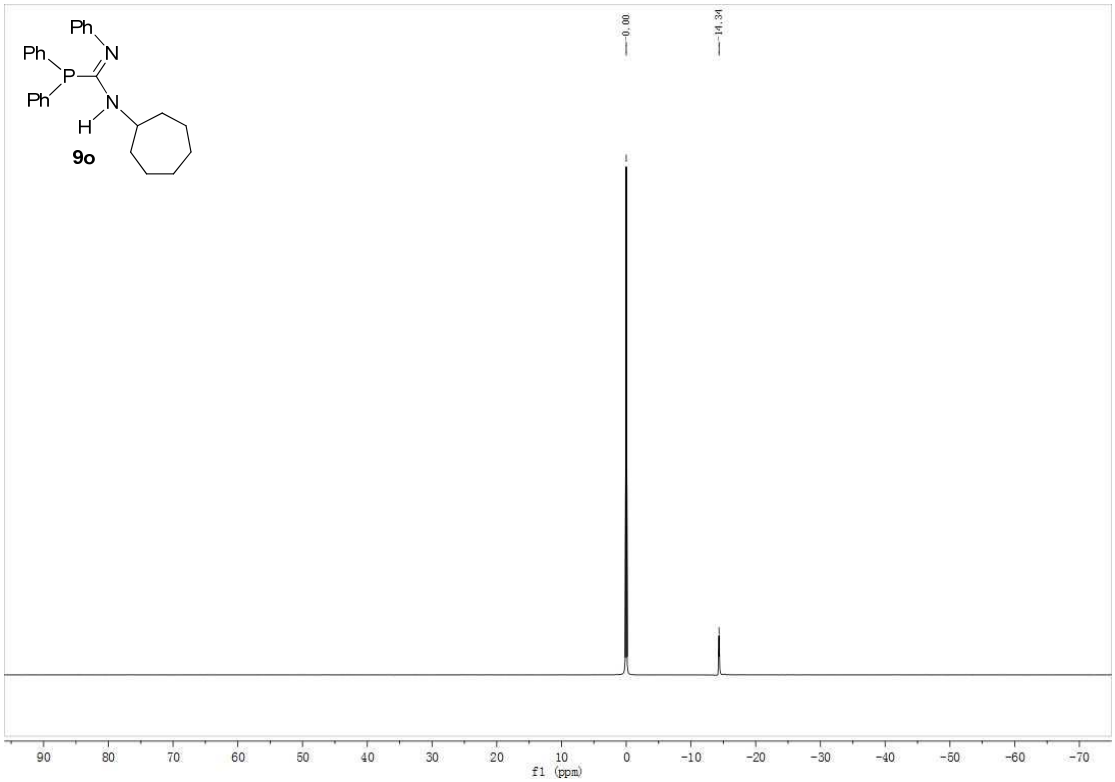
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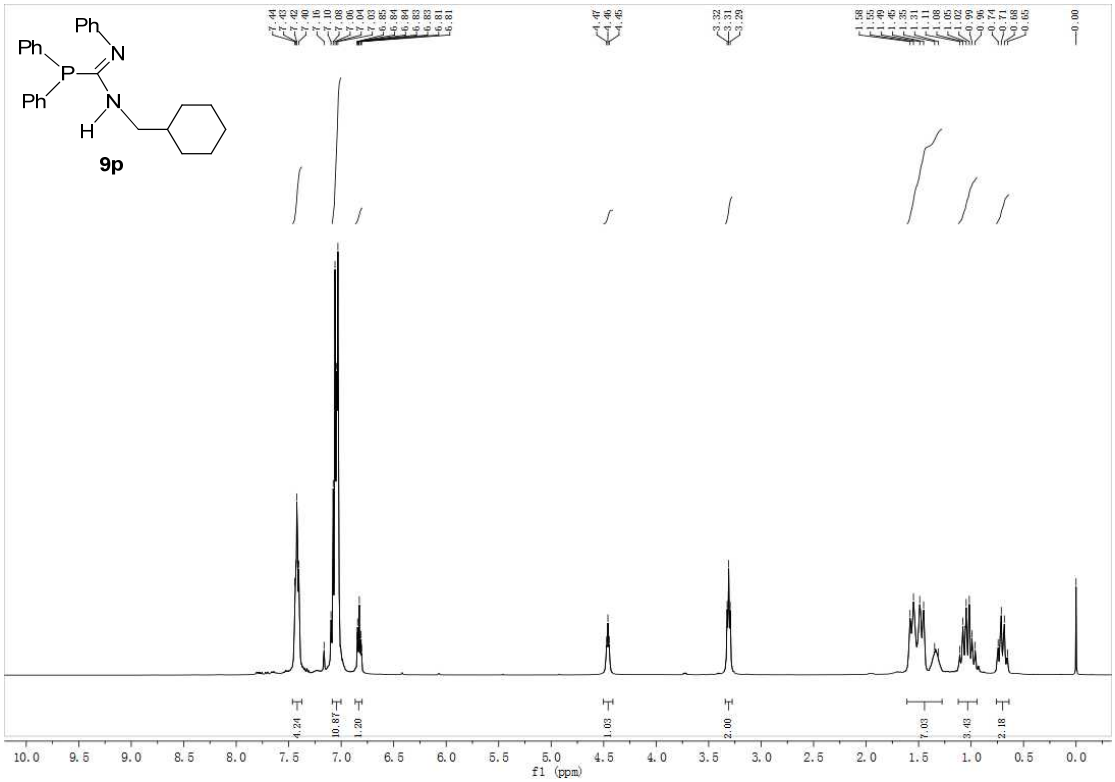
f1 (ppm)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9.0
8.5
8.0
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6.0
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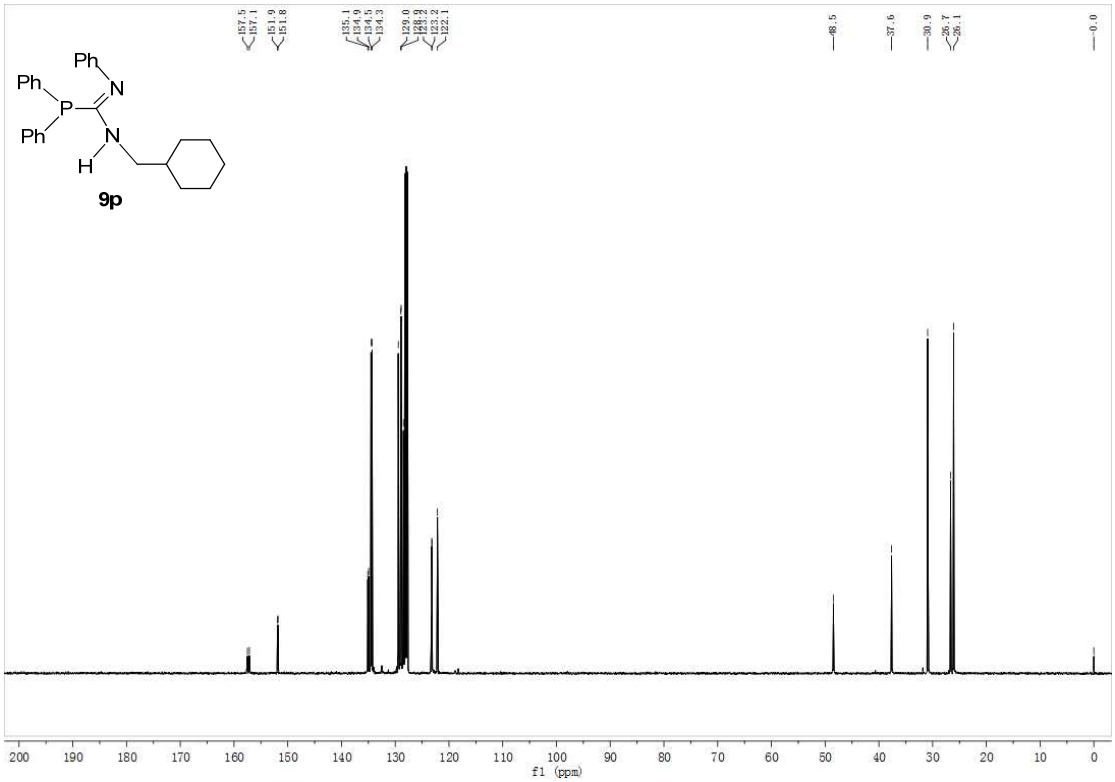
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134.3
129.0
128.9
123.2
123.2
122.2
122.1
48.5
37.6
30.9
26.7
26.1
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190
180
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110
100
90
80
70
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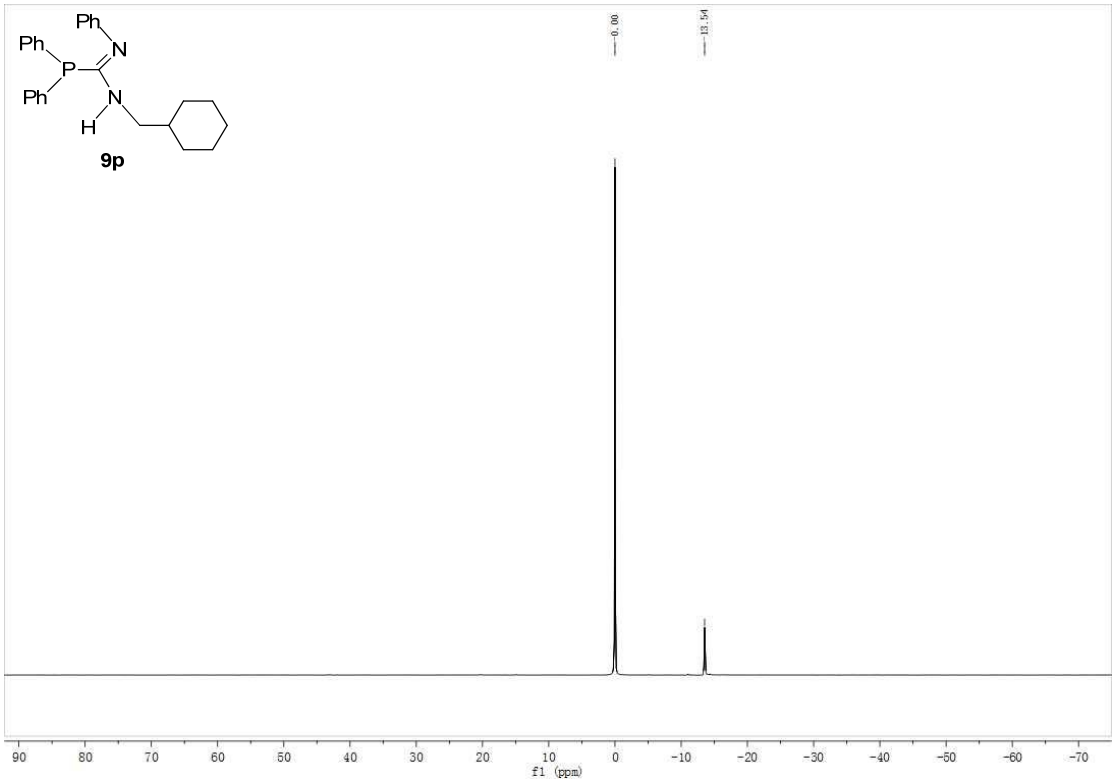
50
40
30
20
10
0
f1 (ppm)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Ph
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13.54
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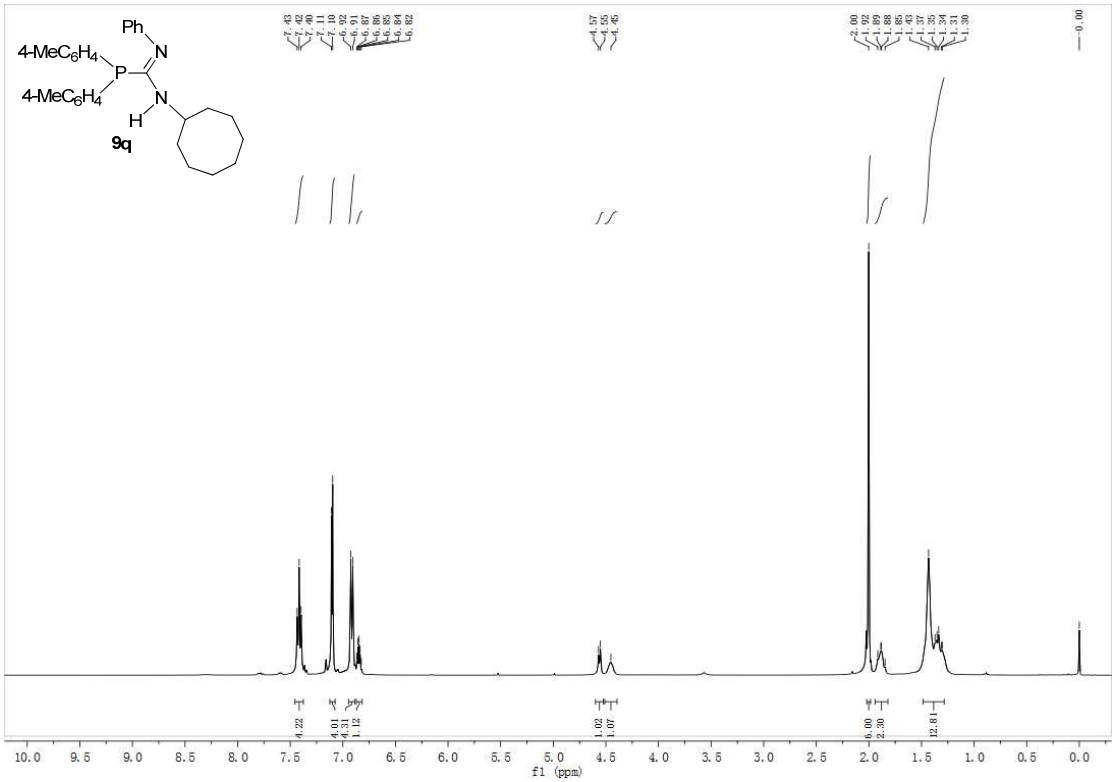
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N
P
4-MeC6H4
N
H
9q
7.43
7.42
7.40
7.11
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6.91
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4.46
2.00
1.92
1.89
1.88
1.65
1.64
1.37
1.35
1.34
1.31
1.30
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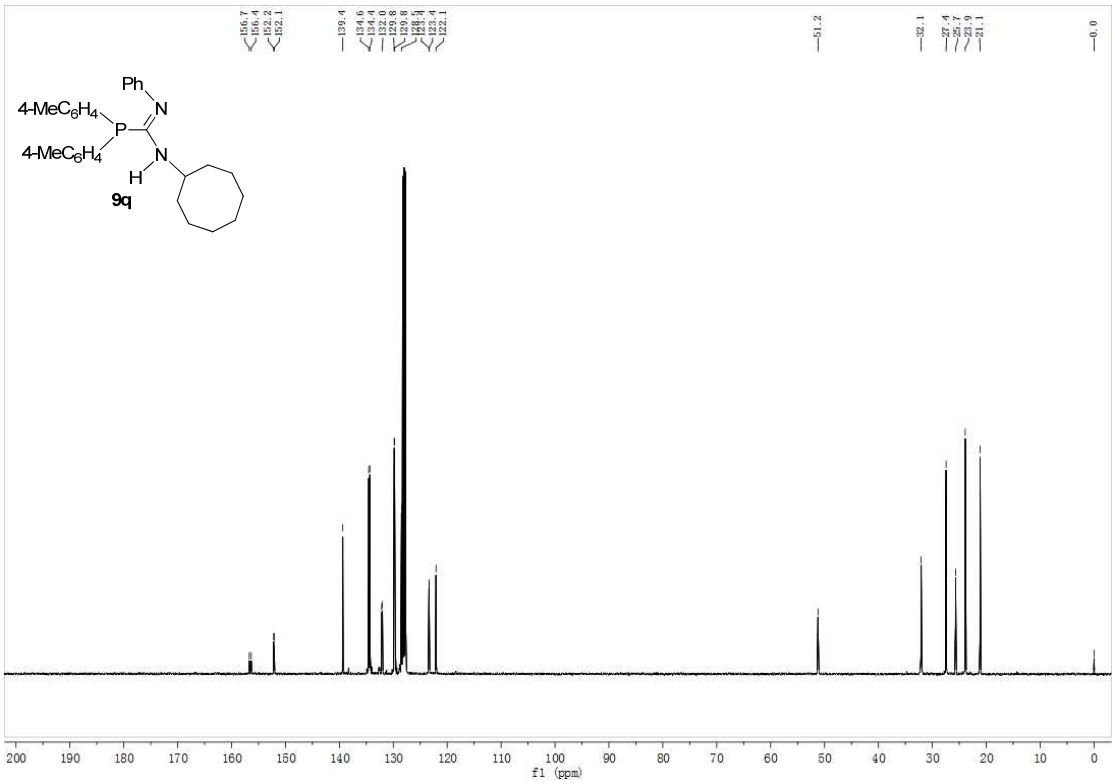
1.12
1.02
1.07
6.00
2.30
12.81
f1 (ppm)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P
4-MeC6H4
N
H
9q
156.7
156.4
152.2
152.1
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134.6
134.4
132.0
129.8
123.4
122.1
51.2
32.1
27.4
25.7
21.9
21.1
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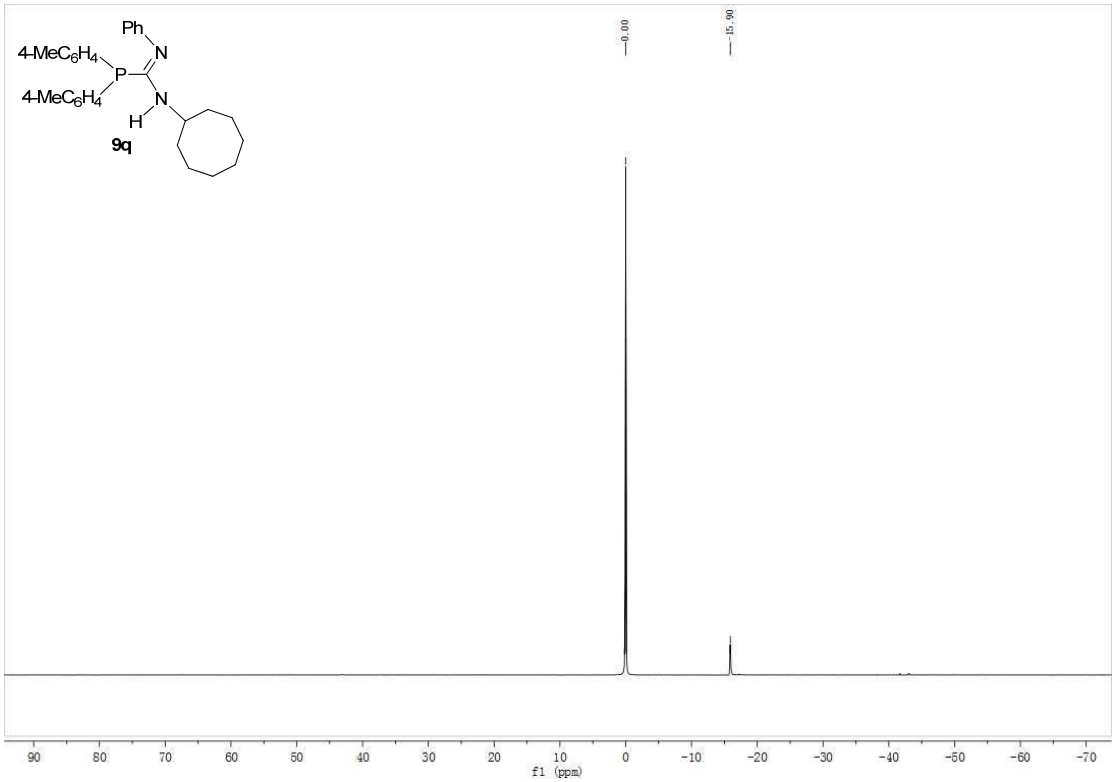
f1 (ppm)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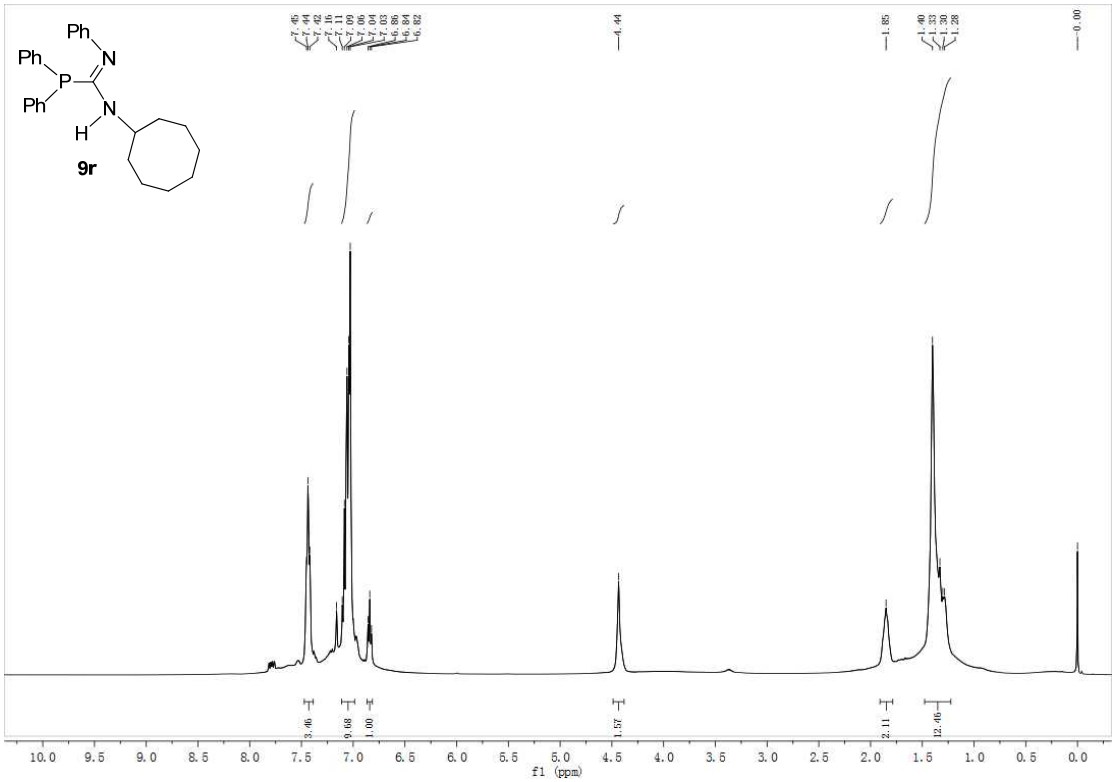
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6.84
6.82
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1.85
1.40
1.33
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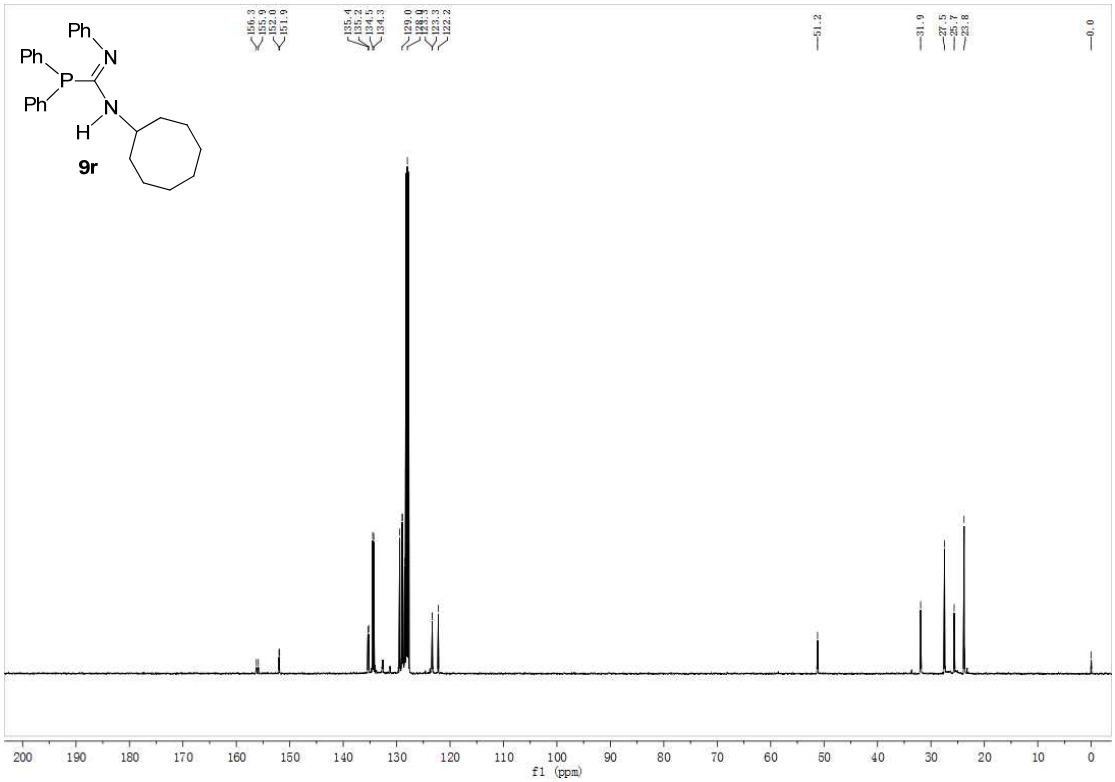
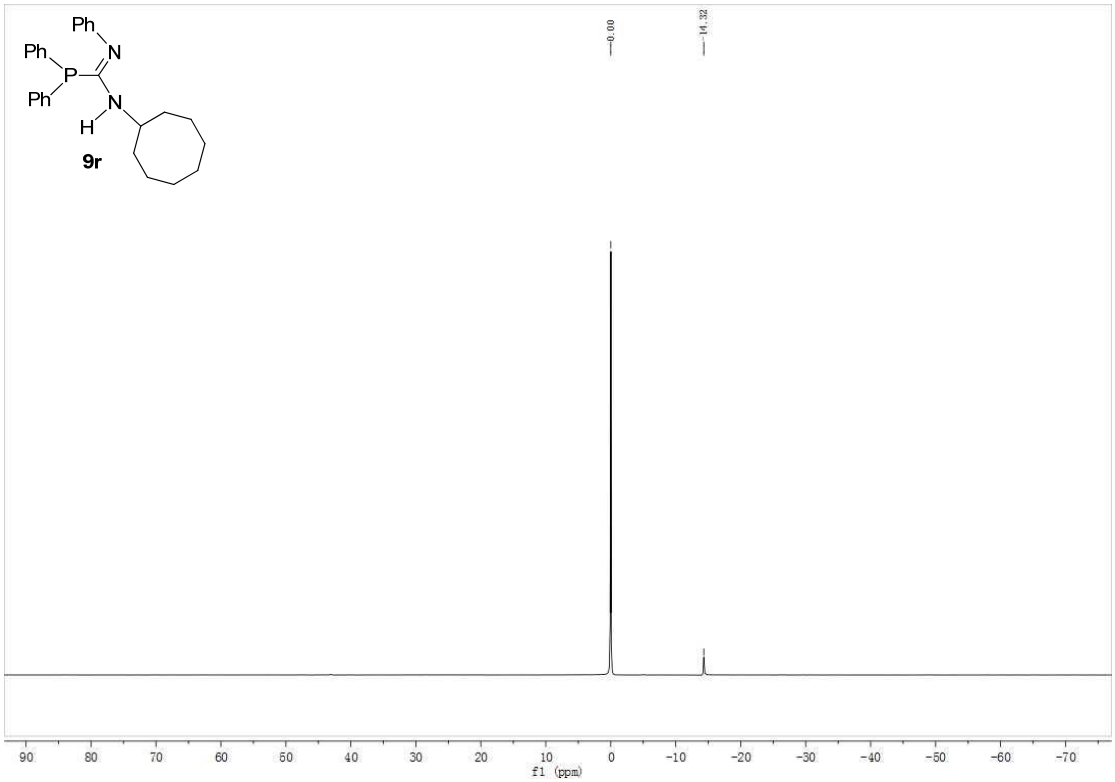
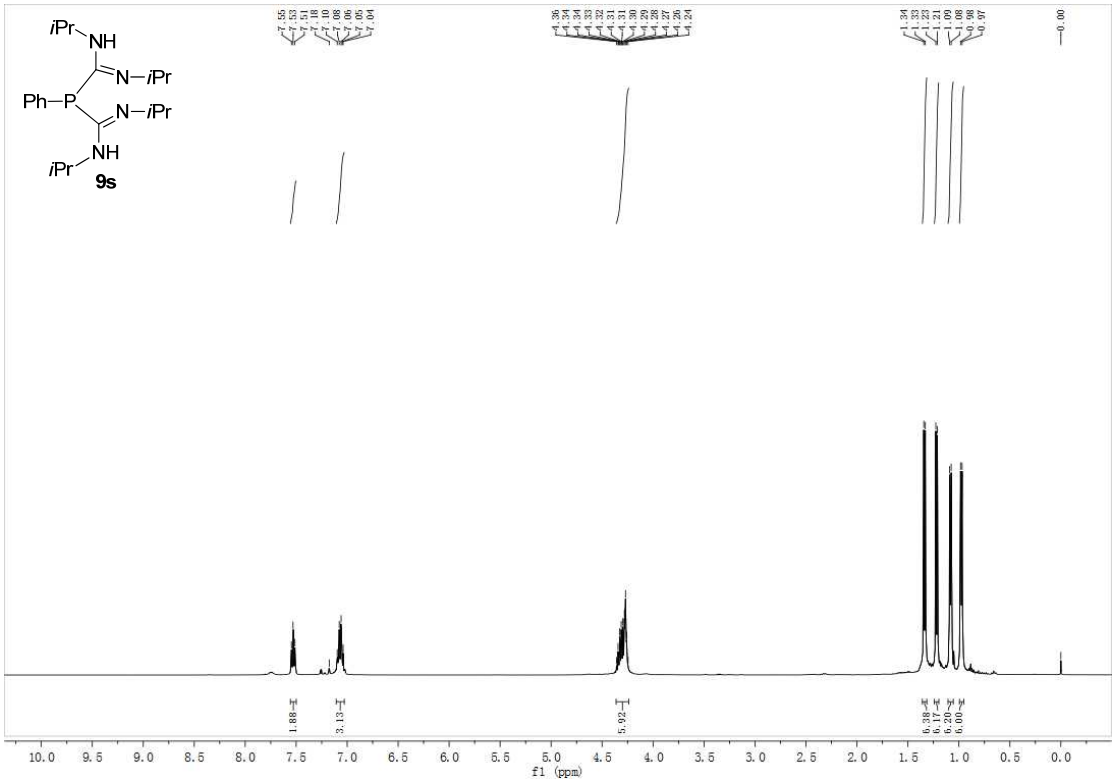
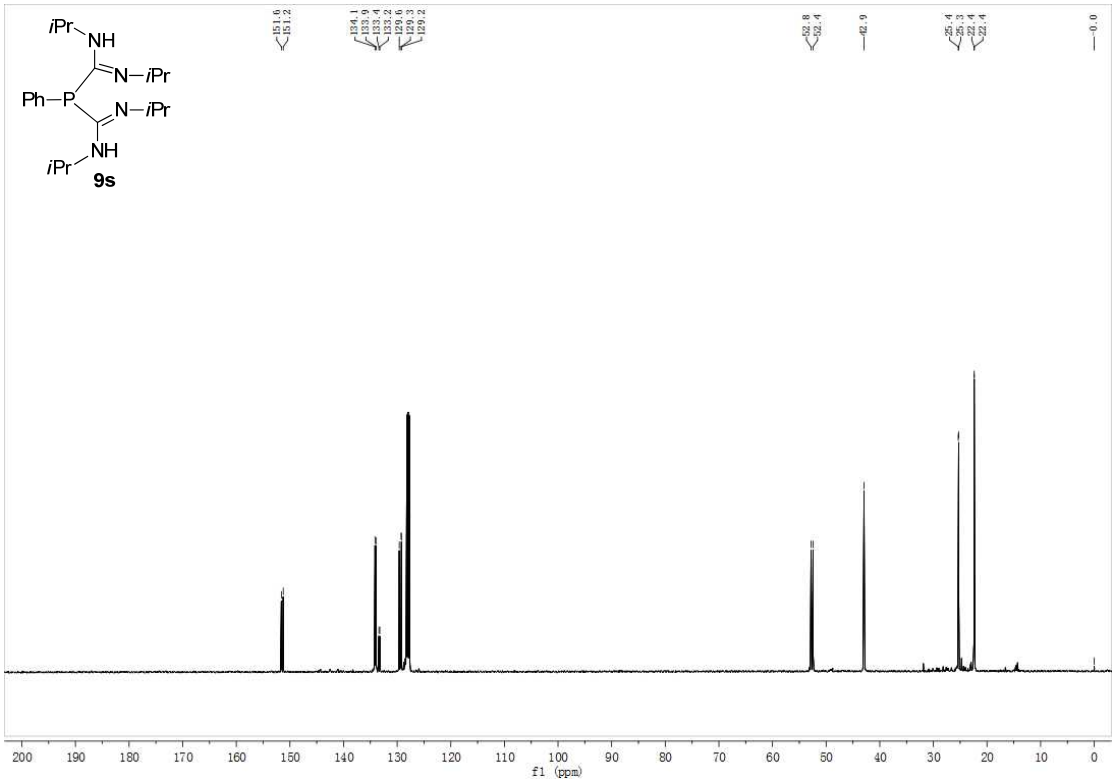
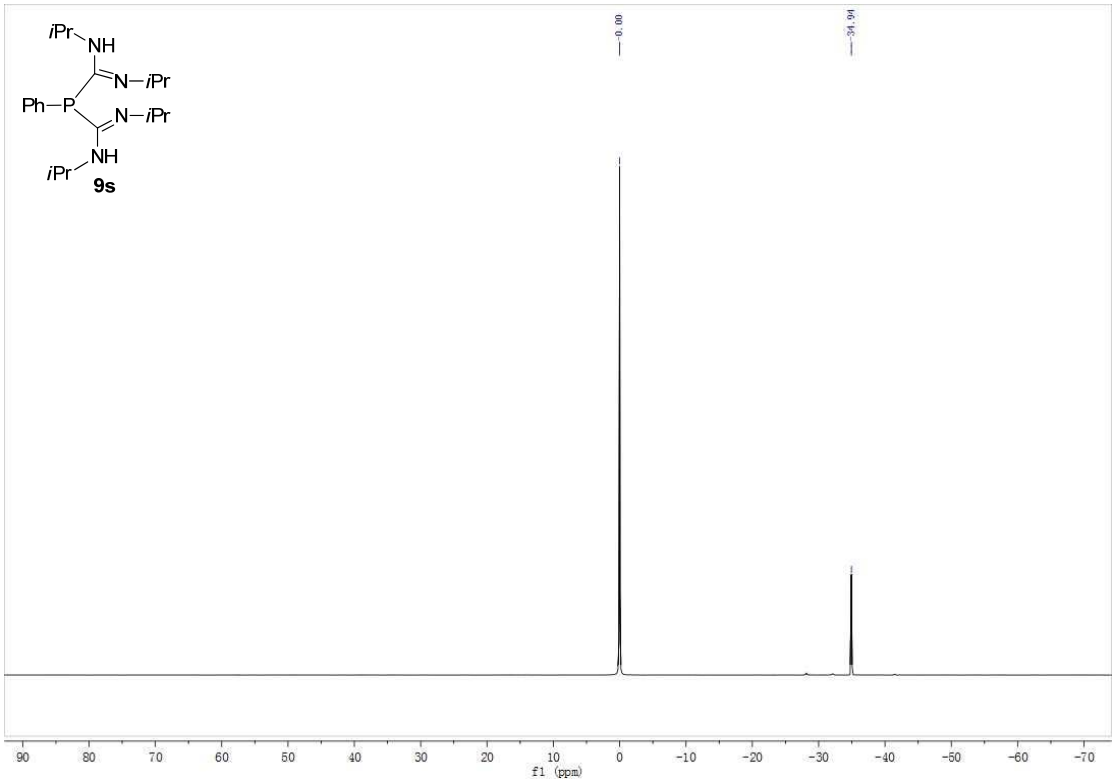
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Ph
N
Ph
P
Ph
N
H
9r
156.3
155.9
152.0
151.9
135.4
135.2
134.5
134.3
129.0
128.9
128.4
128.3
122.3
122.2
51.2
31.9
27.5
25.7
23.8
0.0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

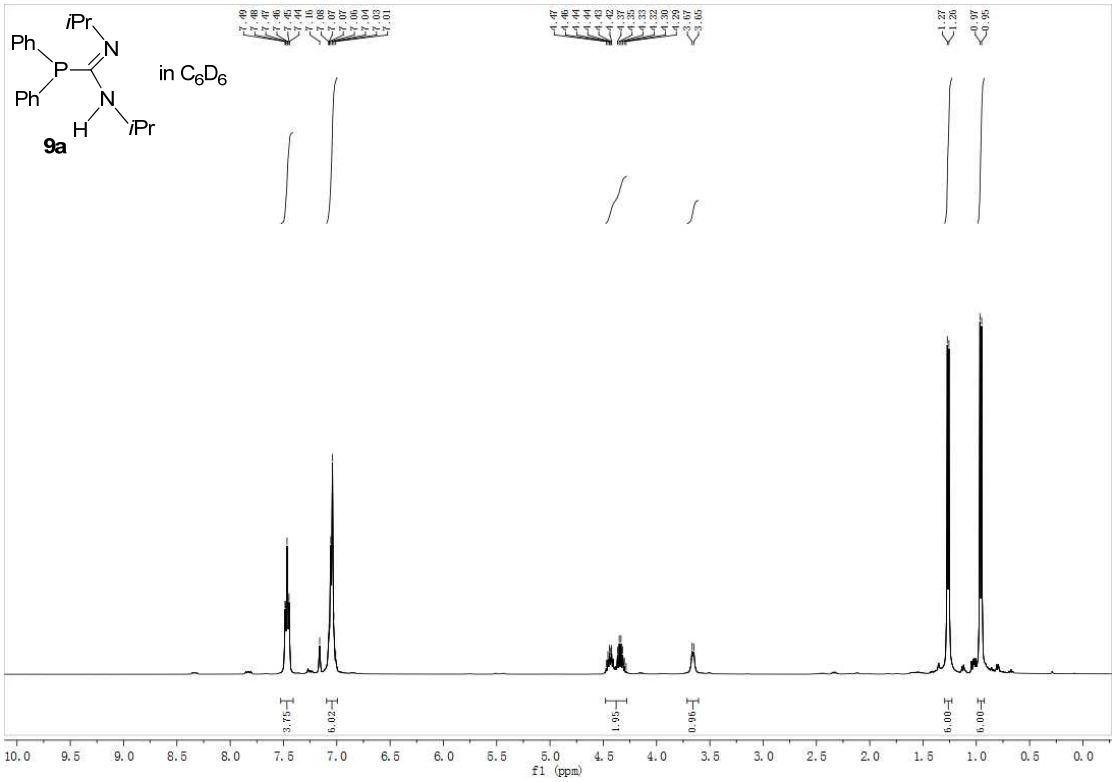

Ph
Ph
P
N
Ph
N
H
9r
0.00
14.32
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70
f1 (ppm)

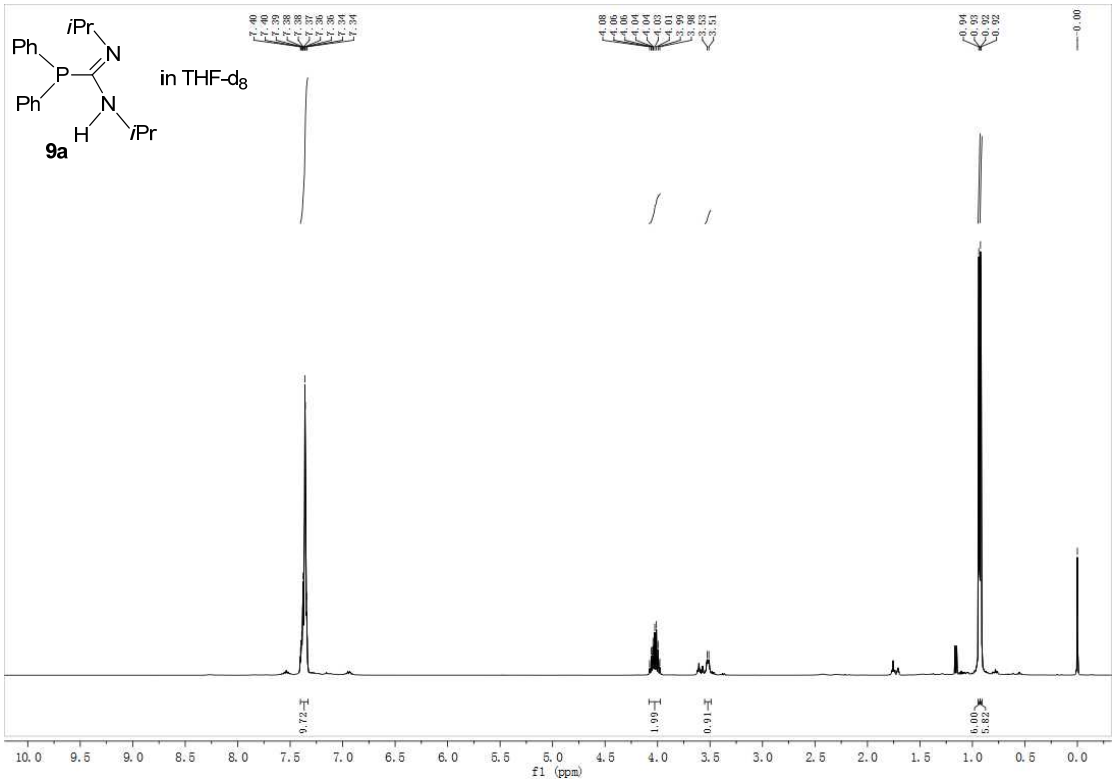

iPr
NH
N—iPr
Ph—P
N—iPr
NH
iPr
9s
7.55
7.53
7.51
7.18
7.10
7.08
7.06
7.05
7.04
4.36
4.34
4.34
4.33
4.32
4.31
4.30
4.29
4.28
4.27
4.26
4.24
1.34
1.33
1.32
1.21
1.09
1.08
0.98
0.97
0.00
1.88
3.13
5.92
6.38
6.17
6.20
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

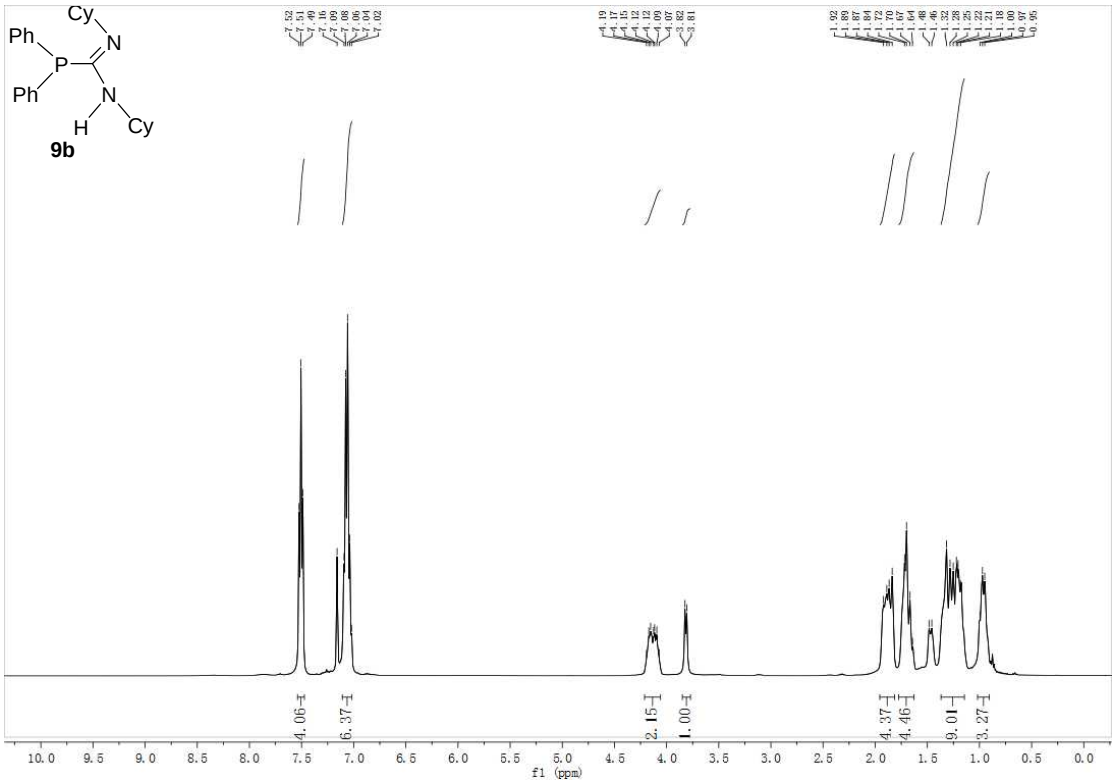

iPr
NH
N—iPr
Ph—P
N—iPr
NH
iPr
9s
151.6
151.2
134.1
133.9
133.4
133.2
129.6
129.3
129.2
52.8
52.4
42.9
25.4
25.3
22.4
22.4
0.0
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

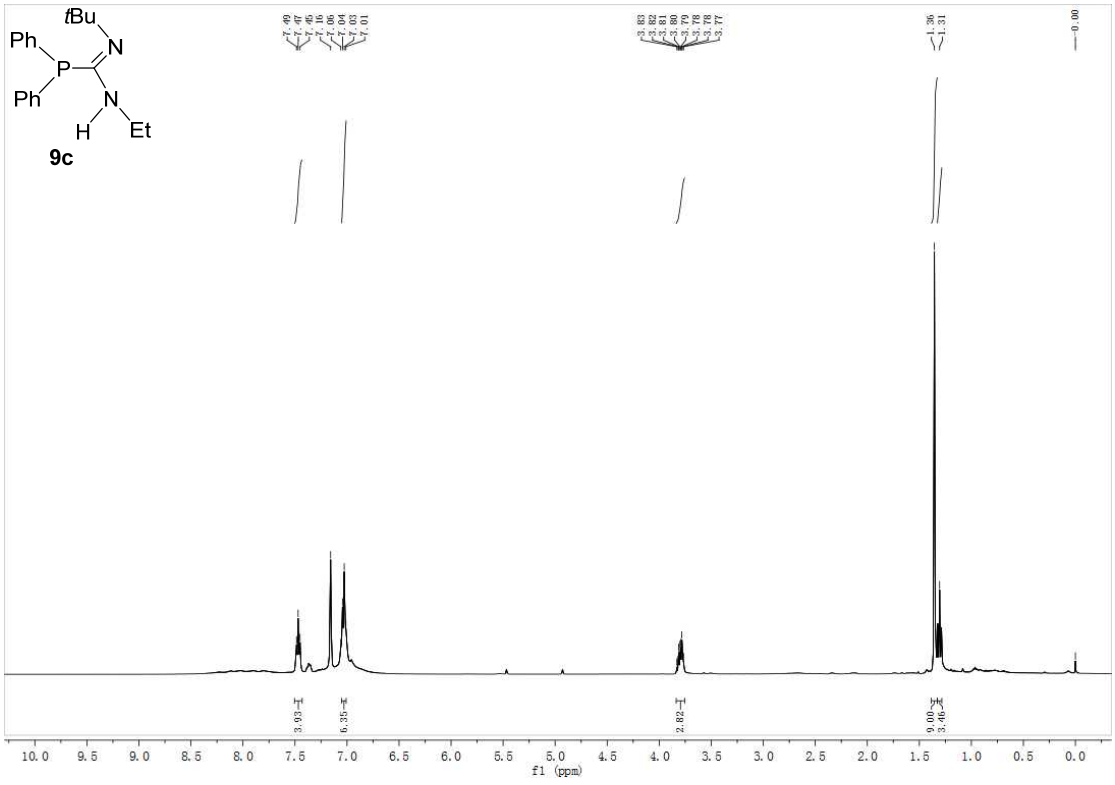

iPr
NH
N—iPr
Ph—P
N—iPr
NH
iPr
9s
0.00
-34.94
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70
f1 (ppm)

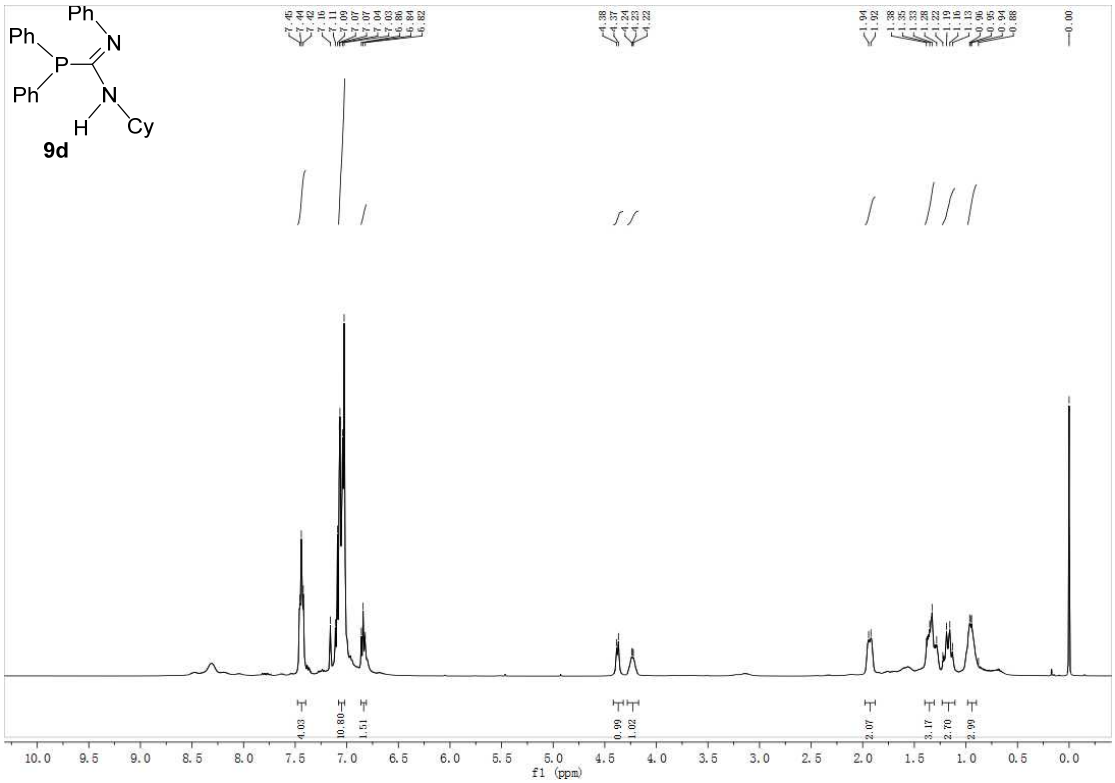
## 2) Copies of $^{1}$H NMR Spectra of All Reported Compounds

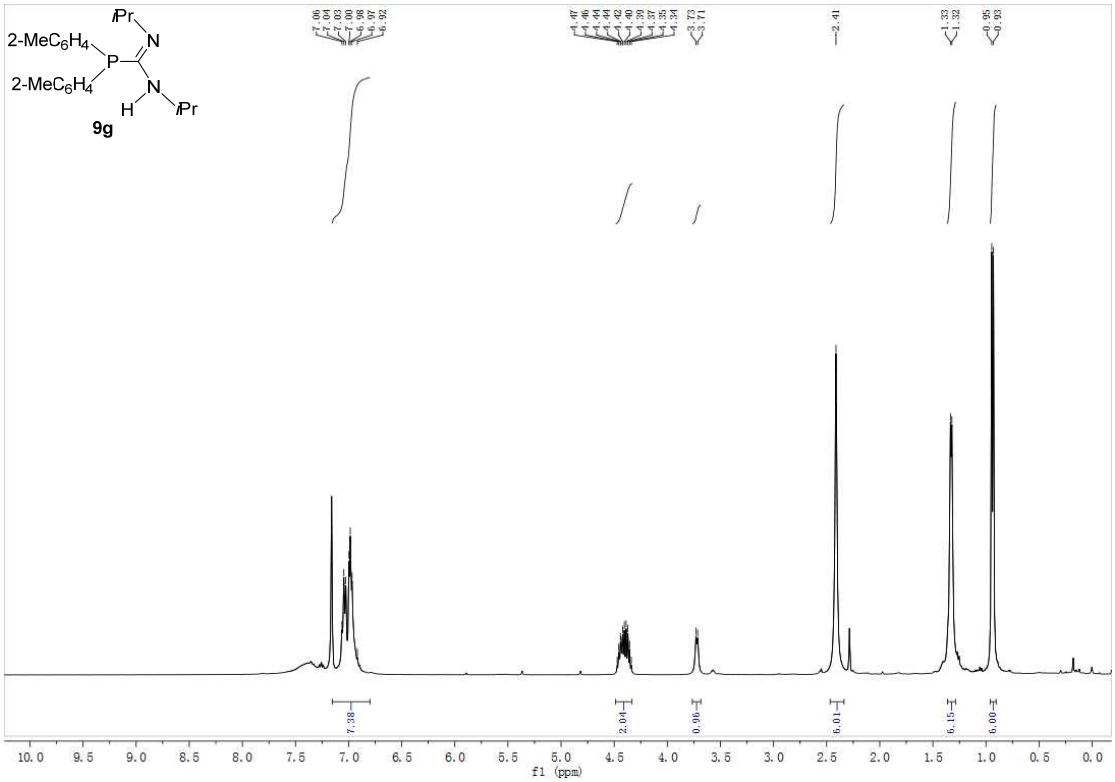


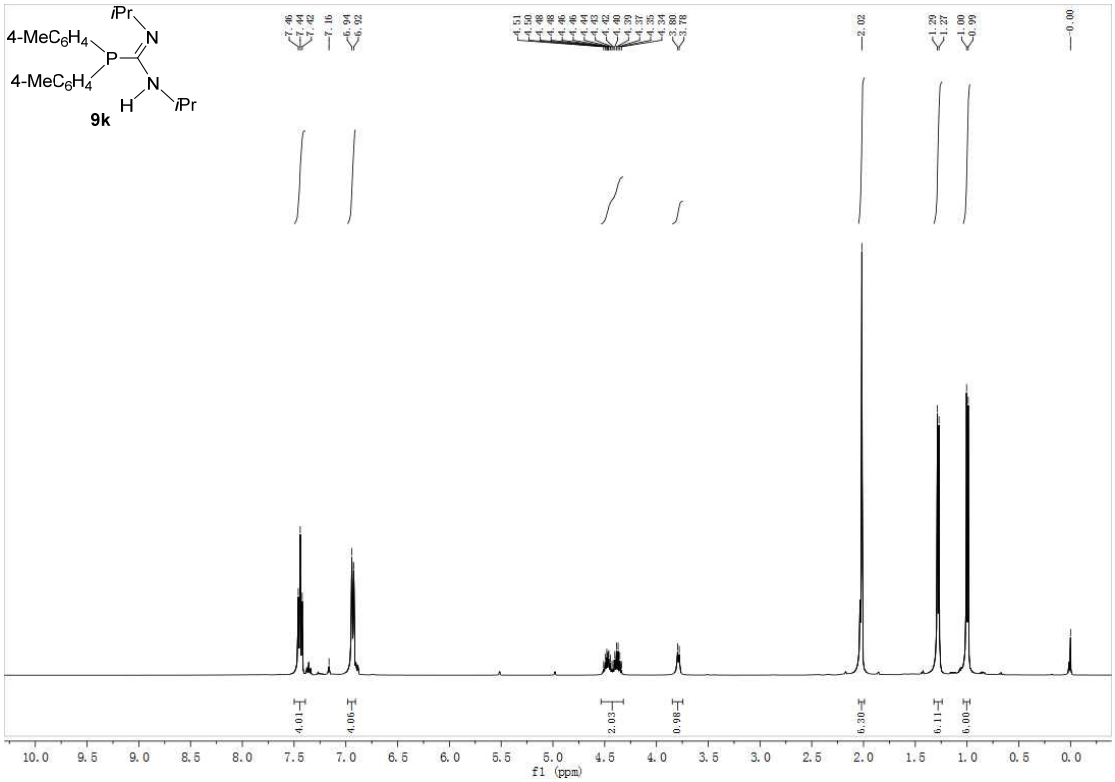



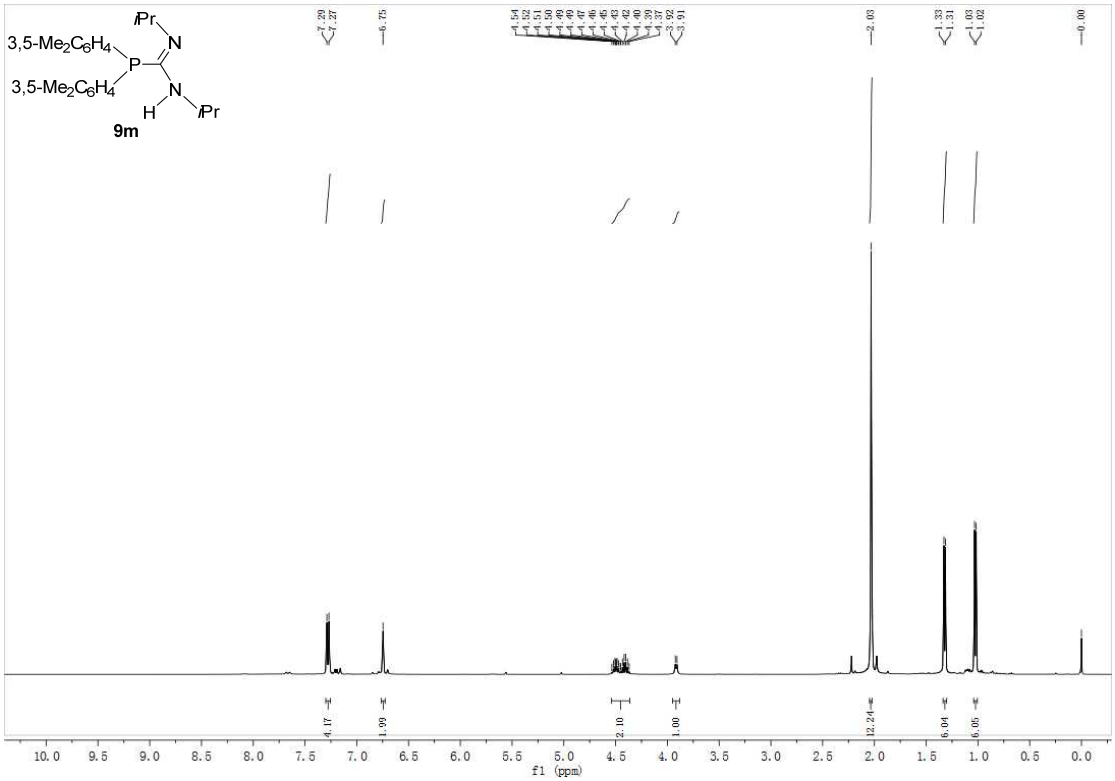

Cy
N
Ph
P
Ph
N
H
Cy
9b
4.06
6.37
2.15
1.00
4.37
4.46
9.01
3.27
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


tBu
N
Ph
P
Ph
N
H
Et
9c
3.03
6.35
2.82
9.00
3.46
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

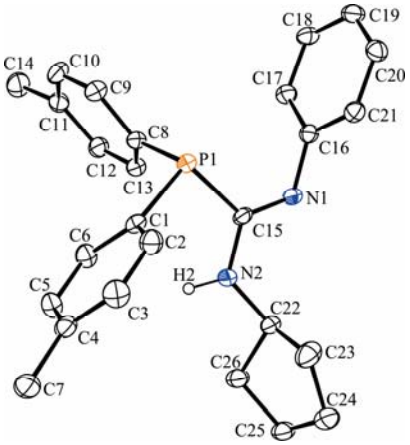

Ph
Ph
P
N
Ph
N
H
Cy
9d
f1 (ppm)


iPr
2-MeC6H4
P
N
2-MeC6H4
N
H
iPr
9g
f1 (ppm)


iPr
N
4-MeC6H4
P
4-MeC6H4
N
H
iPr
9k
f1 (ppm)


iPr
N
3,5-Me2C6H4
P
3,5-Me2C6H4
N
H
iPr
9m
f1 (ppm)

**4) X-ray Crystallographic Studies for 9i**




**SFig. 1** ORTEP drawing of **9i** with 30% ellipsoids. Hydrogen atoms, except that on nitrogen atom N2, are omitted for clarity.

**STable 1** Crystal data and structure refinement for **9i.**

| | |
|---|---|
| Identification code | **9i** |
| Empirical formula | $C_{26}H_{29}N_2P$ |
| Formula weight | 400.48 |
| Temperature/K | 180 (2) |
| Crystal system | monoclinic |
| Space group | $P2_1$ |
| a/Å | 6.1617(8) |
| b/Å | 10.5098(13) |
| c/Å | 17.3476(17) |
| α/° | 90 |
| β/° | 98.607(10) |
| γ/° | 90 |
| Volume/Å$^3$ | 1110.7(2) |
| Z | 2 |
| $\rho_{calc}$mg/mm$^3$ | 1.197 |
| m/mm$^{-1}$ | 0.138 |
| F(000) | 428.0 |
| Crystal size/mm$^3$ | 0.2×0.2×0.2 |
| 2Θ range for data collection | 6.132 to 50.042° |
| Index ranges | $-7 \le h \le 7$, $-12 \le k \le 12$, $-20 \le l \le 20$ |
| Reflections collected | 16480 |
| Independent reflections | 3941[R(int) = 0.0864] |
| Data/restraints/parameters | 3941/1/264 |
| Goodness-of-fit on $F^2$ | 1.039 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0508, $wR_2$ = 0.1192 |
| Final R indexes [all data] | $R_1$ = 0.0618, $wR_2$ = 0.1290 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.28/-0.36 |

**STable 2.** Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **9i**. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| P1 | 1394.9(17) | 5711.7(11) | 2261.7(5) | 32.2(3) |
| N1 | 2826(6) | 5116(3) | 3814.1(17) | 34.0(9) |
| N2 | 4382(6) | 3917(4) | 2940.7(19) | 38.0(9) |
| C1 | 1804(7) | 4618(4) | 1469(2) | 31.2(9) |
| C2 | 212(7) | 3689(5) | 1261(2) | 40.2(11) |
| C3 | 477(8) | 2773(5) | 711(3) | 44.7(12) |
| C4 | 2331(7) | 2753(4) | 351(2) | 37.6(11) |
| C5 | 3883(7) | 3691(5) | 538(2) | 39.9(11) |
| C6 | 3641(7) | 4609(5) | 1092(2) | 36.7(10) |
| C7 | 2673(9) | 1734(5) | -231(2) | 48.9(12) |
| C8 | 3243(7) | 7017(4) | 2108(2) | 32.7(10) |
| C9 | 2368(8) | 7986(5) | 1608(2) | 39.6(11) |
| C10 | 3653(8) | 8993(5) | 1444(3) | 45.2(12) |
| C11 | 5865(8) | 9081(4) | 1765(2) | 38.8(11) |
| C12 | 6696(8) | 8137(4) | 2275(2) | 38.5(11) |
| C13 | 5428(7) | 7114(4) | 2440(2) | 35.3(10) |
| C14 | 7279(10) | 10154(5) | 1550(3) | 53.7(13) |
| C15 | 3012(6) | 4863(4) | 3111(2) | 28.7(9) |
| C16 | 1421(7) | 6102(4) | 4001(2) | 30.4(10) |
| C17 | 2135(7) | 7364(4) | 4071(2) | 35.7(10) |
| C18 | 824(7) | 8281(5) | 4336(2) | 39.4(11) |
| C19 | -1160(7) | 7969(5) | 4551(2) | 39.4(11) |
| C20 | -1895(7) | 6730(5) | 4468(2) | 38.7(11) |
| C21 | -597(6) | 5808(5) | 4204.9(19) | 32.7(9) |
| C22 | 5314(7) | 2959(4) | 3499(2) | 36.6(10) |
| C23 | 3835(8) | 1794(5) | 3521(3) | 54.3(14) |
| C24 | 5351(8) | 709(6) | 3814(3) | 51.7(12) |
| C25 | 7662(8) | 1132(4) | 3705(3) | 41.5(11) |
| C26 | 7410(7) | 2404(5) | 3281(3) | 40.1(11) |

**STable 3.** Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **9i**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

| Atom | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| P1 | 36.7(6) | 29.0(6) | 31.7(5) | 4.3(5) | 7.4(4) | 6.5(5) |
| N1 | 48(2) | 26(2) | 29.1(18) | 2.8(14) | 7.4(14) | 11.8(17) |
| N2 | 48(2) | 36(2) | 31.9(18) | 7.1(16) | 12.3(15) | 17.8(19) |
| C1 | 33(2) | 28(2) | 32(2) | 7.1(17) | 2.6(16) | 7(2) |
| C2 | 39(3) | 39(3) | 44(2) | 3(2) | 10.0(18) | -4(2) |
| C3 | 46(3) | 40(3) | 47(3) | -7(2) | 5(2) | -15(2) |
| C4 | 50(3) | 32(3) | 30(2) | 3.9(18) | 1.2(18) | 5(2) |
| C5 | 43(3) | 45(3) | 33(2) | -3(2) | 11.3(18) | -4(2) |
| C6 | 38(2) | 37(3) | 36(2) | -2.6(19) | 8.0(17) | -7(2) |
| C7 | 71(3) | 36(3) | 39(2) | -6(2) | 6(2) | 4(3) |
| C8 | 41(2) | 27(3) | 30(2) | 1.0(17) | 7.3(17) | 8.1(19) |
| C9 | 42(3) | 37(3) | 39(2) | 5(2) | 4.4(18) | 8(2) |
| C10 | 63(3) | 33(3) | 40(2) | 12(2) | 8(2) | 7(3) |
| C11 | 55(3) | 28(3) | 35(2) | -3.8(19) | 11.7(19) | 1(2) |
| C12 | 49(3) | 35(3) | 31(2) | -1.2(19) | 3.8(18) | 3(2) |
| C13 | 42(3) | 33(3) | 31(2) | 2.1(18) | 6.4(17) | 8(2) |
| C14 | 76(4) | 33(3) | 54(3) | -2(2) | 18(2) | -9(3) |
| C15 | 31(2) | 21(2) | 34(2) | 6.6(17) | 5.1(16) | 2.6(17) |
| C16 | 37(2) | 32(3) | 21.9(19) | 0.8(15) | 1.5(15) | 6.6(19) |
| C17 | 39(2) | 28(3) | 41(2) | 1.0(19) | 9.0(17) | 2(2) |
| C18 | 49(3) | 25(2) | 44(2) | 0.1(19) | 8.7(19) | 7(2) |
| C19 | 42(3) | 37(3) | 40(2) | -2(2) | 6.1(18) | 13(2) |
| C20 | 35(2) | 47(3) | 35(2) | 1(2) | 5.5(17) | 6(2) |
| C21 | 39(2) | 29(2) | 30.2(19) | -1(2) | 2.4(15) | -1(2) |
| C22 | 48(3) | 30(3) | 32(2) | 5.1(18) | 7.2(17) | 11(2) |
| C23 | 42(3) | 53(4) | 68(3) | 19(3) | 7(2) | 4(3) |
| C24 | 60(3) | 33(3) | 65(3) | 5(3) | 20(2) | 4(3) |
| C25 | 51(3) | 33(3) | 39(2) | 2.2(18) | 2.2(19) | 14(2) |
| C26 | 41(3) | 32(3) | 48(2) | 3(2) | 8.0(19) | 7(2) |

**STable 4.** Bond Lengths for **9i**.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| P1 | C8 | 1.828(4) | C9 | C10 | 1.377(7) |
| P1 | C1 | 1.839(4) | C10 | C11 | 1.396(7) |
| P1 | C15 | 1.876(4) | C11 | C12 | 1.376(6) |
| N1 | C15 | 1.270(5) | C11 | C14 | 1.506(7) |
| N1 | C16 | 1.419(5) | C12 | C13 | 1.384(6) |
| N2 | C15 | 1.365(5) | C16 | C21 | 1.377(6) |
| N2 | C22 | 1.455(5) | C16 | C17 | 1.397(6) |
| C1 | C6 | 1.390(6) | C17 | C18 | 1.380(6) |
| C1 | C2 | 1.393(6) | C18 | C19 | 1.371(7) |
| C2 | C3 | 1.382(6) | C19 | C20 | 1.379(7) |
| C3 | C4 | 1.382(6) | C20 | C21 | 1.377(6) |
| C4 | C5 | 1.378(6) | C22 | C26 | 1.516(6) |
| C4 | C7 | 1.507(6) | C22 | C23 | 1.530(7) |
| C5 | C6 | 1.385(6) | C23 | C24 | 1.512(7) |
| C8 | C13 | 1.387(6) | C24 | C25 | 1.530(7) |
| C8 | C9 | 1.393(6) | C25 | C26 | 1.523(6) |

**STable 5.** Bond Angles for **9i**.

| Atom | Atom | Atom | Angle/˚ | Atom | Atom | Atom | Angle/˚ |
|---|---|---|---|---|---|---|---|
| C8 | P1 | C1 | 101.66(19) | C10 | C11 | C14 | 121.2(4) |
| C8 | P1 | C15 | 101.65(18) | C11 | C12 | C13 | 121.8(4) |
| C1 | P1 | C15 | 100.00(18) | C12 | C13 | C8 | 120.9(4) |
| C15 | N1 | C16 | 121.2(3) | N1 | C15 | N2 | 120.5(4) |
| C15 | N2 | C22 | 123.7(3) | N1 | C15 | P1 | 122.8(3) |
| C6 | C1 | C2 | 117.7(4) | N2 | C15 | P1 | 116.7(3) |
| C6 | C1 | P1 | 124.7(3) | C21 | C16 | C17 | 118.4(4) |
| C2 | C1 | P1 | 117.5(3) | C21 | C16 | N1 | 120.0(4) |
| C3 | C2 | C1 | 121.0(4) | C17 | C16 | N1 | 121.2(4) |
| C2 | C3 | C4 | 120.9(4) | C18 | C17 | C16 | 119.9(4) |
| C5 | C4 | C3 | 118.3(4) | C19 | C18 | C17 | 120.9(5) |
| C5 | C4 | C7 | 120.3(4) | C18 | C19 | C20 | 119.3(4) |
| C3 | C4 | C7 | 121.5(4) | C21 | C20 | C19 | 120.1(4) |
| C4 | C5 | C6 | 121.3(4) | C16 | C21 | C20 | 121.2(4) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C5 | C6 | C1 | 120.7(4) | N2 | C22 | C26 | 111.5(3) |
| C13 | C8 | C9 | 117.8(4) | N2 | C22 | C23 | 113.1(4) |
| C13 | C8 | P1 | 125.6(3) | C26 | C22 | C23 | 103.4(4) |
| C9 | C8 | P1 | 116.6(3) | C24 | C23 | C22 | 105.7(4) |
| C10 | C9 | C8 | 120.7(4) | C23 | C24 | C25 | 106.2(4) |
| C9 | C10 | C11 | 121.7(4) | C26 | C25 | C24 | 106.5(4) |
| C12 | C11 | C10 | 117.1(4) | C22 | C26 | C25 | 104.2(4) |
| C12 | C11 | C14 | 121.7(4) | | | | |