**Electronic Supplementary Information for:**

**Synthesis and characterization of 2-*t*-butylimino-functionalized indolyl rare-earth metal amido complexes for the catalytic addition of terminal alkynes to carbodiimides: the dimeric complexes with the alkynide species in the $\mu$-$\eta^1$:$\eta^2$ bonding modes**

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**Contents**

**NMR spectra of complexes 3, 5, 6 and 11.**

$^1$H NMR

300 M, C$_6$D$_6$

**3**

Figure S1. $^1$H NMR spectrum of complex **3**.



$^{13}$C{$^1$H} NMR

75 M, C$_6$D$_6$

**3**

Figure S2. $^{13}$C{$^1$H} NMR spectrum of complex **3**.

¹H NMR
300 M, C₆D₆

**5**

Figure S3. ¹H NMR spectrum of complex **5**.



¹³C{¹H} NMR
75 M, C₆D₆

**5**

Figure S4. ¹³C{¹H} NMR spectrum of complex **5**.

$^1$H NMR
500 M, C$_6$D$_6$

**6**

Figure S5. $^1$H NMR spectrum of complex **6**.



$^{13}$C{$^1$H} NMR
125 M, C$_6$D$_6$

**6**

Figure S6. $^{13}$C{$^1$H} NMR spectrum of complex **6**.

Figure S7. $^1$H NMR spectrum of complex **11**.
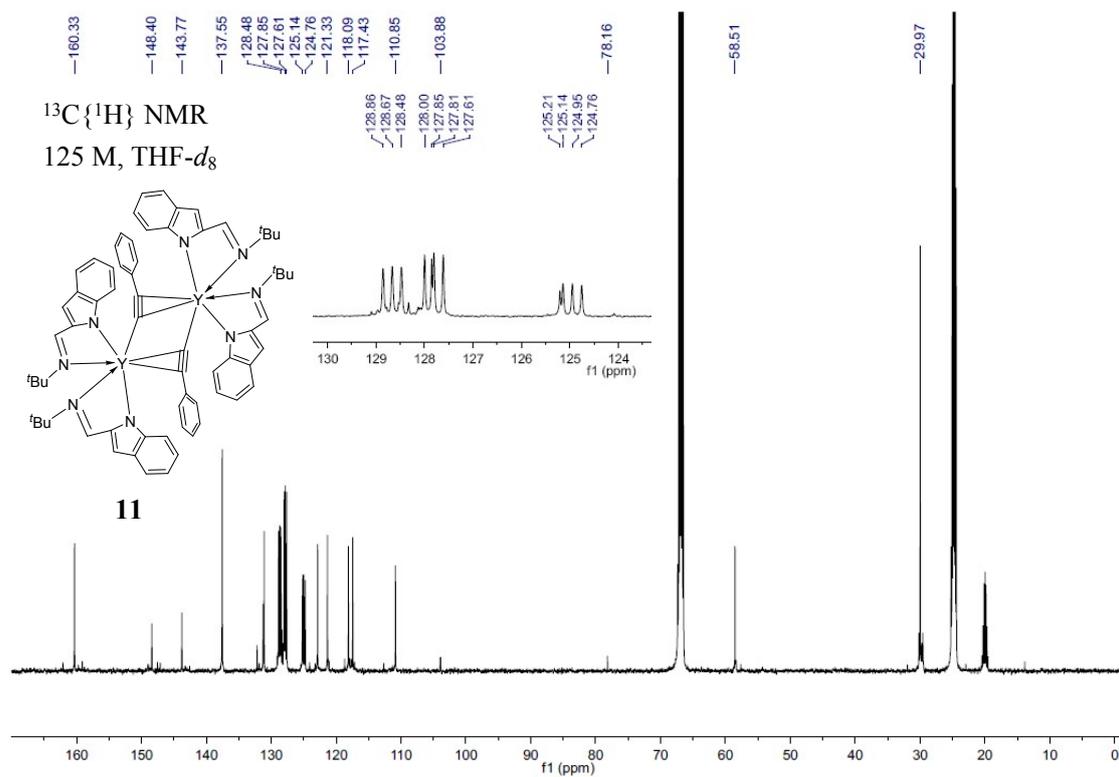


Figure S8. $^{13}$C{$^1$H} NMR spectrum of complex **11**.

# NMR spectra of substituted propiolamidines.

¹H NMR
500 M, CDCl₃

**9a**

7.51 7.50 7.49 7.49 7.39 7.38 7.38 7.37 7.36 7.34 7.34 7.26
4.00 3.99 3.97 3.96 3.95 3.94 3.92
1.17 1.16

1.00 1.52
0.98
6.05
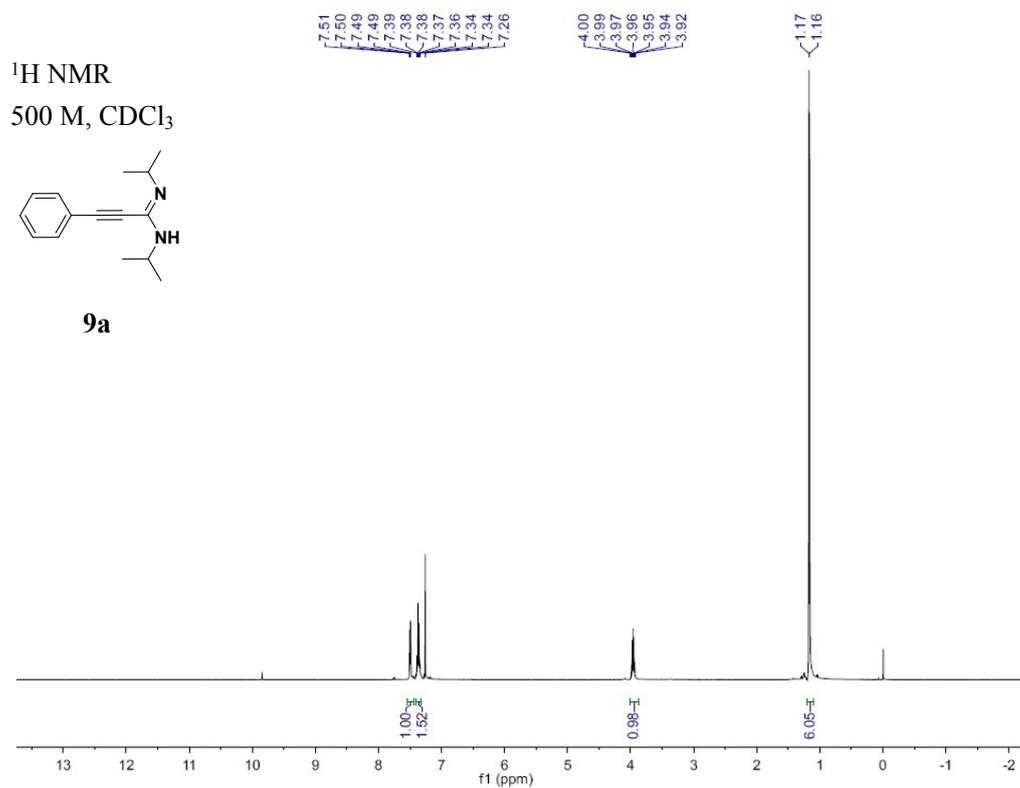
Figure S9. ¹H NMR spectrum of compound **9a**.

¹³C{¹H} NMR
125 M, CDCl₃

**9a**

41.76
42.37 39.75 38.87 31.83
92.17
79.70 77.75 77.70 77.50 77.24
48.19
24.31
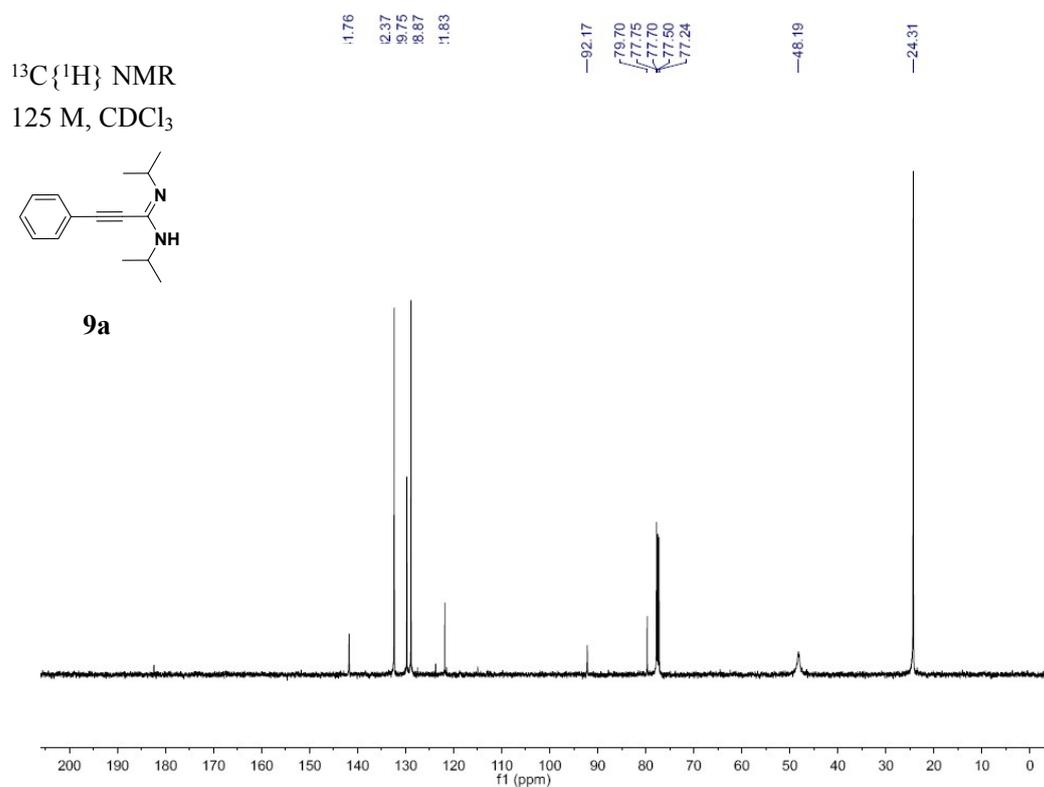
Figure S10. ¹³C{¹H} NMR spectrum of compound **9a**.

<sup>1</sup>H NMR
500 M, CDCl<sub>3</sub>

**9ba**
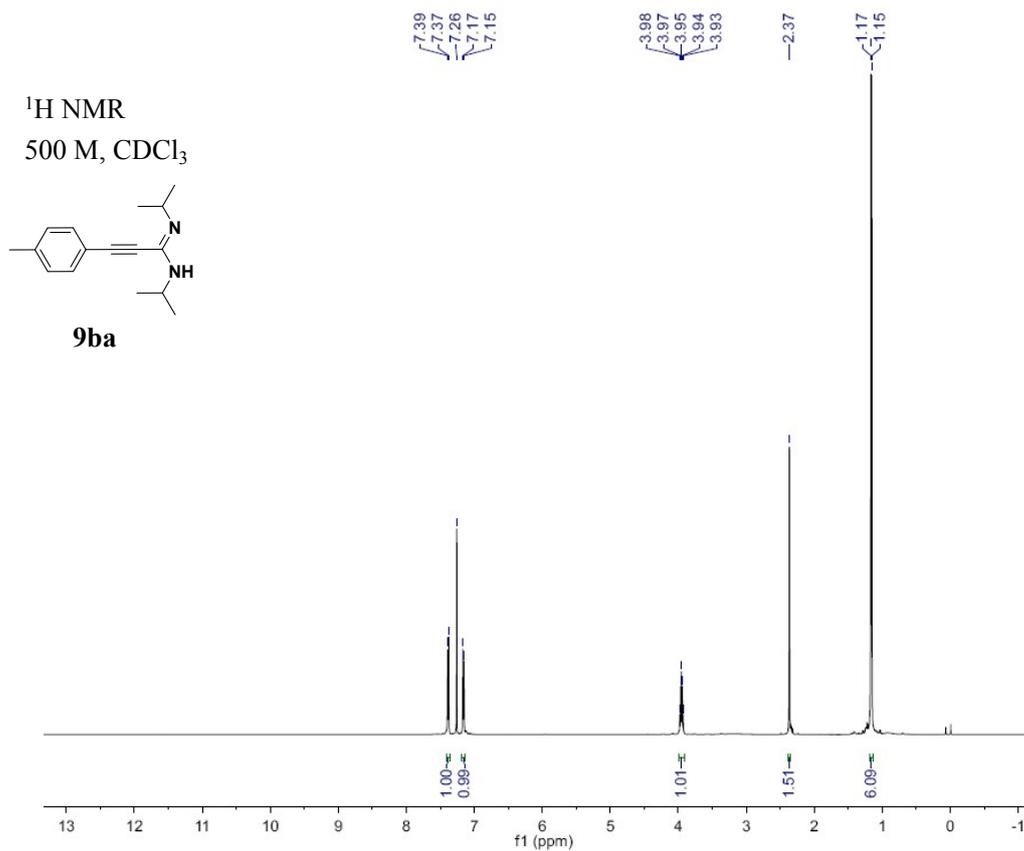
Figure S11. <sup>1</sup>H NMR spectrum of compound **9ba**.

<sup>13</sup>C{<sup>1</sup>H} NMR
125 M, CDCl<sub>3</sub>

**9ba**
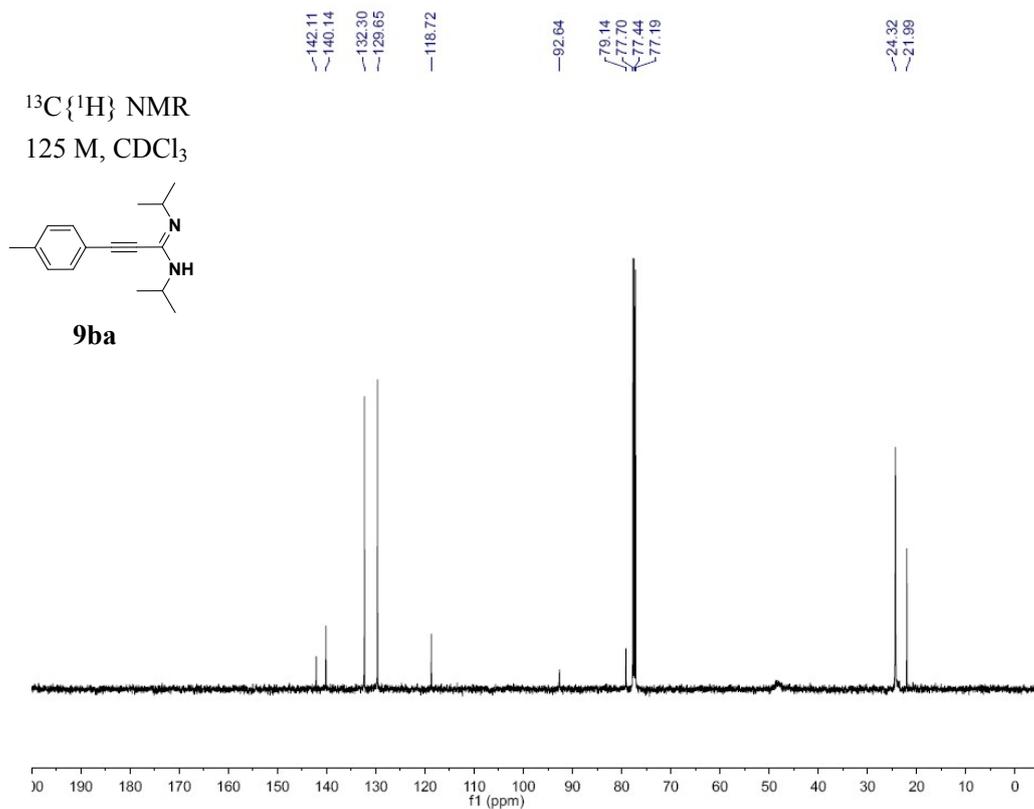
Figure S12. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of compound **9ba**.

7.44
7.42
7.26

3.97
3.96
3.95
3.93
3.92
3.83

1.17
1.15

$^1$H NMR

500 M, CDCl$_3$

**9ca**

1.00  0.99   1.02  1.51   6.00

12  11  10  9  8  7  6  5  4  3  2  1  0  -1
f1 (ppm)
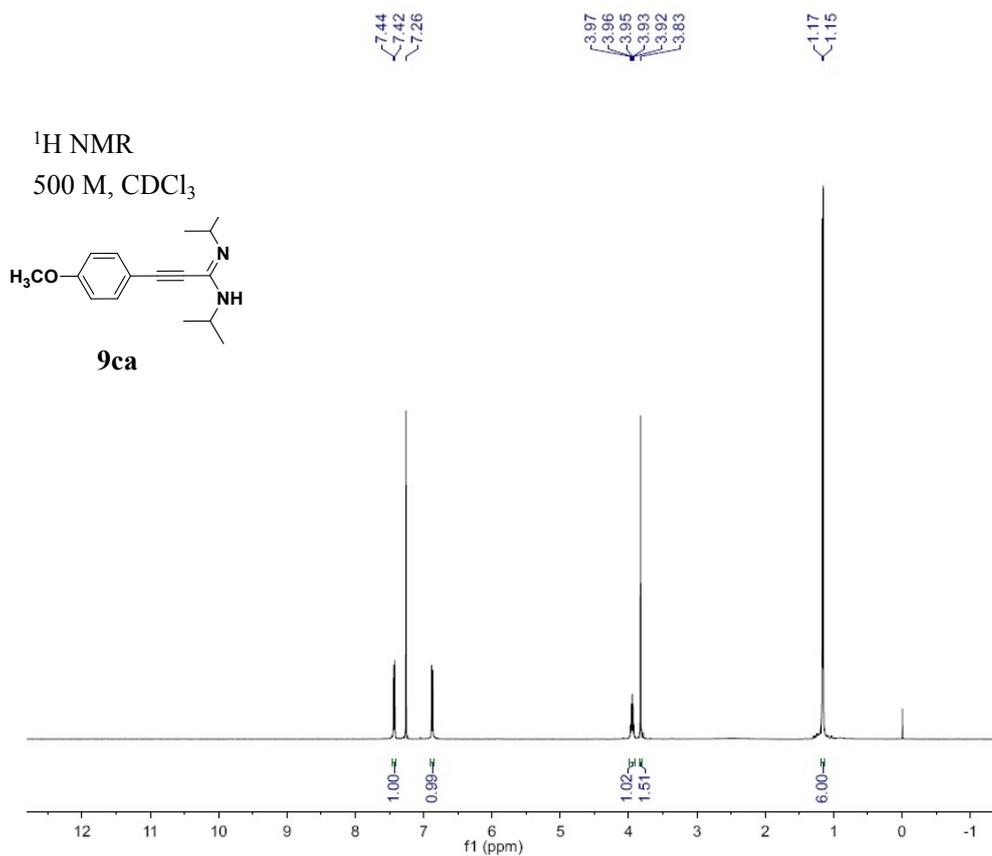
Figure S13. $^1$H NMR spectrum of compound **9ca**.

160.82

142.18
133.94

114.50
113.71

92.57

78.68
77.84
77.79
77.59
77.33

55.64

48.05

24.28

$^{13}$C{$^1$H} NMR

125 M, CDCl$_3$

**9ca**

0  190  180  170  160  150  140  130  120  110  100  90  80  70  60  50  40  30  20  10  0
f1 (ppm)
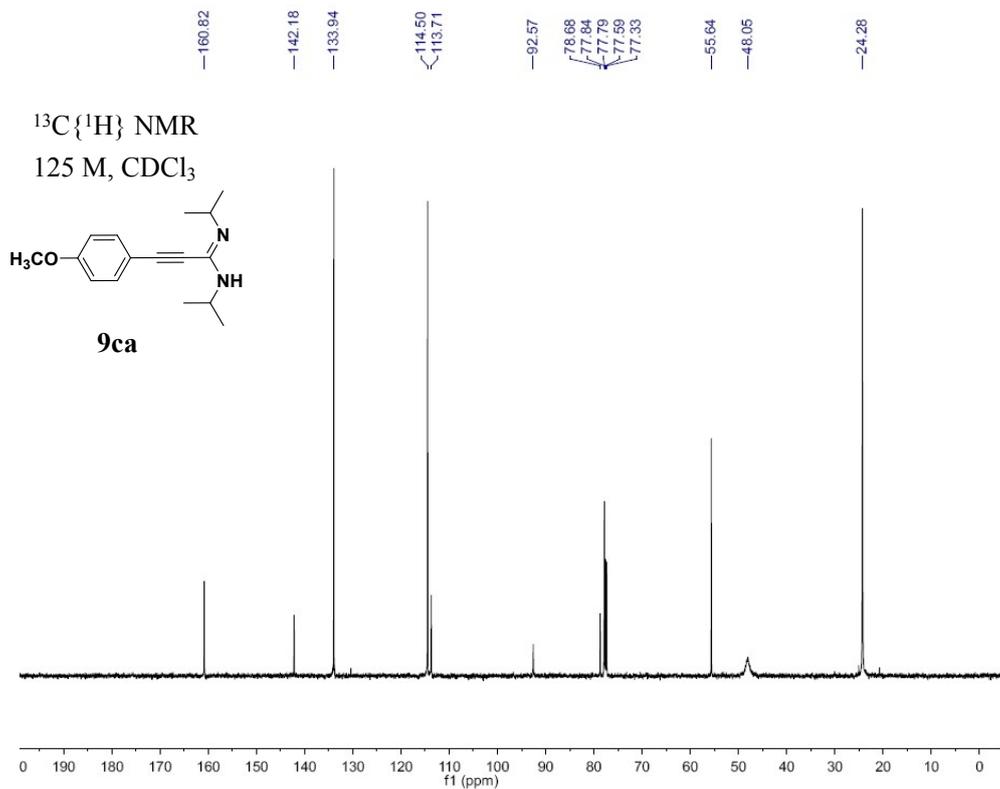
Figure S14. $^{13}$C{$^1$H} NMR spectrum of compound **9ca**.

<sup>1</sup>H NMR

7.50, 7.50, 7.49, 7.36, 7.35, 7.34, 7.26

3.97, 3.96, 3.94, 3.93, 3.92, 3.91

1.16, 1.15

<sup>1</sup>H NMR

500 M, CDCl₃

**9da**

1.00, 1.01

1.00

6.02

13  12  11  10  9  8  7  6  5  4  3  2  1  0  -1
f1 (ppm)
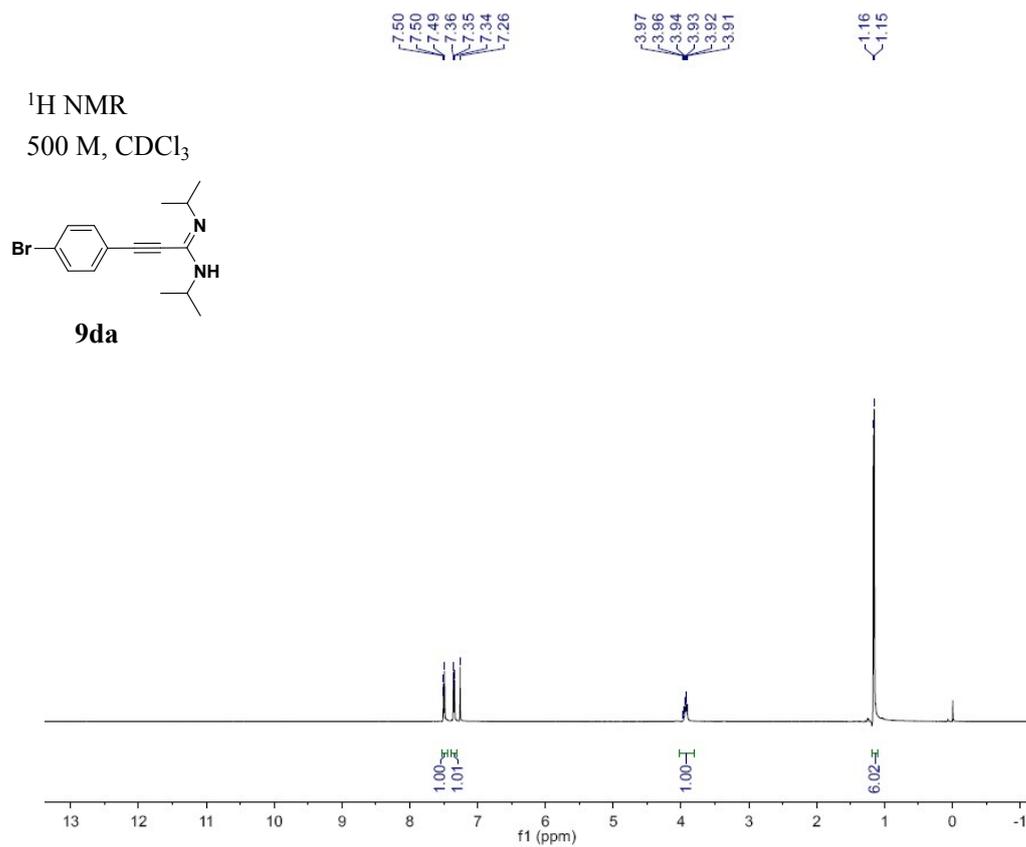
Figure S15. ¹H NMR spectrum of compound **9da**.

141.39

133.75, 132.21

124.23, 120.76

90.90

80.72, 77.68, 77.63, 77.42, 77.17

24.28

¹³C{¹H} NMR

125 M, CDCl₃

**9da**

190  180  170  160  150  140  130  120  110  100  90  80  70  60  50  40  30  20  10  0
f1 (ppm)
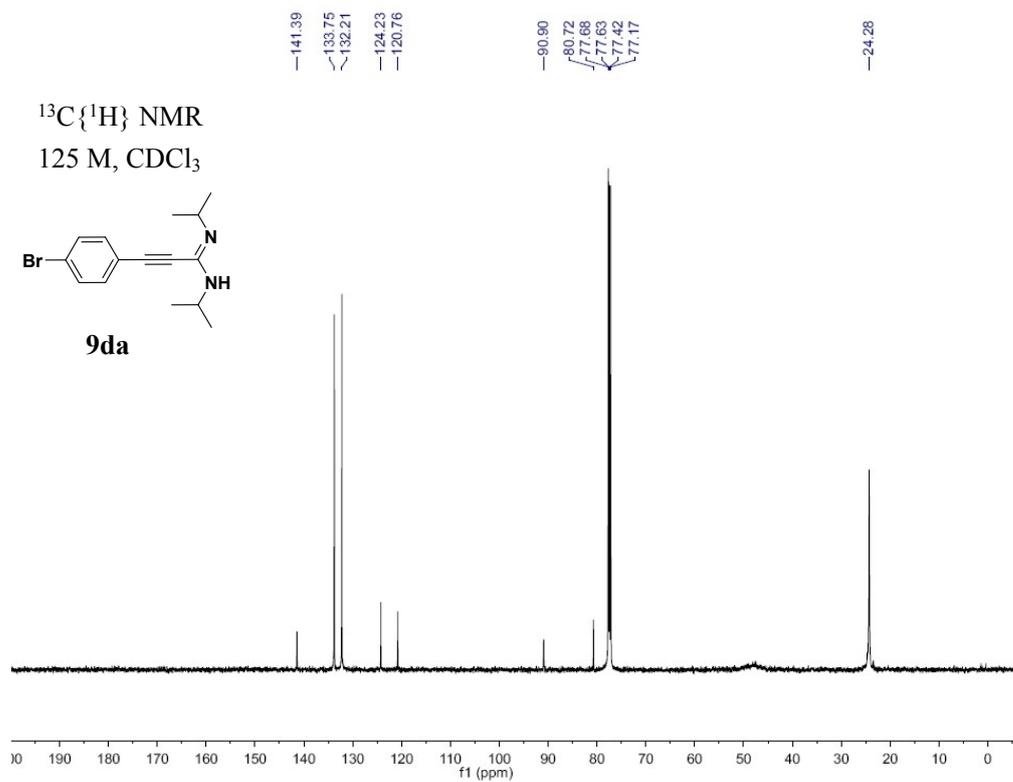
Figure

S16. ¹³C{¹H} NMR spectrum of compound **9da**.

7.50
7.48
7.48
7.41
7.40
7.38
7.37
7.35
7.26

3.62
3.60
3.59
3.58

1.90
1.88
1.76
1.75
1.74
1.73
1.72
1.62
1.59
1.39
1.36
1.32
1.28
1.25
1.23
1.20
1.18

¹H NMR
500 M, CDCl₃

**9ab**

1.00
1.47

0.98

2.01
2.04
1.03
5.14
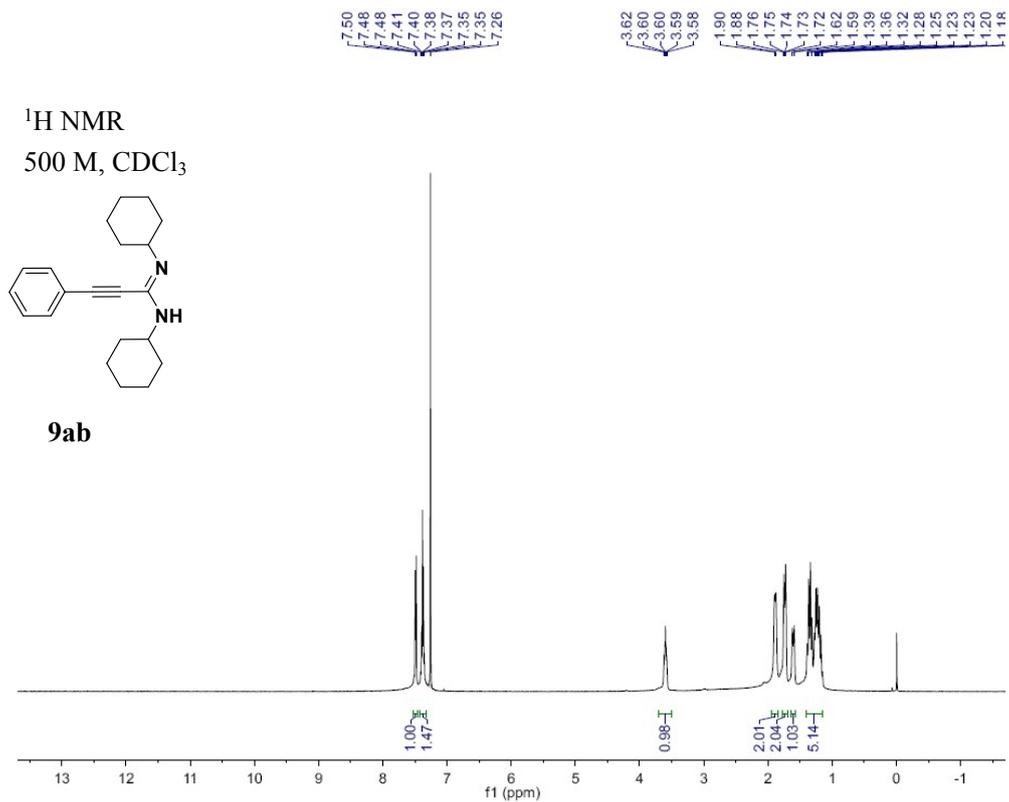
Figure S17. ¹H NMR spectrum of compound **9ab**.

142.07
132.36
129.74
128.89
121.92

92.38
79.83
77.92
77.88
77.67
77.42

56.38

34.69

26.23
25.53

¹³C{¹H} NMR
125 M, CDCl₃

**9ab**
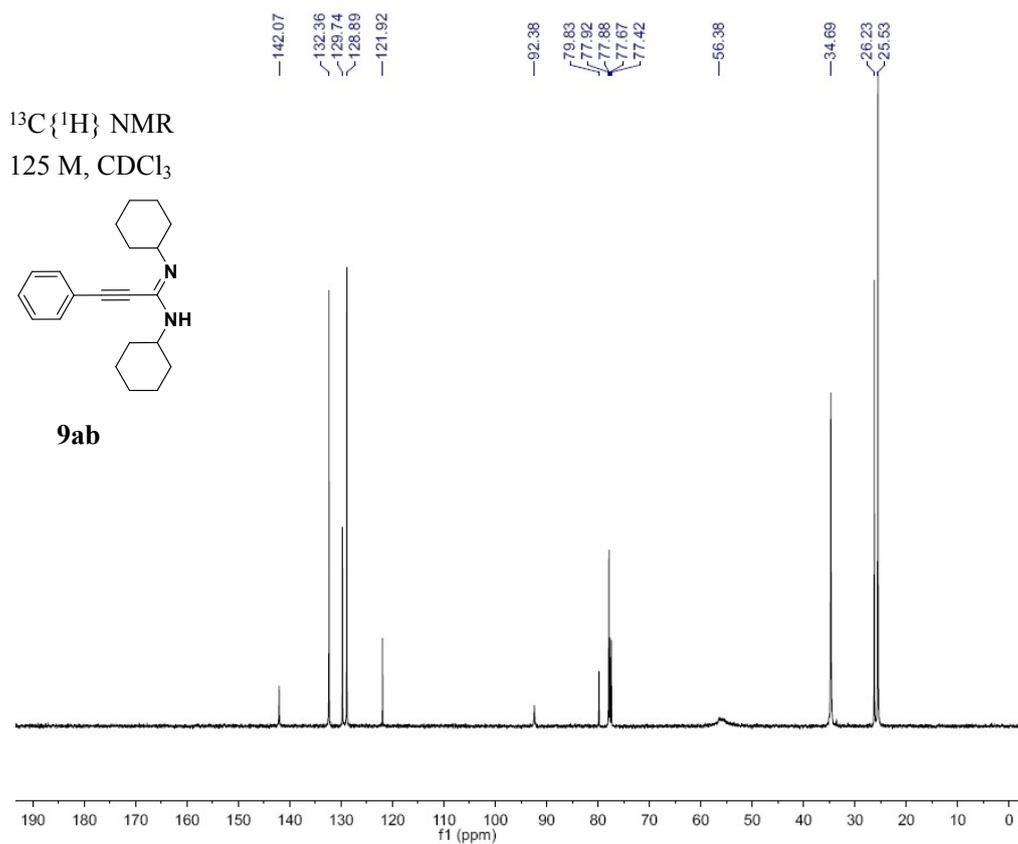
Figure S18. ¹³C{¹H} NMR spectrum of compound **9ab**.

## ¹H NMR
500 M, CDCl₃

**9bb**
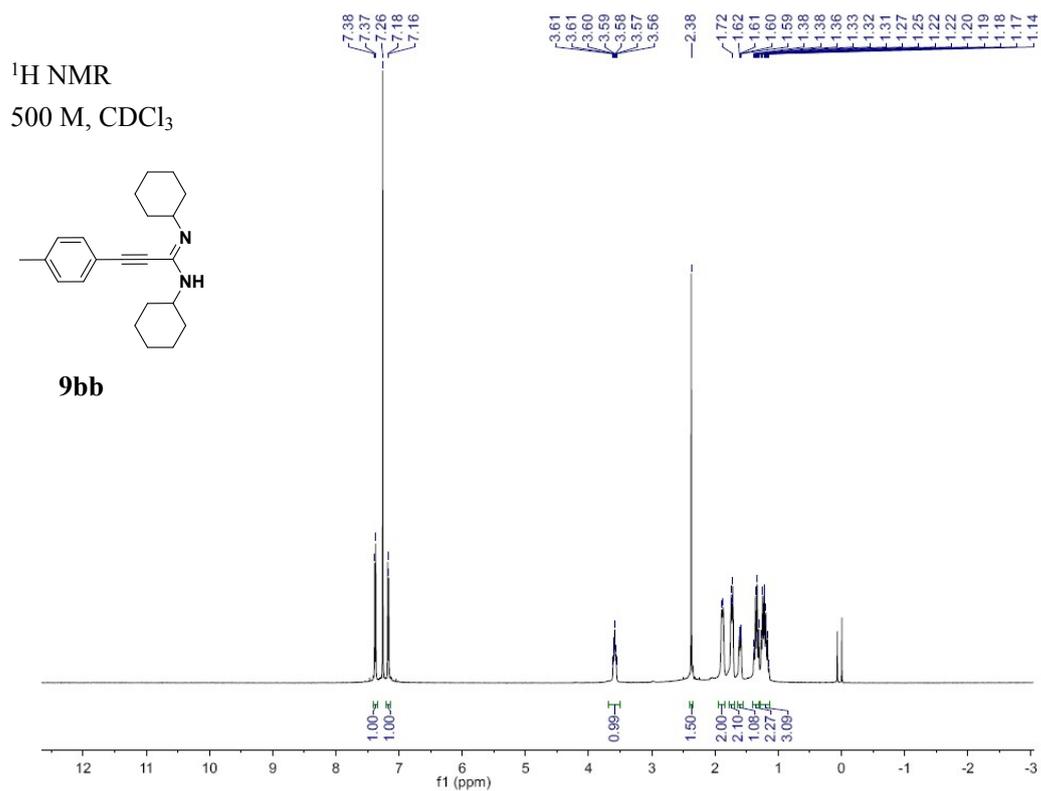


Figure S19. ¹H NMR spectrum of compound **9bb**.

## ¹³C{¹H} NMR
125 M, CDCl₃

**9bb**
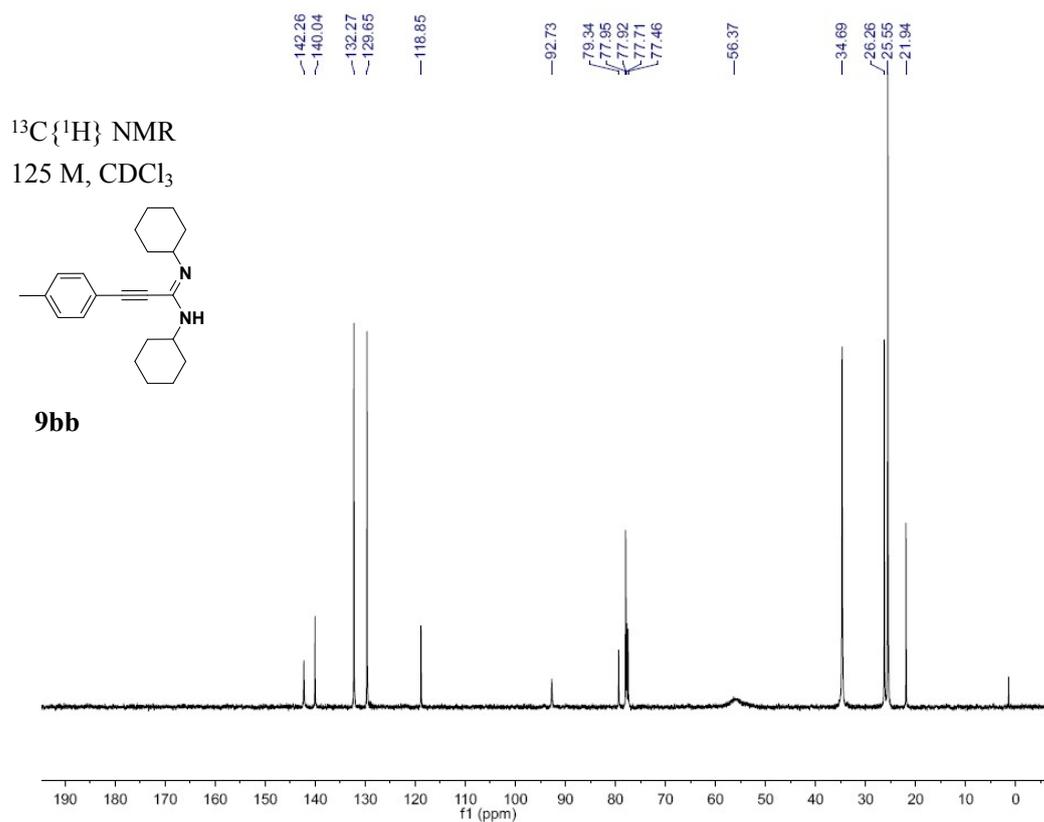


Figure S20. ¹³C{¹H} NMR spectrum of compound **9bb**.

<sup>1</sup>H NMR

500 M, CDCl<sub>3</sub>

**9cb**
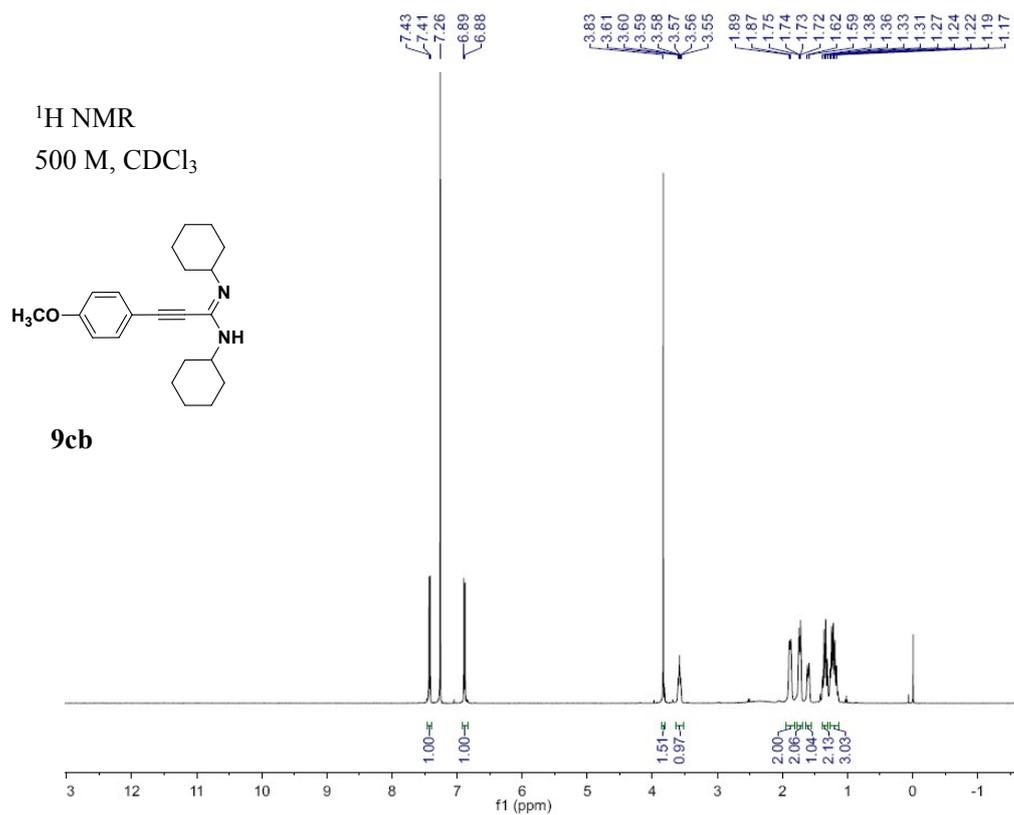
Figure S21. <sup>1</sup>H NMR spectrum of compound **9cb**.

<sup>13</sup>C{<sup>1</sup>H} NMR

125 M, CDCl<sub>3</sub>

**9cb**
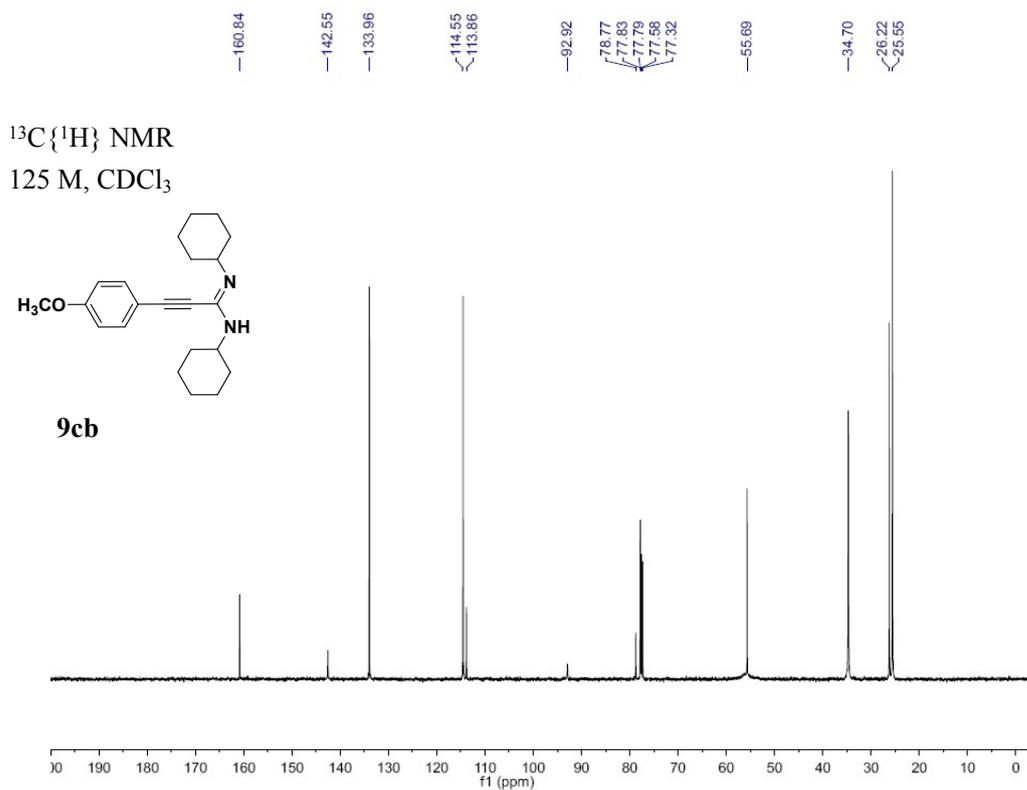
Figure S22. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of compound **9cb**.

<sup>1</sup>H NMR spectrum peaks: 7.51, 7.50, 7.49, 7.35, 7.33, 7.33, 7.26, 3.56, 1.87, 1.87, 1.75, 1.74, 1.72, 1.72, 1.62, 1.60, 1.38, 1.35, 1.33, 1.30, 1.27, 1.25, 1.22, 1.20, 1.17

<sup>1</sup>H NMR
500 M, CDCl<sub>3</sub>

**9db**

Integrations: 1.00, 1.05, 0.95, 1.93, 2.08, 1.13, 5.46
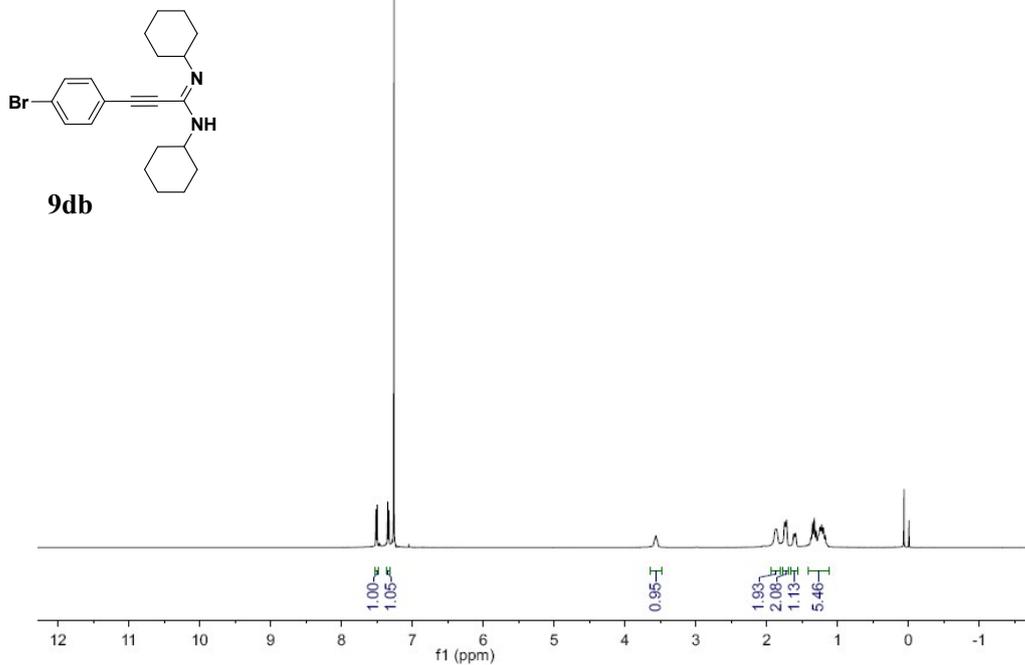
Figure S23. <sup>1</sup>H NMR spectrum of compound **9db.**

<sup>13</sup>C{<sup>1</sup>H} NMR
125 M, CDCl<sub>3</sub>

**9db**

<sup>13</sup>C peaks: 141.66, 133.71, 132.20, 124.22, 124.18, 120.87, 120.82, 91.10, 80.85, 77.76, 77.71, 77.51, 77.46, 77.25, 77.20, 34.67, 26.20, 26.15, 25.50
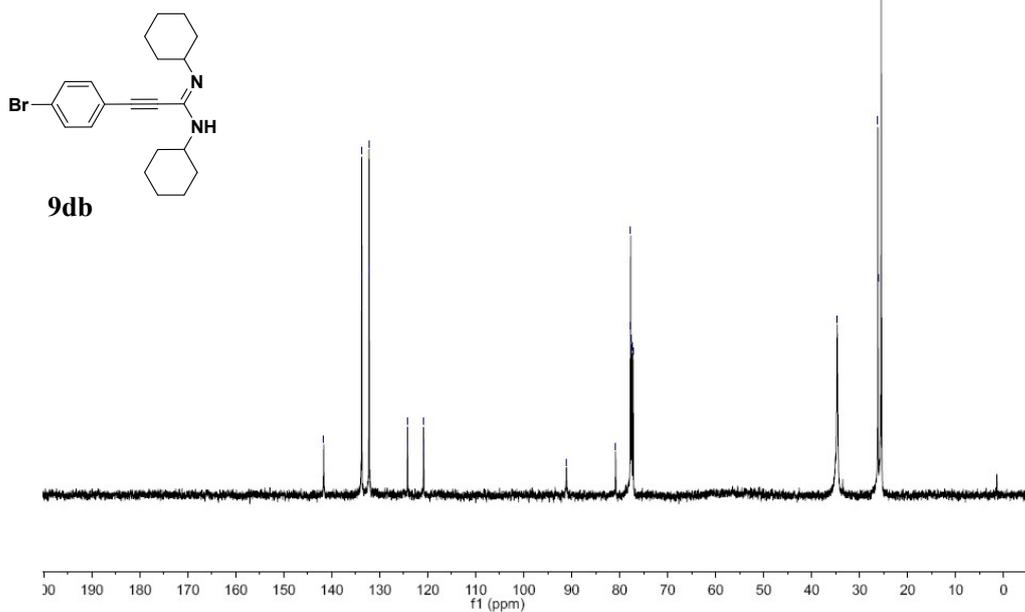
Figure S24. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of compound **9db**.

<sup>1</sup>H NMR
500 M, CDCl<sub>3</sub>

**9ac**
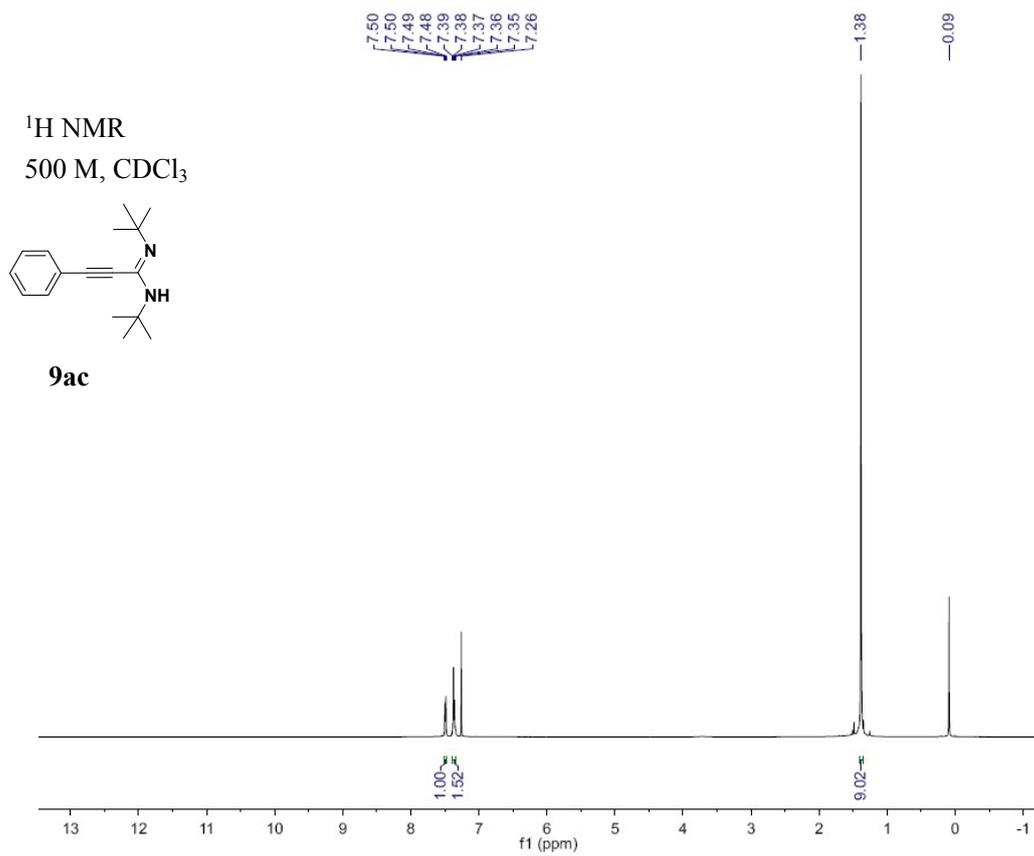
Figure S25. <sup>1</sup>H NMR spectrum of compound **9ac.**

<sup>13</sup>C{<sup>1</sup>H} NMR
125 M, CDCl<sub>3</sub>

**9ac**
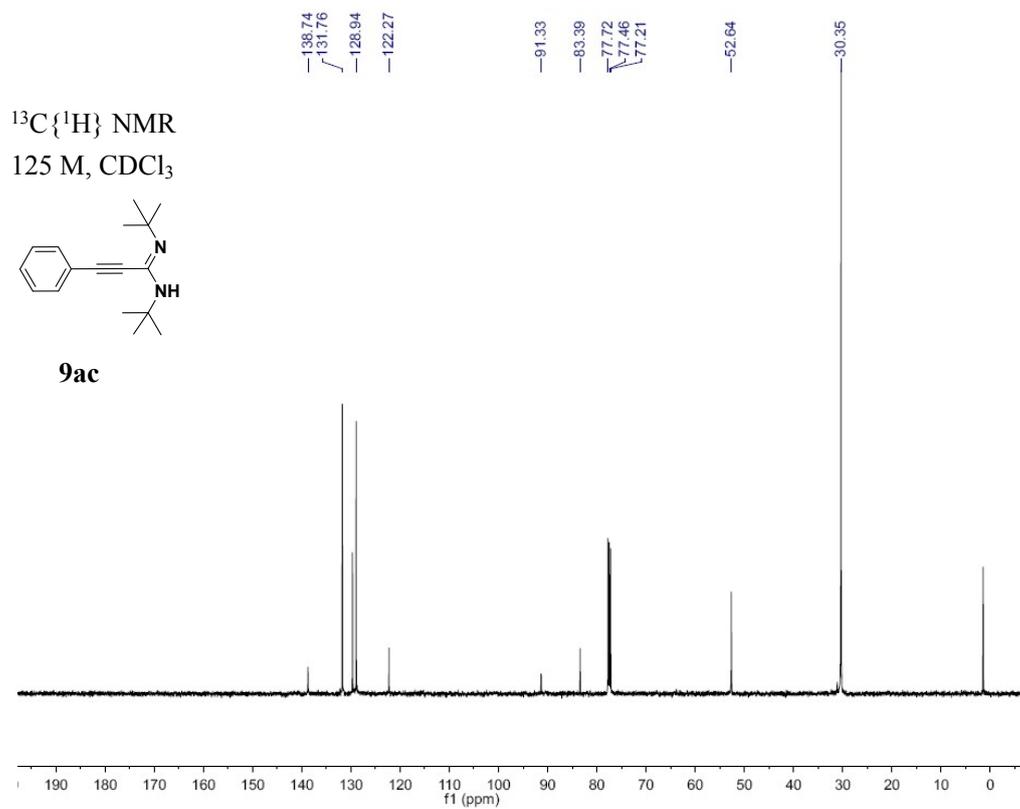
Figure S26. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of compound **9ac**.

<sup>1</sup>H NMR
500 M, CDCl<sub>3</sub>

**9bc**
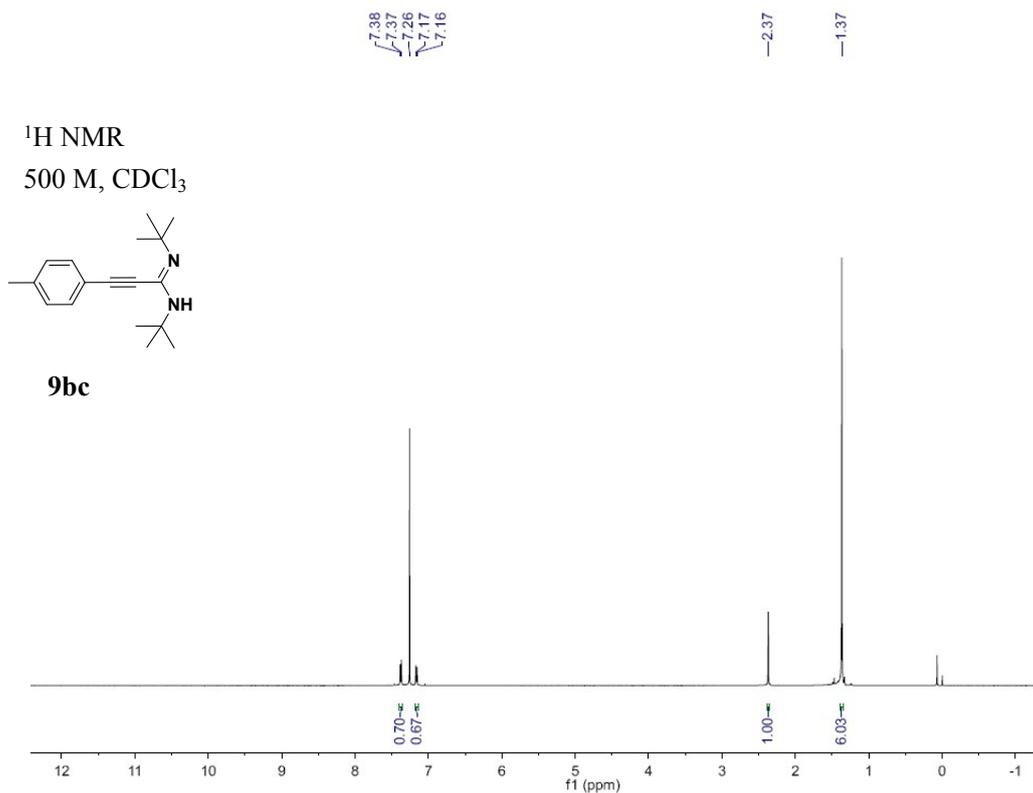
Figure S27. <sup>1</sup>H NMR spectrum of compound **9bc.**

<sup>13</sup>C{<sup>1</sup>H} NMR
125 M, CDCl<sub>3</sub>

**9bc**
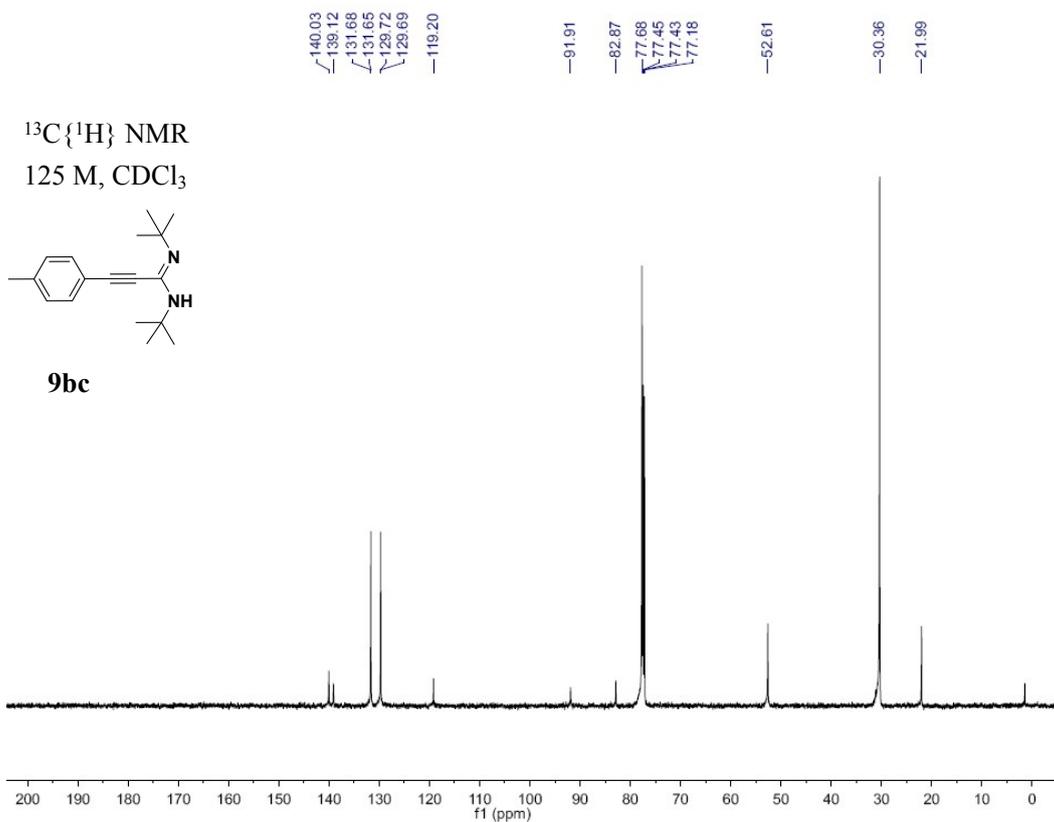
Figure S28. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of compound **9bc**.
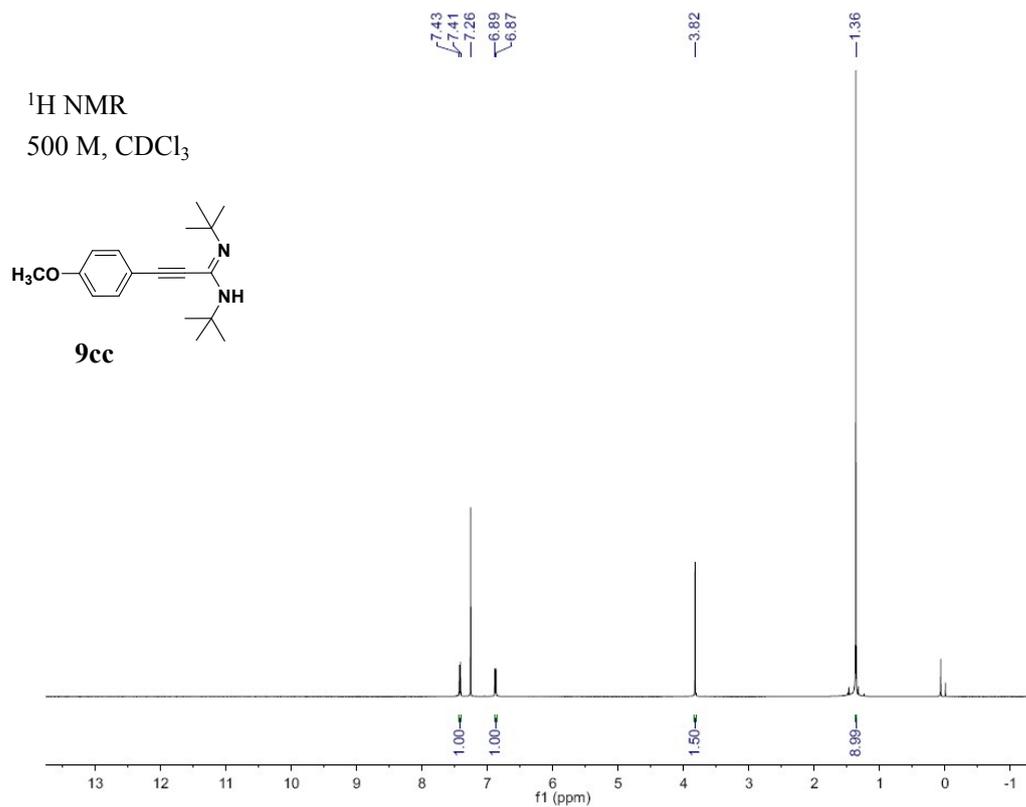
Figure S29. ¹H NMR spectrum of compound **9cc.**
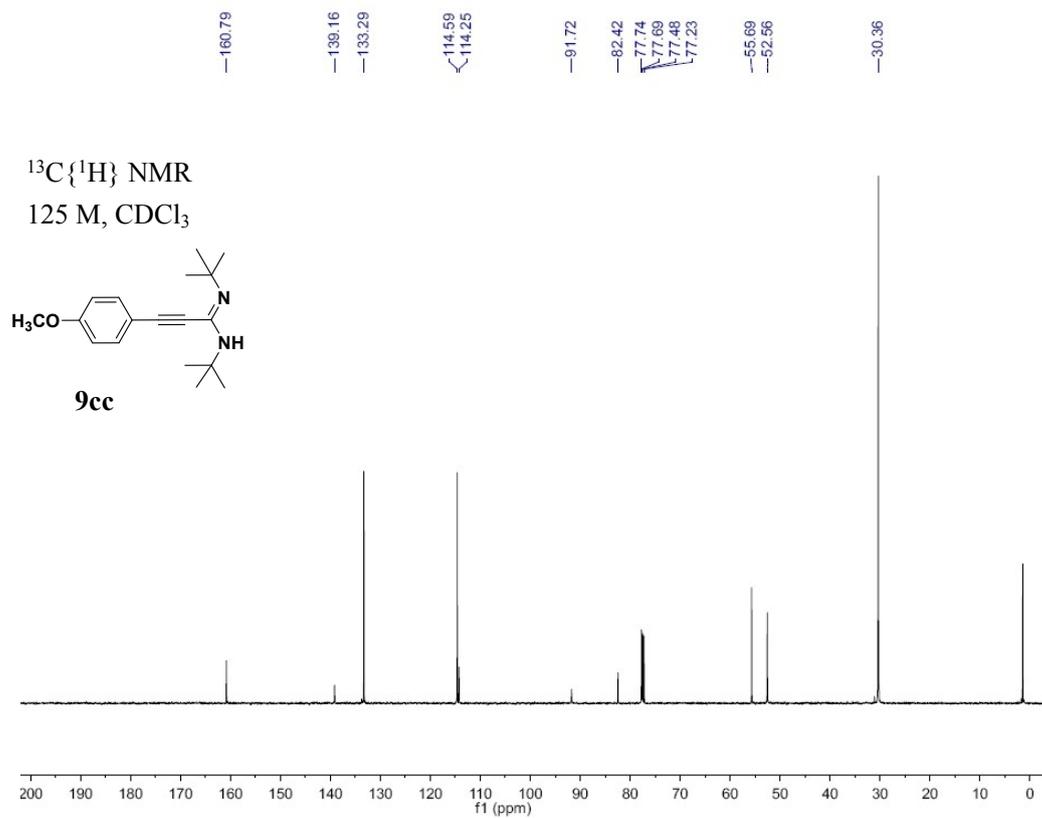


Figure S30. ¹³C{¹H} NMR spectrum of compound **9cc**.
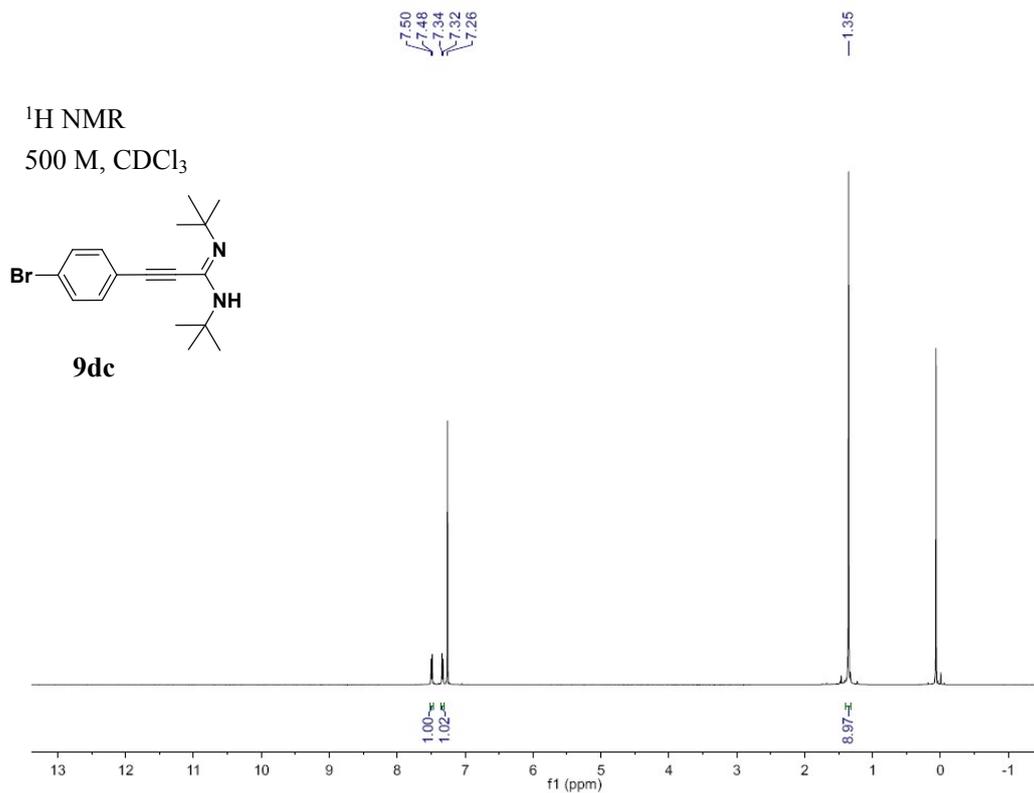
<sup>1</sup>H NMR
500 M, CDCl<sub>3</sub>



Figure S31. <sup>1</sup>H NMR spectrum of compound **9dc.**

<sup>13</sup>C{<sup>1</sup>H} NMR
125 M, CDCl<sub>3</sub>
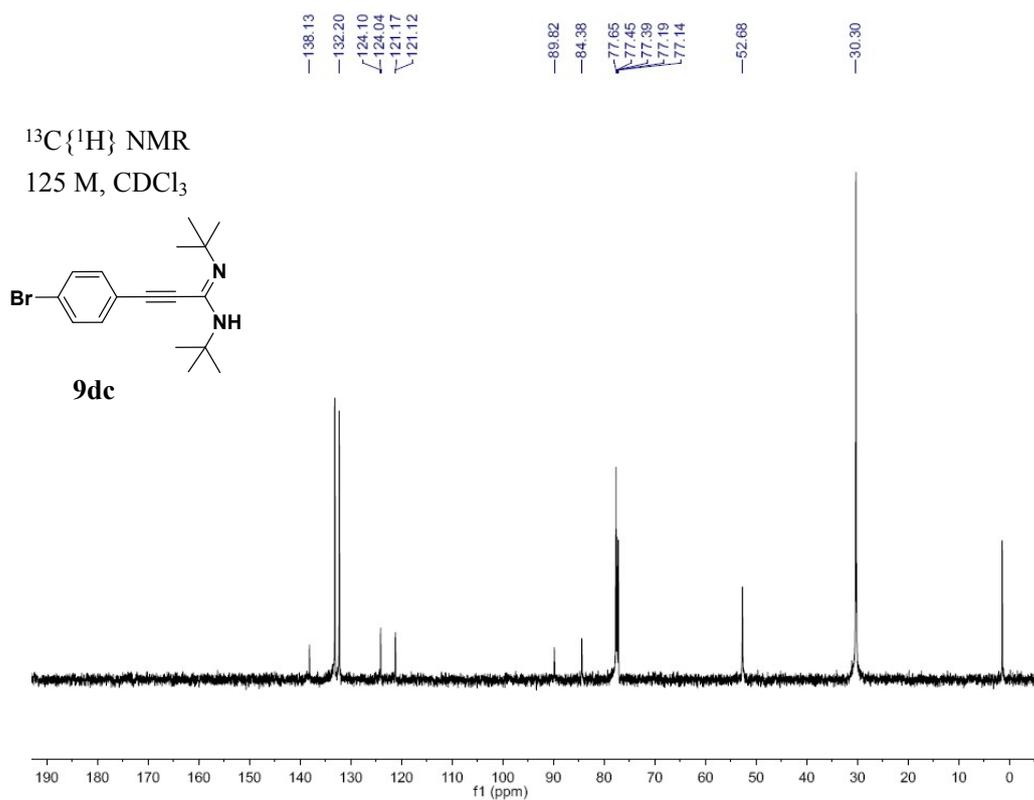


Figure S32. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of compound **9dc**.

<sup>1</sup>H NMR
500 M, CDCl<sub>3</sub>

**9ad**
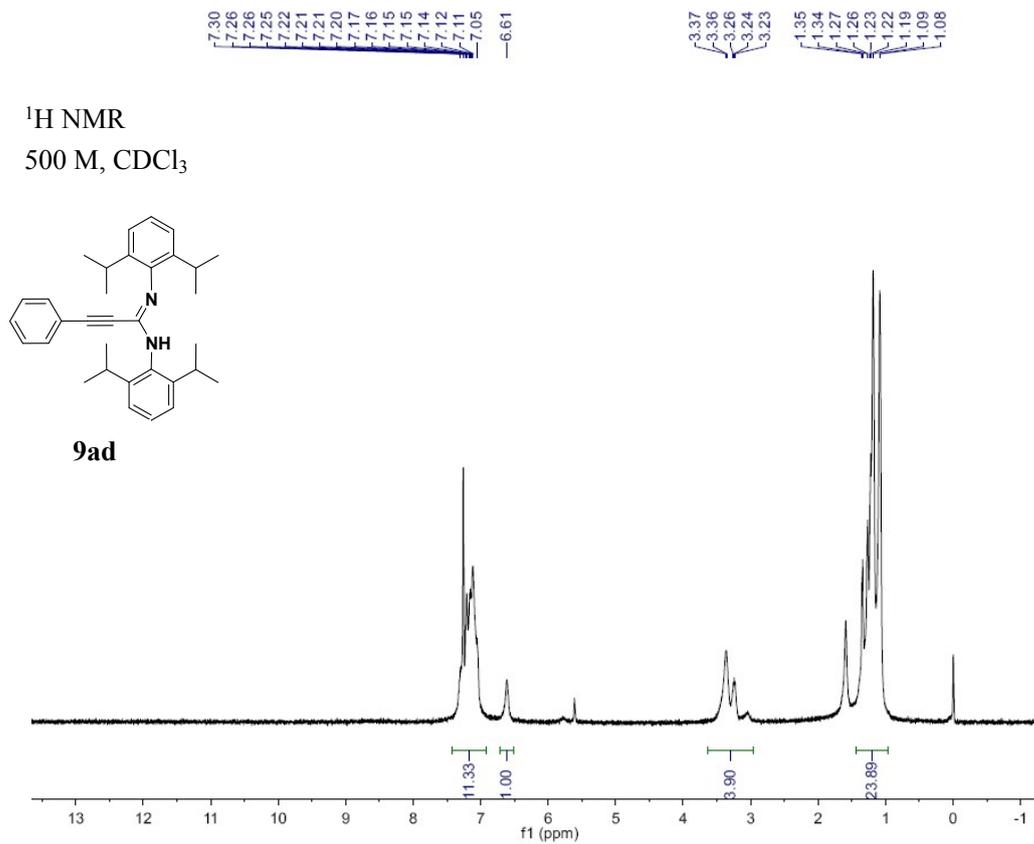
Figure S33. <sup>1</sup>H NMR spectrum of compound **9ad.**

<sup>13</sup>C{<sup>1</sup>H} NMR
125 M, CDCl<sub>3</sub>

**9ad**
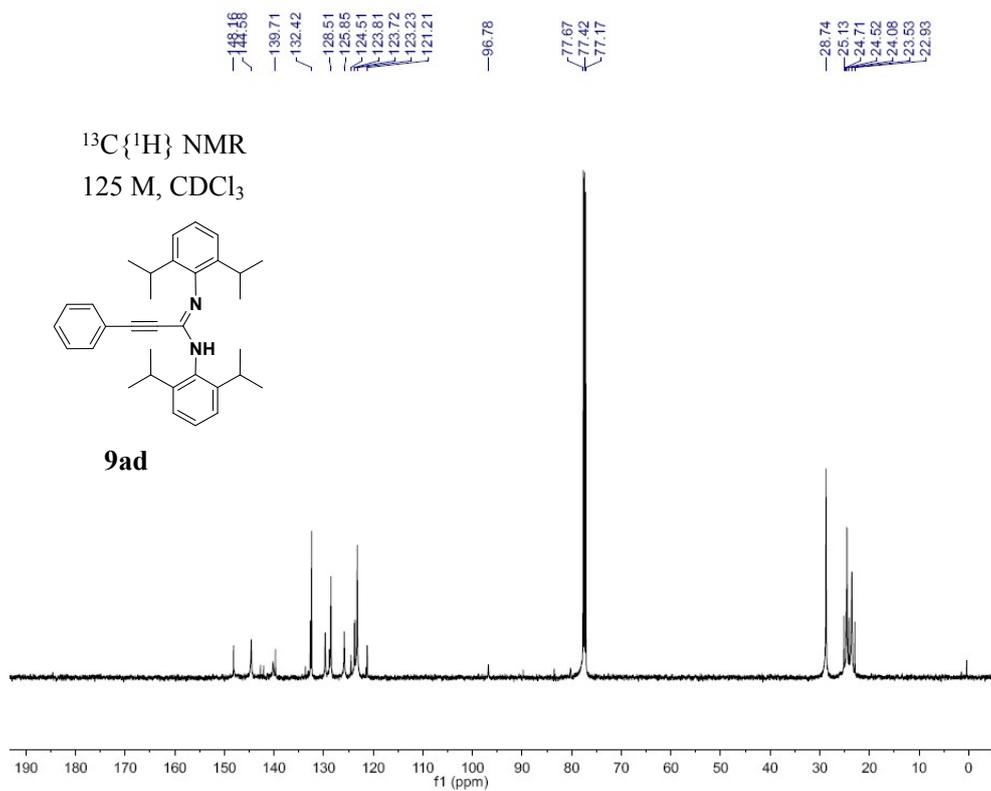
Figure S34. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of compound **9ad**.

**Molecular structures and selected bond distances and angles of the complexes 2–6, 10, 11, 12.**
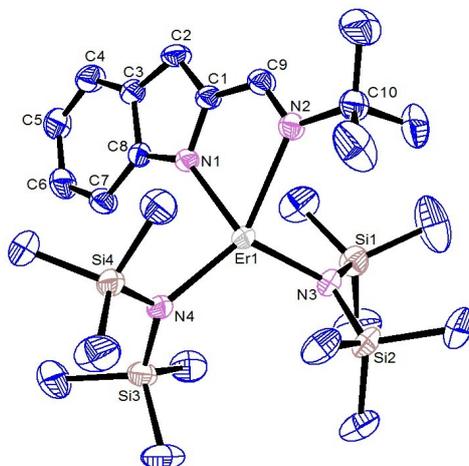


**Figure S35.** Structure of complex **2** (Ellipsoids at 30% probability level). Hydrogen atoms were omitted for clarity. Selected bond distances (Å) and angles (°): Er(1)−N(1) 2.271(2), Er(1)−N(2) 2.493(2), Er(1)−N(3) 2.197(2), Er(1)−N(4) 2.197(2), C(9)−N(2) 1.282(4), N(2)–C(9)–C(1) 123.0(3), N(1)−Er(1)−N(2) 72.94(8), N(3)−Er(1)−N(2) 100.73(9), N(4)−Er(1)−N(2) 143.46(8), N(3)−Er(1)−N(1) 120.63(9), N(4)−Er(1)−N(1) 97.86(9), N(4)−Er(1)−N(3) 113.81(9).
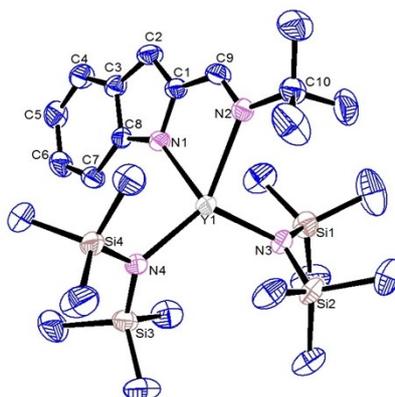


**Figure S36.** Structure of complex **3** (Ellipsoids at 30% probability level). Hydrogen atoms were omitted for clarity. Selected bond distances (Å) and angles (°): Y(1)−N(1) 2.293(2), Y(1)−N(2) 2.513(2), Y(1)−N(3) 2.208(2), Y(1)−N(4) 2.214(2), C(9)−N(2) 1.282(4), N(2)−C(9)−C(1) 123.1(3), N(1)−Y(1)−N(2) 72.04(8), N(3)−Y(1)−N(2) 100.61(9), N(4)−Y(1)−N(2) 142.73(9), N(3)−Y(1)−N(1) 121.87(9), N(4)−Y(1)−N(1) 98.12(9), N(4)−Y(1)−N(3) 114.41(10).
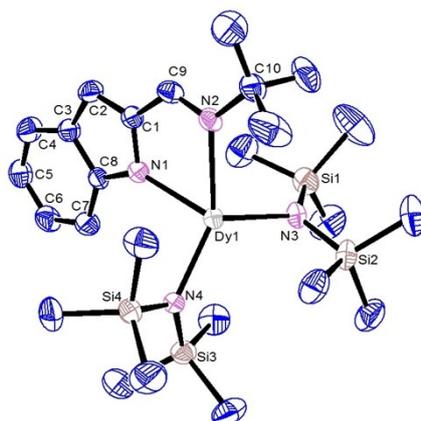
**Figure S37.** Structure of complex **4** (Ellipsoids at 30% probability level). Hydrogen atoms were omitted for clarity. Selected bond distances (Å) and angles (°): Dy(1)−N(1) 2.306(5), Dy(1)−N(2) 2.520(5), Dy(1)−N(3) 2.230(5), Dy(1)−N(4) 2.221(5), C(9)−N(2) 1.260(7), N(2)−C(9)−C(1) 122.9(6), N(1)−Dy(1)−N(2) 71.91(16), N(3)−Dy(1)−N(2) 100.01(18), N(4)−Dy(1)−N(2) 142.33(17), N(3)−Dy(1)−N(1) 122.65(18), N(4)−Dy(1)−N(1) 97.31(16), N(4)−Dy(1)−N(3) 115.45(19).
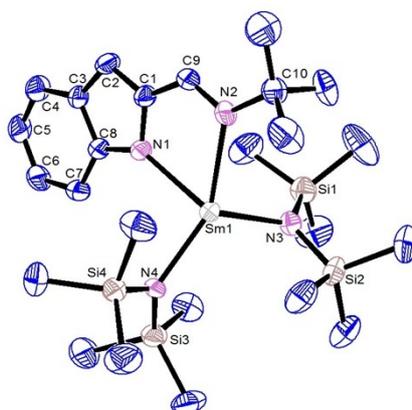


**Figure S38**. Structure of complex **5** (Ellipsoids at 30% probability level). Hydrogen atoms were omitted for clarity. Selected bond distances (Å) and angles (°): N(1)−Sm(1) 2.368(6), N(2)−Sm(1) 2.586(6), N(3)−Sm(1) 2.255(6), N(4)−Sm(1) 2.271(5), C(9)−N(2) 1.274(9), N(2)−C(9)−C(1) 123.7(7), N(1)−Sm(1)−N(2) 70.1(2), N(4)−Sm(1)−N(2) 140.7(2), N(3)−Sm(1)−N(2) 100.8(2), N(4)−Sm(1)−N(1) 97.3(2), N(3)−Sm(1)−N(1) 125.4(2), N(3)−Sm(1)−N(4) 115.9(2).
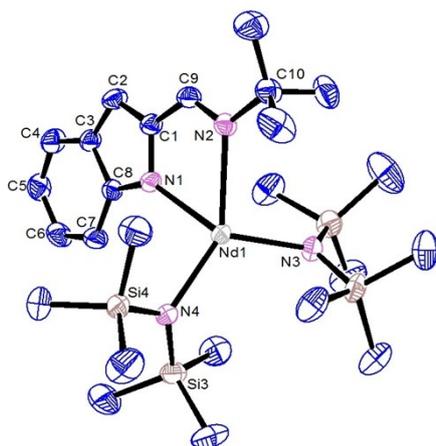
**Figure S39**. Structure of complex **6** (Ellipsoids at 30% probability level). Hydrogen atoms were omitted for clarity. Selected bond distances (Å) and angles (°): N(1)−Nd(1) 2.3967(19), N(2)−Nd(1) 2.611(2), N(3)−Nd(1) 2.292(2), N(4)−Nd(1) 2.2865(19), C(9)−N(2) 1.279(3), N(2)−C(9)−C(1) 123.4(2), N(1)−Nd(1)−N(2) 69.30(6), N(3)−Nd(1)−N(2) 101.34(7), N(4)−Nd(1)−N(2) 139.22(7), N(3)−Nd(1)−N(1) 125.97(7), N(4)−Nd(1)−N(1) 97.69(7), N(4)−Nd(1)−N(3) 116.49(7).
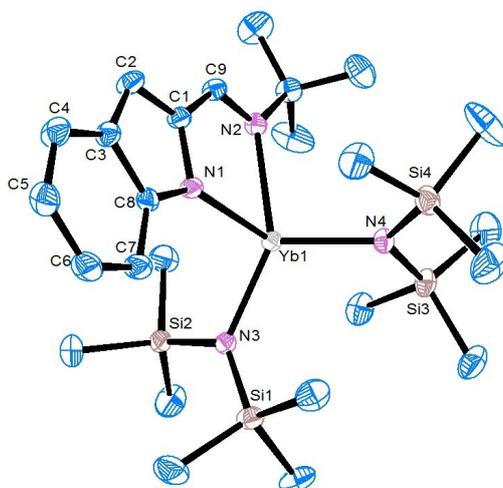


**Figure S40**. Structure of complex **10** (Ellipsoids at 30 % probability level). Hydrogen atoms were omitted for clarity. Selected bond distances (Å) and angles (°): N(1)−Yb(1) 2.258(2), N(2)−Yb(1) 2.471(2), N(3)−Yb(1) 2.174(2), N(4)−Yb(1) 2.169(2), C(9)−N(2) 1.282(3), N(2)−C(9)−C(1) 122.9(3), N(1)−Yb(1)−N(2) 73.15(7), N(3)−Yb(1)−N(2) 143.37(8), N(3)−Yb(1)−N(1) 97.87(8), N(4)−Yb(1)−N(2) 100.27(8), N(4)−Yb(1)−N(1) 122.81(8), N(4)−Yb(1)−N(3) 113.72(9).

**Figure S41**. Structure of complex **11** (Ellipsoids at 15 % probability level). Hydrogen atoms were omitted for clarity. Selected bond distances (Å) and angles (°): N(1)−Y(1) 2.325(6), N(2)−Y(1) 2.470(7), N(3)−Y(1) 2.328(6), N(4)−Y(1) 2.494(6), N(5)−Y(2) 2.324(6), N(6)−Y(2) 2.429(6), N(7)−Y(2) 2.347(6), N(8)−Y(2) 2.508(6), C(9)−N(2) 1.253(11), C(22)−N(4) 1.268(10), C(43)−N(6) 1.293(9), C(56)−N(8) 1.295(9), C(27)−Y(1) 2.524(8), C(28)−Y(1) 2.877(8), C(27)−C(28) 1.198(10), C(27)−Y(2) 2.483(8), C(61)−Y(1) 2.502(8), C(61)−Y(2) 2.513(8), C(62)−Y(2) 2.943(8), C(61)−C(62) 1.176(10), N(2)−C(9)−C(1) 125.7(10), N(4)−C(22)−C(14) 123.7(8), N(6)−C(43)−C(35) 123.0(8), N(8)−C(56)−C(48) 123.6(7), N(3)−Y(1)−N(1) 167.1(2), N(3)−Y(1)−N(2) 103.2(2), N(1)−Y(1)−N(2) 72.3(2), N(3)−Y(1)−N(4) 71.6(2), N(1)−Y(1)−N(4) 96.2(2), N(2)−Y(1)−N(4) 91.7(2), N(3)−Y(1)−C(61) 91.2(3), N(1)−Y(1)−C(27) 89.2(2), N(3)−Y(1)−C(27) 98.4(2), N(1)−Y(1)−C(61) 100.4(2), N(5)−Y(2)−N(7) 164.3(2), N(5)−Y(2)−N(6) 72.8(2), N(7)−Y(2)−N(6) 106.2(2), N(5)−Y(2)−N(8) 93.0(2), N(7)−Y(2)−N(8) 71.3(2), N(6)−Y(2)−N(8) 92.15(19), N(5)−Y(2)−C(27) 103.2(2), N(7)−Y(2)−C(61) 97.0(2), N(7)−Y(2)−C(27) 92.3(2), C(28)−C(27)−Y(2) 166.2(7), C(62)−C(61)−Y(1)    161.9(7).

**Figure S42**. Structure of complex **12** (Ellipsoids at 15 % probability level). Hydrogen atoms were omitted for clarity. Selected bond distances (Å) and angles (°): N(1)−Yb(1) 2.285(3), N(2)−Yb(1) 2.504(4), N(3)−Yb(1) 2.292(3), N(4)−Yb(1) 2.404(3), N(5)−Yb(2) 2.300(3), N(6)−Yb(2) 2.493(3), N(7)−Yb(2) 2.287(3), N(8)−Yb(2) 2.422(3), C(9)−N(2) 1.285(6), C(22)−N(4) 1.288(5), C(40)−N(6) 1.292(5), C(53)−N(8) 1.281(5), C(27)−Yb(1) 2.483(4), C(28)−Yb(1) 2.954(4), C(27)−Yb(2) 2.479(4), C(27)−C(28) 1.216(5), C(58)−Yb(2) 2.473(4), C(59)−Yb(2) 3.035(4), C(58)−Yb(1) 2.488(4), C(58)−C(59) 1.205(5), N(2)−C(9)−C(1) 123.4(4), N(4)−C(22)−C(14) 123.3(4), N(6)−C(40)−C(32) 123.2(4), N(8)−C(53)−C(45) 122.4(4), N(1)−Yb(1)−N(3) 165.29(13), N(1)−Yb(1)−N(4) 107.22(12), N(3)−Yb(1)−N(4) 73.95(12), N(1)−Yb(1)−N(2) 72.28(13), N(3)−Yb(1)−N(2) 93.23(12), N(4)−Yb(1)−N(2) 88.08(12), N(1)−Yb(1)−C(27) 97.01(12), N(1)−Yb(1)−C(58) 91.63(13), N(3)−Yb(1)−C(27) 86.99(12), N(3)−Yb(1)−C(58) 103.02(12), N(5)−Yb(2)−N(6) 72.90(11), N(7)−Yb(2)−N(5) 164.76(11), N(5)−Yb(2)−N(8) 104.28(11), N(7)−Yb(2)−N(6) 91.97(11), N(8)−Yb(2)−N(6) 90.66(11), N(7)−Yb(2)−N(8) 73.41(11), N(5)−Yb(2)−C(27) 92.40(12), N(7)−Yb(2)−C(27) 102.29(11), N(5)−Yb(2)−C(58) 98.31(12), N(7)−Yb(2)−C(58) 88.24(12), C(28)−C(27)−Yb(2) 161.4(3), C(59)−C(58)−Yb(1) 156.1(4).

**Table S1**. Crystallographic data for **2–4**.

| | 2 | 3 | 4 |
|---|---|---|---|
| formula | $C_{25}H_{51}ErN_4Si_4$ | $C_{25}H_{51}N_4Si_4Y$ | $C_{25}H_{51}N_4Si_4Dy$ |
| Fw | 687.31 | 608.96 | 682.55 |
| $T$(K) | 293(2) | 293(2) | 293(2) |
| $\lambda$ (Å) | 0.71073 | 0.71073 | 0.71073 |
| crystal system | Monoclinic | Monoclinic | Monoclinic |
| space group | $P2_1/c$ | $P2_1/c$ | $P2_1/c$ |
| $a$ (Å) | 18.1565(16) | 18.1922(16) | 18.233(3) |
| $b$ (Å) | 11.6742(10) | 11.6913(10) | 11.728(2) |
| $c$ (Å) | 17.3053(15) | 17.2934(15) | 17.281(3) |
| $\alpha$(deg) | 90 | 90 | 90 |
| $\beta$(deg) | 109.1190(10) | 108.9890(10) | 108.947(2) |
| $\gamma$(deg) | 90 | 90 | 90 |
| $V$ (Å$^3$) | 3465.7(5) | 3478.0(5) | 3495.2(11) |
| $Z$ | 4 | 4 | 4 |
| $D_{calcd}$ (mg/m$^3$) | 1.317 | 1.163 | 1.297 |
| $\mu$(mm$^{-1}$) | 2.578 | 1.833 | 2.293 |
| $F$(000) | 1412 | 1296 | 1404 |
| $\theta$ range (deg) | 2.11–27.68 | 2.11–27.58 | 2.10–27.66 |
| reflections collected / unique | 29320/8062 | 29572/7994 | 28487/8052 |
| $R$(int) | 0.0326 | 0.0610 | 0.0660 |
| goodness-of-fit on $F^2$ | 1.031 | 1.002 | 1.005 |
| $R_1, wR_2$ [$I > 2\sigma(I)$] | 0.0285, 0.0700 | 0.0460, 0.0909 | 0.0530, 0.1324 |
| $R_1, wR_2$(all data) | 0.0356, 0.0744 | 0.1020, 0.1080 | 0.0875, 0.1586 |
| Largest diff. peak and hole (e Å$^{-3}$) | 0.755 and -1.232 | 0.402 and -0.405 | 3.194 and -2.020 |

**Table S2**. Crystallographic data for **5**, **6**, **10**.

| | 5 | 6 | 10 |
|---|---|---|---|
| formula | $C_{25}H_{51}N_4Si_4Sm$ | $C_{25}H_{51}N_4Si_4Nd$ | $C_{25}H_{51}N_4Si_4Yb$ |
| Fw | 670.40 | 664.29 | 693.09 |
| $T$(K) | 293(2) | 293(2) | 293(2) |
| $\lambda$ (Å) | 0.71073 | 0.71073 | 0.71073 |
| crystal system | Monoclinic | Monoclinic | Monoclinic |
| space group | $P2_1/c$ | $P2_1/c$ | $P2_1/c$ |
| $a$ (Å) | 18.356(4) | 18.3322(11) | 18.1425(13) |
| $b$ (Å) | 11.757(3) | 11.7260(7) | 11.6936(8) |
| $c$ (Å) | 17.248(4) | 17.2138(10) | 17.2342(12) |
| $\alpha$(deg) | 90 | 90 | 90 |
| $\beta$(deg) | 108.672(3) | 108.5360(10) | 109.0750(10) |
| $\gamma$(deg) | 90 | 90 | 90 |
| $V$ (Å$^3$) | 3526.6(14) | 3508.4(4) | 3455.5(4) |
| $Z$ | 4 | 4 | 4 |
| $D_{calcd}$ (mg/m$^3$) | 1.263 | 1.258 | 1.332 |
| $\mu$(mm$^{-1}$) | 1.819 | 1.635 | 2.864 |
| $F$(000) | 1388 | 1380 | 1420 |
| $\theta$ range (deg) | 2.09–27.66 | 2.10–27.63 | 2.11–27.62 |
| reflections collected / unique | 28465/8093 | 29901/8097 | 29236/7948 |
| $R$(int) | 0.0899 | 0.0264 | 0.0298 |
| goodness-of-fit on $F^2$ | 1.028 | 1.016 | 1.036 |
| $R_1,wR_2$ [$I > 2\sigma(I)$] | 0.0573, 0.1298 | 0.0257, 0.0606 | 0.0251, 0.0598 |
| $R_1,wR_2$(all data) | 0.1386, 0.1671 | 0.0369, 0.0657 | 0.0335, 0.0641 |
| Largest diff. peak and hole (e Å$^{-3}$) | 2.166 and -1.584 | 0.519 and -0.644 | 0.407 and -1.088 |

**Table S3**. Crystallographic data for **11**, **12**.

| | 11 | 12 |
|---|---|---|
| formula | $C_{68}H_{70}N_8Y_2$ | $C_{62}H_{78}N_8Si_2Yb_2$ |
| Fw | 1177.14 | 1337.58 |
| $T$(K) | 293(2) | 293(2) |
| $\lambda$ (Å) | 0.71073 | 0.71073 |
| crystal system | Monoclinic | Triclinic |
| space group | $P2_1/c$ | $P\bar{1}$ |
| $a$ (Å) | 12.995(3) | 12.6269(9) |
| $b$ (Å) | 20.995(5) | 12.9123(10) |
| $c$ (Å) | 23.338(6) | 22.4030(17) |
| $\alpha$(deg) | 90 | 77.3030(10) |
| $\beta$(deg) | 106.16 | 80.6500(10) |
| $\gamma$(deg) | 90 | 61.7530(10) |
| $V$ (Å$^3$) | 6116(3) | 3131.7(4) |
| $Z$ | 4 | 2 |
| $D_{calcd}$ (mg/m$^3$) | 1.278 | 1.418 |
| $\mu$(mm$^{-1}$) | 1.935 | 3.049 |
| $F$(000) | 2448 | 1348 |
| $\theta$ range (deg) | 1.63–25.03 | 1.82–25.41 |
| reflections collected / unique | 43976/10794 | 31940/11514 |
| $R$(int) | 0.1758 | 0.0267 |
| goodness-of-fit on $F^2$ | 0.993 | 1.036 |
| $R_1,wR_2$ [$I > 2\sigma(I)$] | 0.0725, 0.1799 | 0.0282, 0.0608 |
| $R_1,wR_2$(all data) | 0.1724, 0.2264 | 0.0388, 0.0654 |
| Largest diff. peak and hole (e Å$^{-3}$) | 0.847 and -0.767 | 1.323 and -0.811 |