Electronic Supplementary Material (ESI) for Chemical Science.
This journal is © The Royal Society of Chemistry 2024

Rare-earth metal complexes bearing electrophilic and nucleophilic carbon centres and their unique reactivity patterns towards pyridine derivatives

Weikang Wu,[a] Thayalan Rajeshkumar,[d] Shan Zhu,[a] Fuxiang Chai,[a] Dongjing Hong,[a] Zeming Huang,[b] Qingbing Yuan,[a] Laurent Maron,*[d] Shaowu Wang*[bc]

[a]Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, College of Chemistry and Materials Science, Anhui Normal University, Wuhu 241000, Anhui, P. R. China.
E-mail: swwang@mail.ahnu.edu.cn

[b]Anhui Laboratory of Clean Catalytic Engineering, Anhui Laboratory of Functional Coordinated Complexes for Materials Chemistry and Application, College of Chemical and Environmental Engineering, Anhui Polytechnic University, Wuhu 241000, Anhui, P. R. China.
E-mail: wsw@ahpu.edu.cn

[c]State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, P. R. China.

[d]LPCNO, CNRS & INSA, Université Paul Sabatier, 135 Avenue de Rangueil, 31077 Toulouse, France.
E-mail: laurent.maron@irsamc.ups-tlse.fr

Table of Contents

1. General Reaction Methods 1
2. Synthesis of Ligands and Complexes 1
3. ^{1}H, $^{13}C\{^{1}H\}$, 2D HSQC, and ^{89}Y NMR Spectra of Ligands and Complexes 14
4. DFT Calculations 40
5. Olex2 Drawing of Complexes 133
6. Electron Paramagnetic Resonance and UV/vis Absorption Spectra 154
7. GC-MS 155
8. Tables of Crystal Data and Structure Refinement 155
9. IR Spectra 163
10. References 170

1. General Reaction Methods

Materials and Methods. All syntheses and manipulations of air- and moisture-sensitive materials were performed under dry argon and oxygen-free atmosphere, using standard Schlenk techniques or in a glovebox unless otherwise stated. All solvents were refluxed and distilled over sodium benzophenone ketyl under argon prior to use unless otherwise noted. $RECl_3$,[1] $LiCH_2SiMe_3$,[2] $RE(CH_2SiMe_3)_3(THF)_2$ (RE = Lu, Yb, Er, Y, Dy, Gd)[3] were prepared according to the literature methods. All other chemicals were commercially available and used as received unless otherwise specified. Elemental analyses data were obtained on an Elemental Model Vario EL III automatic elemental analyzer. ^{1}H NMR, and $^{13}C\{^1H\}$ NMR spectra for analyses of compounds were recorded on a Bruker Model AV-500 NMR spectrometer (500 MHz for ^{1}H; 125 MHz for $^{13}C\{^1H\}$) in C_6D_6 or THF-d_8 for lanthanide complexes and in $CDCl_3$ for organic compounds. Chemical shifts (δ) were reported in ppm. J values are reported in Hz. IR spectra were recorded on a Shimadzu Model FTIR-8400s or Bruker OPTIK GmbH spectrometer (KBr pellet). HRMS measurements were conducted with an Agilent Model 6220 ESI-TOF mass spectrometer.

Single Crystal X-ray Crystallographic and refinements.

Data Collection: Data collection was performed at 300 K on Bruker D8 Venture diffractometer (S1 and S2) and Bruker SMART APEX II diffractometer (complexes) with a CCD area detector, using graphite monochromated Mo K_α radiation (λ = 0.71073 Å).

Data Reduction: The determination of the crystal class and unit cell parameters was carried out by the SMART program package.[4] The raw frame data were processed using SAINT[5] and absorption corrections using SADABS[6] to yield the reflection data file.

Structure Solution: The structures were solved by using structure program ShelXT with Intrinsic Phasing method[7] in the OLEX2 software.[8]

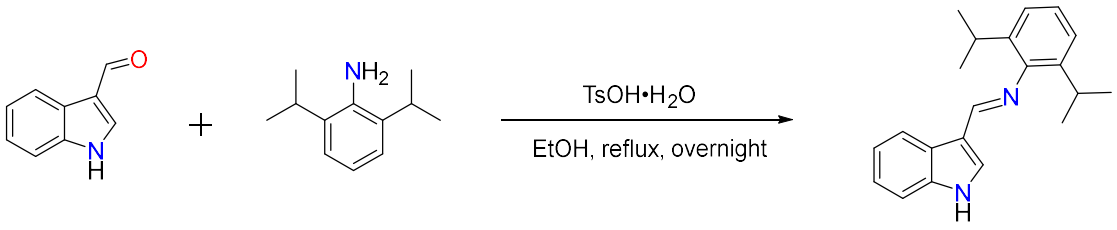
Structure Refinement: Refinements were performed on F^2 anisotropically for all the non-hydrogen atoms by the full-matrix least-squares method using SHELXL program in OLEX2 software.[8]

CCDC numbers: 2278697(**1a**), 2278699(**1b**), 2278698(**1c**), 2278700(**1e**), 2278701(**1d**), 2348805(**2a**), 2348806(**2b**), 2348807(**2c**), 2348808(**2d**), 2348809(**2e**), 2348810(**3a**), 2348811(**3b**), 2348812(**3c**), 2348813(**3d**), 2348814(**3e**), 2348816(**4a**), 2348817(**4b**), 2348818(**4c**), 2348819(**4d**), 2348820(**5a**), 2348821(**5b**), 2348822(**5c**), 2348823(**5d**), 2348824(**6a**), 2348825(**6b**), 2348826(**6c**), 2348827(**6d**), 2348828(**7a**), 2348829(**7b**), 2348830(**10b**), 2348831(**10a**), 2348832(**10c**), 2348833(**11**), 2348834(**8a**), 2348835(**8b**), 2348836(**9**), 2348837(**12a**), 2348838(**12b**), 2348839(**12c**), 2348840(**12d**), 2348841(**13**), 2348842(**14a**), 2348843(**14b**), 2348844(**14c**).

2. Synthesis of Ligands and Complexes

Synthesis of 1H-3-(2,6-^{i}Pr$_2$C$_6$H$_3$N=CH)-C$_8$H$_5$N (S1). According to the literature,[9] to a 500 mL flask was added 2,6-diisopropylphenylaniline (21.27 g, 22.7 mL, 120 mmol), 1*H*-indole-3-carbaldehyde (14.52 g, 100 mmol), 150 mL EtOH and catalytic amount of $TsOH{\cdot}H_2O$. Then the mixture was reflux overnight. The yellow suspensions were gradually transferred to dark-red with large amount white salt-like crystals precipitated. The reaction process was monitored by TLC (PE/EA = 1/1, v/v, PE = petroleum ether, EA = ethyl acetate, R_f = 0.42). The mixture was allowed to be cooled to ambient temperature and filtered, and the filter cake was washed with ice-cold EtOH (150 mL × 3) followed petroleum ether (150 mL × 3). The volatiles were removed under reduced pressure to give the product **S1** as a white salt-like crystalline solid (30.14 g) in 99% yield. M.P.: 240 °C. IR (KBr pellets, cm^{-1}): ν 3228(m), 3063(w), 2958(m), 2923(m), 2863(w), 1683(w), 1621(s), 1580(m), 1525(w), 1456(m), 1425(s), 1361(m), 1317(w), 1245(m), 1173(w), 1105(w), 1046(w),

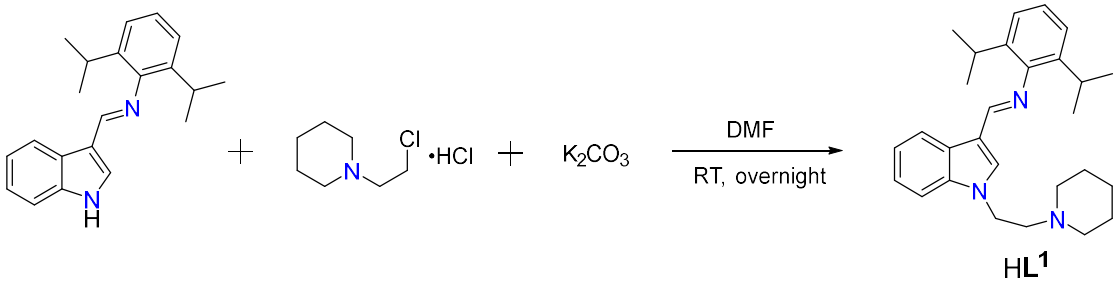
1008(w), 972(w), 932(w), 883(w), 851(m), 795(w), 744(m). ^{1}H NMR (500 MHz, $CDCl_3$, ppm, 298 K): δ 8.54 (d, J = 7.5 Hz, 1H), 8.47 (s, 1H, -N*H*-), 8.36 (s, 1H, -C*H*=N-), 7.61 (s, 1H, -$C_{2\text{-indolyl}}H$), 7.45 (d, J = 10.0 Hz, 1H), 7.35-7.28 (m, 2H), 7.18-7.16 (m, 2H), 7.11-7.08 (m, 1H), 3.13 (hept, J = 5.0 Hz, 2H, -C*H*$(CH_3)_2$), 1.18 (d, J = 5.0 Hz, 12H, -CH(C*H*$_3)_2$). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, ppm, 298 K): δ 156.3 (-*C*H=N-), 150.9 (2-indolyl-C_{sp2}), 138.5, 137.2, 130.1, 125.8, 124.1, 123.9, 123.3, 122.9, 122.2, 116.8, 111.7, 28.3, 24.0. HR-MS (APCI) *m/z* calcd. for $C_{21}H_{25}N_2$ (M+H$^+$): 305.2012, found: 305.2019.



S1

Scheme S1. Synthesis of **S1**.

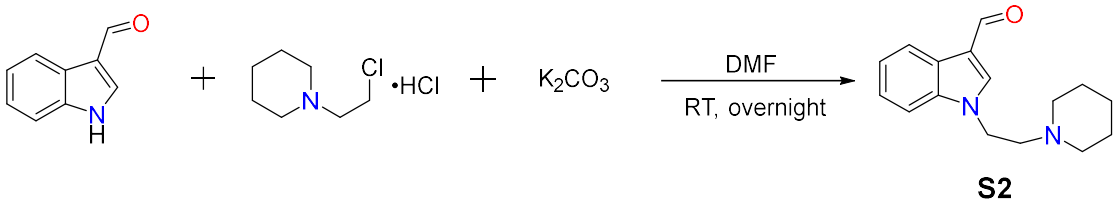
Synthesis of [1-(2-$C_5H_{10}NCH_2CH_2$)-3-(2,6-$^{i}Pr_2C_6H_3N$=CH)-C_8H_5N] (HL^1). According to the literature,[10] anhydrous K_2CO_3 (13.8 g, 100 mmol) and **S1** (15 g, 50 mmol) were added to a 500 mL flask, followed by addition of 125 mL anhydrous *N*,*N*-dimethylformamide as a solvent. The mixture was stirred at room temperature for 30 min. Then 1-(2-chloroethyl) piperidine hydrochloride (11.25 g, 60 mmol) was added and the mixture was reacted overnight at room temperature. With the progress of the reaction, the light-yellow suspension solution gradually turns into light pink emulsion. The reaction process was monitored by TLC (PE/EA = 3/1, v/v, PE = petroleum ether, EA = ethyl acetate, R_f = 0.60). When the reaction finished, it was gradually diluted with 200 mL of water and extracted with ethyl acetate (100 mL × 3). The combined organic phase was washed with brine (100 mL × 3) and dried over anhydrous $MgSO_4$. The $MgSO_4$ was filtered and the solvent of the filtrate was evaporated under reduced pressure on a rotary evaporator to obtain H**L^1** as a yellow solid which was recrystallized from a mixture of ethyl acetate and petroleum ether to afford a light yellow crystalline solid (19.7 g) in 95% yield. M.P.: 80 °C. IR (KBr pellets, cm^{-1}): ν 3119(m), 3052(w), 2957(m), 2932(m), 2862(w), 2369(w), 1622(s), 1589(m), 1572(m), 1535(w), 1468(m), 1441(s), 1395(m), 1352(w), 1165(m), 1034(m), 854(w), 789(w), 743(m). ^{1}H NMR (500 MHz, $CDCl_3$, ppm, 298 K): δ 8.49 (d, J = 5.0 Hz, 1H), 8.32 (s, 1H, -C*H*=N-), 7.58 (s, 1H, -$C_{2\text{-indolyl}}H$), 7.41 (d, J = 10.0 Hz, 1H), 7.35-7.31 (m, 1H), 7.29-7.26 (m, 1H), 7.16-7.15 (m, 2H), 7.09-7.06 (m, 1H), 4.28 (t, J = 7.5 Hz, 2H, -CH_2-), 3.13 (hept, J = 7.5 Hz, 2H, -C*H*$(CH_3)_2$), 2.76 (t, J = 7.5 Hz, 2H, -CH_2-), 2.49-2.46 (m, 4H, -CH_2-), 1.62-1.58 (m, 4H, -CH_2-), 1.48-1.44 (m, 2H, -CH_2-), 1.18 (d, J = 5.0 Hz, 12H, -CH(C$H_3)_2$). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, ppm, 298 K): δ 155.7 (-*C*H=N-), 150.7 (2-indolyl-C_{sp2}), 138.2, 137.2, 133.6, 126.2, 123.4, 123.2, 122.9, 122.6, 121.5, 114.8, 109.6, 58.4, 54.9, 44.6, 27.9, 26.0, 24.2, 23.6. HR-MS(APCI) *m/z* calcd. for $C_{28}H_{38}N_3$(M+H$^+$): 416.3060, found: 416.3056.



HL^1

Scheme S2. Synthesis of H**L^1**.

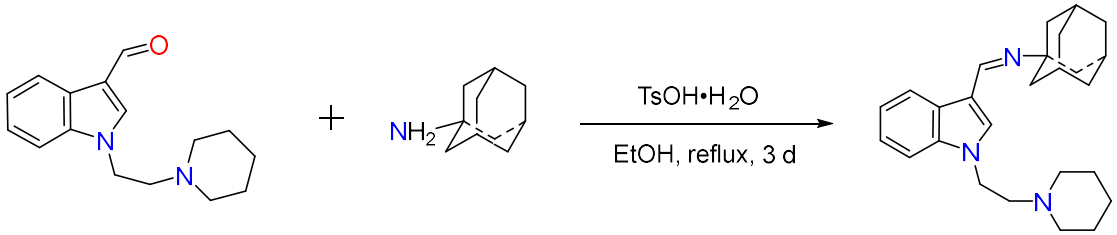
Synthesis of [1-(2-$C_5H_{10}NCH_2CH_2$)-3-(CHO)-C_8H_5N] (S2). To a 500 mL flask was added 1*H* indole-3-carbaldehyde (7.25 g, 50 mmol), Anhydrous K_2CO_3 (13.8 g, 100 mmol) and 125 mL anhydrous DMF. The mixture was stirred at room temperature for 30 min. Then 1-(2-chloroethyl) piperidine hydrochloride (11.25 g, 60 mmol) was added and the mixture was reacted overnight at room temperature. The reaction process was monitored by TLC. When the reaction finished, it was gradually diluted with 200 mL of water and extracted with ethyl acetate (100 mL × 3). The combined organic phase was washed with brine (100 mL × 3) and dried over anhydrous $MgSO_4$. The $MgSO_4$ was filtered and the solvent of the filtrate was evaporated under reduced pressure on a rotary evaporator to obtain **S2** as a yellow solid which was recrystallized with ethyl acetate and petroleum ether to afford a light yellow crystalline solid (12.2 g) in 95% yield. M.P.: 65-72 °C. IR (KBr pellets, cm^{-1}): ν 3285, 3076, 3016, 2930, 2855, 2779, 2359, 1651, 1531, 1470, 1402, 1389, 1182, 1059, 777, 746. ^{1}H NMR (500 MHz, $CDCl_3$, ppm, 298 K): δ 10.01 (s, 1H, -*CHO*), 8.30 (d, J = 10.0 Hz, 1H, 4-indole-*H*), 7.82 (s, 1H, indole-NC*H*), 7.38-7.28 (m, 3H, Ph-*H*), 4.26 (t, J = 5.0 Hz, 2H), 2.74 (t, J = 5.0 Hz, 2H), 2.44 (t, J = 5.0 Hz, 4H), 1.58 (quint, J = 5.0 Hz, 4H), 1.45 (m, 2H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, ppm, 298 K): δ 185.0 (-*C*HO), 138.6, 137.7, 125.7, 124.3, 123.3, 122.6, 118.5, 110.3, 58.4, 55.2, 45.2, 26.3, 24.5. HR-MS(ESI) *m/z* calcd. for $C_{16}H_{21}N_2O(M+H^+)$: 257.1648, found: 257.1646.



S2

Scheme S3. Synthesis of **S2**.

Synthesis of [1-(2-$C_5H_{10}NCH_2CH_2$)-3-($C_{10}H_{15}N$=CH)-C_8H_5N] (HL^2). To a 500 mL flask was added 2,6-diisopropylphenylaniline (8.51 g, 9.1 mL, 48 mmol), **S2** (10.2 g, 40 mmol), 100 mL EtOH and catalytic amount of $TsOH·H_2O$. Then the mixture was reflux for three days. After the reaction was completed and cooled to room temperature, the solvent was removed by rotary evaporation and a large amount of petroleum ether was added to continuously precipitate white powder. After filtration, the desired product HL^2 was obtained (14.0 g) in 90% yield. M.P.: 62-65 °C. IR (KBr pellets, cm^{-1}): ν 3128, 3072, 2976, 2892, 2845, 2402, 1645, 1605, 1589, 1552, 1486, 1467, 1402, 1387, 1235, 1088, 872, 768, 752. ^{1}H NMR (400 MHz, $CDCl_3$, ppm, 298 K): δ 8.52 (s, 1H, -C*H*=N-), 8.36 (d, J = 8.0 Hz, 2H, 4-indole-*H*), 7.47 (s, indole-NC*H*, 1H), 7.35-7.18 (m, 3H), 4.24 (t, J = 8.0 Hz, 2H), 2.70 (t, J = 6.0 Hz, 2H), 2.45 (s, 4H), 2.17 (s, 3H), 1.84 (d, J = 8.0 Hz, 6H), 1.76-1.69 (m, 6H), 1.59 (quint, J = 4.0 Hz, 4H), 1.47-1.43 (m, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm, 298 K): δ 148.9, 137.0, 130.8, 126.5, 122.5, 121.8, 120. 8, 115.2, 109. 3, 58.6, 56.9, 54.9, 44.4, 43.5, 36.8, 29.8, 26.0, 24.2. HR-MS(ESI) *m/z* calcd. for $C_{26}H_{26}N_3(M+H^+)$: 390.2909, found: 390.2900.



HL^2

Scheme S4. Synthesis of HL^2.

Preparation of (κ^2-L^1)Lu(CH_2SiMe_3)$_2$(THF)$_2$ (1a).[10] To a mixture of H**L**^{1} (207 mg, 0.5 mmol) and Lu(CH_2SiMe_3)$_3$(THF)$_2$ (0.5 mmol, 310 mg) was added 3 mL tetrahydrofuran, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (10 mL) and THF (0.2 mL). Light yellow crystals were obtained at 0 °C by standing the extraction for several days (295 mg, 85%). M.P. (sealed): 126 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3060(w), 3042(m), 2963(s), 2892(s), 2816(m), 2326(w), 1608(s), 1582(m), 1560(m), 1510(m), 1420(m), 1425(m), 1380(m), 1326(m), 1143(m), 1020(m), 886(s), 753(s), 743(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.54 (s, 1H, -C*H*=N-), 7.54-7.52 (m, 1H), 7.33-7.31 (m, 1H), 7.20-7.19 (m, 2H), 7.11-7.10 (m, 3H), 4.36 (br, 2H, -CH_2-), 3.59-3.56 (m, 8H, THF), 3.40-3.37 (m, 2H, -C*H*(CH_3)$_2$), 3.02-3.00 (m, 2H, -CH_2-), 2.65 (br, 4H, -CH_2-), 1.41 (br, 4H, -CH_2-), 1.31-1.30 (m, 8H, -CH(CH_3)$_2$ & -CH_2-), 1.29-1.28 (m, 8H, THF), 1.10-1.09 (m, 6H, -CH(CH_3)$_2$), 0.27 (s, 18H, -Si(CH_3)$_3$), -0.33 (s, 4H, -CH_2Si(CH_3)$_3$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 214.2 (s, 2-indolyl-C_{sp2}), 169.2 (imine *C*), 156.2, 148.4, 142.3, 141.6, 138.4, 129.8, 126.3, 123.9, 123.3, 121.9, 121.7, 116.9, 111.2, 68.9, 58.3, 54.9, 53.3, 48.5, 47.7, 44.5, 28.9, 28.6, 28.4, 26.0, 25.4, 24.4, 23.8, 22.8, 4.6 (s, -Si(*C*H_3)$_3$). Anal. Calcd for $C_{44}H_{74}LuN_3O_2Si_2$: C, 58.19; H, 8.21; N, 4.63. Found: C, 58.23; H, 8.46; N, 4.50.

Preparation of (κ^2-L^1)Yb(CH_2SiMe_3)$_2$(THF)$_2$ (1b).[10] A similar procedure to that for the preparation of complex **1a** was used. Red crystals were obtained at 0 °C by standing the extraction for several days (235 mg, 78%). M.P. (sealed): 123 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3065(w), 3047(m), 2953(s), 2915(s), 2834(m), 2330(w), 1605(s), 1574(m), 1566(m), 1506(m), 1433(m), 1425(m), 1388(m), 1345(m), 1159(m), 1022(m), 846(s), 776(s), 737(s). Anal. Calcd for $C_{44}H_{74}YbN_3O_2Si_2$: C, 58.31; H, 8.23; N, 4.64. Found: C, 58.23; H, 8.43; N, 4.37.

Preparation of (κ^2-L^1)Er(CH_2SiMe_3)$_2$(THF)$_2$ (1c).[10] A similar procedure to that for the preparation of complex **1a** was used. Light yellow crystals were obtained at 0 °C by standing the extraction for several days (324 mg, 79%). M.P. (sealed): 128 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3062(w), 3045(m), 2946(s), 2933(s), 2845(m), 2350(w), 1621(s), 1553(m), 1545(m), 1521(m), 1455(m), 1432(m), 1385(m), 1342(m), 1152(m), 1028(m), 850(s), 763(s), 741(s). Anal. Calcd for $C_{44}H_{74}ErN_3O_2Si_2$: C, 58.69; H, 8.28; N, 4.67. Found: C, 58.88; H, 8.52; N, 4.46.

Preparation of (κ^2-L^1)Y(CH_2SiMe_3)$_2$(THF)$_2$ (1d).[10] A similar procedure to that for the preparation of complex **1a** was used. Light yellow crystals were obtained at 0 °C by standing the extraction for several days (205 mg, 76%). M.P. (sealed): 132 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3071(w), 3055(m), 2956(s), 2932(s), 2846(m), 2342(w), 1606(s), 1565(m), 1540(m), 1514(m), 1462(m), 1431(m), 1375(m), 1346(m), 1145(m), 1018(m), 834(s), 756(s), 738(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.51(s, 1H, -C*H*=N-), 7.55-7.53 (m, 1H), 7.33-7.31 (m, 1H), 7.20-7.18 (m, 2H), 7.13-7.11 (m, 3H), 4.36 (br, 2H, -CH_2-), 3.61-3.59 (m, 8H, THF), 3.39-3.34 (m, 2H, -C*H*(CH_3)$_2$), 2.99-2.96 (m, 2H, -CH_2-), 2.65-2.63 (m, 4H, -CH_2-), 1.48-1.43 (m, 4H, -CH_2-), 1.32-1.31 (m, 8H, -CH(CH_3)$_2$ & -CH_2-), 1.30-1.27 (m, 8H, THF), 1.12-1.11 (m, 6H, -CH(CH_3)$_2$), 0.28 (s, 18H, -Si(CH_3)$_3$), -0.20 (d, $J_{Y\text{-}C}$ = 5.0 Hz, 4H, -CH_2Si(CH_3)$_3$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 204.1 (d, $J_{Y\text{-}C}$ = 43.8 Hz, 2-indolyl-C_{sp2}), 168.7 (imine *C*), 148.5, 142.1, 141.1, 130.2, 129.3, 126.1, 125.7, 123.9, 123.1, 121.7, 121.6, 116.8, 110.9, 69.0, 59.1, 58.3, 56.6, 55.1, 54.9, 53.6, 47.7, 40.8 (d, $J_{Y\text{-}C}$ = 36.3 Hz, -*C*H$_2$Si(CH_3)$_3$), 28.8, 26.4, 26.3, 25.9, 25.5, 24.5, 23.8, 22.9, 21.4, 20.9, 4.5 (s, -Si(*C*H_3)$_3$). ^{89}Y NMR (24.5 MHz, C_6D_6, ppm, 298 K): δ 1101.5. Anal. Calcd for $C_{44}H_{74}YN_3O_2Si_2$: C, 64.28; H, 9.07; N, 5.11. Found: C, 64.57; H, 9.13; N, 4.87.

Preparation of (κ^2-L^1)Dy(CH_2SiMe_3)$_2$(THF)$_2$ (1e).[10] A similar procedure to that for the preparation of complex **1a** was used. Yellow crystals were obtained at 0 °C by standing the

extraction for several days (291 mg, 80%). M.P. (sealed): 139 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3089(w), 3067(m), 2972(s), 2952(s), 2861(m), 2353(w), 1642(s), 1577(m), 1562(m), 1532(m), 1472(m), 1455(m), 1378(m), 1352(m), 1149(m), 1034(m), 854(s), 761(s), 749(s). Anal. Calcd for $C_{44}H_{74}DyN_3O_2Si_2$: C, 59.00; H, 8.33; N, 4.69. Found: C, 59.24; H, 8.10; N, 4.32.

Preparation of (κ^2-L^1)$_2$LuCH$_2$SiMe$_3$ (2a). To a mixture of H**L^1** (0.6 mmol, 249 mg) and $Lu(CH_2SiMe_3)_3(THF)_2$ (0.3 mmol, 182 mg) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (10 mL) and THF (0.2 mL). Light yellow crystals were obtained at 0 ℃ by standing the extraction for several days (213 mg, 65%). M.P. (sealed): 135 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3060(w), 2958(s), 2935(s), 2863(m), 2804(w), 2379(w), 2352(w), 2316(w), 1629(s), 1539(m), 1464(s), 1438(s), 1390(s), 1358(m), 1326(w), 1248(m), 1165(s), 1125(m), 1105(m), 1041(m), 932(w), 858(s), 788(m), 746(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.38 (s, 2H, -C*H*=N-), 7.29-7.27 (m, 2H), 7.13-7.10 (m, 4H), 6.99-6.95 (m, 6H), 6.74-6.73 (m, 2H), 3.64-3.58 (m, 2H, -CH_2-), 3.52-3.46 (m, 2H, -CH_2-), 2.90-2.85 (m, 2H, -CH(CH$_3$)$_2$), 2.70-2.64 (m, 2H, -CH(CH$_3$)$_2$), 2.42 (t, J = 7.5 Hz, 4H, -CH_2-), 2.09 (br, 8H, -CH_2-), 1.51 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), 1.39-1.35 (m, 8H, -CH_2-), 1.17-1.15 (m, 4H, -CH_2-), 1.09 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), 0.81 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), 0.12 (s, 9H, -Si(CH_3)$_3$), 0.11 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), -0.08 (q, J = 15.0 Hz, 2H, -CH_2Si(CH$_3$)$_3$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 216.6 (s, 2-indolyl-C_{sp2}), 169.3 (imine *C*), 147.3, 143.1, 141.8, 130.3, 129.4, 128.6, 126.6, 124.3, 123.6, 123.3, 122.0, 121.8, 116.5, 111.5, 58.9, 56.1, 55.2, 48.1, 30.7, 29.0, 26.4, 26.0, 25.6, 24.9, 24.0, 20.9, 4.5 (s, -Si(*C*H$_3$)$_3$). Anal. Calcd for $C_{60}H_{83}LuN_6Si$: C, 66.03; H, 7.67; N, 7.70. Found: C, 65.77; H, 7.89; N, 7.72.

Preparation of (κ^2-L^1)$_2$YbCH$_2$SiMe$_3$ (2b). A similar procedure to that for the preparation of complex **2a** was used. Red crystals were obtained at 0 °C by standing the extraction for several days (203 mg, 62%). M.P. (sealed): 132 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3060(w), 2957(s), 2932(s), 2860(m), 2814(w), 2372(w), 2349(w), 2316(w), 1628(s), 1536(m), 1462(s), 1435(s), 1390(s), 1356(m), 1327(w), 1248(m), 1166(s), 1128(m), 1106(m), 1042(m), 932(w), 859(s), 789(m), 745(s). Anal. Calcd for $C_{60}H_{83}YbN_6Si$: C, 66.15; H, 7.68; N, 7.71. Found: C, 66.38; H, 7.98; N, 7.68.

Preparation of (κ^2-L^1)$_2$ErCH$_2$SiMe$_3$(THF) (2c). A similar procedure to that for the preparation of complex **2a** was used. Yellow crystals were obtained at 0 °C by standing the extraction for several days (250 mg, 72%). M.P. (sealed): 134 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3061(w), 2958(s), 2934(s), 2858(m), 2804(w), 2371(w), 2349(w), 2315(w), 1626(s), 1535(m), 1461(s), 1435(s), 1390(s), 1355(m), 1324(w), 1246(m), 1165(s), 1129(m), 1106(m), 1041(m), 932(w), 856(s), 785(m), 745(s). Anal. Calcd for $C_{64}H_{91}ErN_6OSi$: C, 66.51; H, 7.94; N, 7.27. Found: C, 66.14; H, 8.13; N, 6.95.

Preparation of (κ^2-L^1)$_2$YCH$_2$SiMe$_3$(THF) (2d). A similar procedure to that for the preparation of complex **2a** was used. Yellow crystals were obtained at 0 °C by standing the extraction for several days (181 mg, 56%). M.P. (sealed): 132 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3060(w), 2956(s), 2935(s), 2856(m), 2803(w), 2370(w), 2349(w), 2314(w), 1626(s), 1534(m), 1460(s), 1438(s), 1390(s), 1356(m), 1322(w), 1245(m), 1166(s), 1127(m), 1106(m), 1042(m), 934(w), 858(s), 788(m), 746(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.51 (s, 2H, -C*H*=N-), 7.45-7.43 (m, 2H), 7.29-7.26 (m, 4H), 7.16-7.11 (m, 6H), 6.91-6.90 (m, 2H), 3.77-3.69 (m, 4H, -CH_2-), 3.64 (br, 4H, THF), 3.07-3.01 (m, 2H, -CH(CH$_3$)$_2$), 2.82-2.77 (m, 2H, -CH(CH$_3$)$_2$), 2.59 (t, J = 7.5 Hz, 4H, -CH_2-), 2.26 (br, 8H, -CH_2-), 1.66 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), 1.55-1.51 (m, 8H, -CH_2-), 1.42 (br, 4H, THF), 1.34-1.31 (m, 4H, -CH_2-), 1.26 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), 0.96 (d, J = 5.0 Hz,

6H, -CH(CH_3)$_2$), 0.29 (s, 9H, -Si(CH_3)$_3$), 0.27 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), -0.53 (br, 1H, -CH_2Si(CH$_3$)$_3$), -0.75 (br, 1H, -CH_2Si(CH$_3$)$_3$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 205.8 (d, $J_{Y\text{-}C}$ = 50.0 Hz, 2-indolyl-C_{sp2}), 168.7 (imine *C*), 147.1, 143.0, 142.6, 141.2, 130.5, 128.3, 126.4, 124.2, 123.7, 123.1, 121.7, 116.4, 111.2, 68.9, 59.1, 55.1, 50.7 (d, $J_{Y\text{-}C}$ = 37.5 Hz, -*C*H$_2$Si(CH$_3$)$_3$), 48.3, 30.6, 29.1, 27.0, 26.4, 26.0, 25.8, 25.5, 24.8, 24.1, 21.0, 4.3 (s, -Si(*C*H$_3$)$_3$). Anal. Calcd for $C_{64}H_{91}YN_6OSi$: C, 71.34; H, 8.51; N, 7.80. Found: C, 71.44; H, 8.13; N, 7.55.

Preparation of (κ^2-L^1)$_2$DyCH$_2$SiMe$_3$(THF) (2e). A similar procedure to that for the preparation of complex **2a** was used. Yellow crystals were obtained at 0 °C by standing the extraction for several days (235 mg, 68%). M.P. (sealed): 136 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3060(w), 2958(s), 2932(s), 2858(m), 2804(w), 2370(w), 2348(w), 2314(w), 1625(s), 1532(m), 1460(s), 1432(s), 1389(s), 1356(m), 1325(w), 1246(m), 1165(s), 1128(m), 1105(m), 1042(m), 935(w), 857(s), 785(m), 746(s). Anal. Calcd for $C_{64}H_{91}DyN_6OSi$: C, 66.78; H, 7.97; N, 7.30. Found: C, 66.99; H, 7.60; N, 7.47.

Preparation of (κ^2-L^2)$_2$YbCH$_2$SiMe$_3$(THF) (3a). To a mixture of H**L^2** (0.6 mmol, 233 mg) and Yb(CH$_2$SiMe$_3$)$_3$(THF)$_2$ (0.3 mmol, 183 mg) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (10 mL) and THF (0.2 mL). Red crystals were obtained at room temperature by standing the extraction for several days (226 mg, 68%). M.P. (sealed): 126 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3051(m), 2905(s), 2847(m), 2808(m), 2674(w), 2314(w), 1635(s), 1573(m), 1537(s), 1463(s), 1388(s), 1346(s), 1307(m), 1247(w), 1176(s), 1124(s), 1095(w), 1036(m), 1005(w), 922(w), 861(s), 811(m), 744(s). Anal. Calcd for $C_{60}H_{87}YbN_6OSi$: C, 64.95; H, 7.90; N, 7.57. Found: C, 64.90; H, 7.62; N, 7.91.

Preparation of (κ^2-L^2)$_2$ErCH$_2$SiMe$_3$(THF) (3b). A similar procedure to that for the preparation of complex **3a** was used. Yellow crystals were obtained at room temperature by standing the extraction for several days (238 mg, 72%). M.P. (sealed): 128 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3050(m), 2906(s), 2845(m), 2807(m), 2672(w), 2314(w), 1636(s), 1572(m), 1537(s), 1463(s), 1389(s), 1345(s), 1306(m), 1246(w), 1175(s), 1126(s), 1098(w), 1035(m), 1003(w), 925(w), 862(s), 810(m), 744(s). Anal. Calcd for $C_{60}H_{87}ErN_6OSi$: C, 65.29; H, 7.95; N, 7.61. Found: C, 65.40; H, 7.63; N, 7.36.

Preparation of (κ^2-L^2)$_2$YCH$_2$SiMe$_3$(THF) (3c). A similar procedure to that for the preparation of complex **3a** was used. Yellow crystals were obtained at room temperature by standing the extraction for several days (178 mg, 58%). M.P. (sealed): 125 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3052(m), 2903(s), 2845(m), 2808(m), 2673(w), 2314(w), 1635(s), 1573(m), 1537(s), 1462(s), 1387(s), 1345(s), 1307(m), 1245(w), 1177(s), 1123(s), 1096(w), 1036(m), 1005(w), 923(w), 862(s), 811(m), 745(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.89 (s, 2H, -C*H*=N-), 7.81 (d, J = 10.0 Hz, 2H, Ph-*H*), 7.41 (br, 2H), 7.29-7.26 (m, 2H), 7.23-7.22 (m, 2H), 4.89 (br, 1H, -CH_2-), 4.52 (br, 1H, -CH_2-), 4.06 (br, 2H, -CH_2-), 3.72 (br, 4H, THF), 2.96 (br, 4H, -CH_2-), 2.44 (br, 8H, -CH_2-), 1.96 (br, 6H), 1.93(br, 12H), 1.42 (br, 4H, THF), 1.39 (br, 12H), 1.29-1.24 (m, 8H, -CH_2-), 1.3-1.22 (m, 4H, -CH_2-), 0.18 (s, 9H, -Si(CH_3)$_3$), -0.11 (br, 2H, -CH_2Si(CH$_3$)$_3$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 205.2 (d, $J_{Y\text{-}C}$ = 50.0 Hz, 2-indolyl-C_{sp2}), 160.2 (imine *C*), 140.8, 130.8, 123.4, 120.6, 120.5, 116.5, 110.3, 70.6, 58.0, 55.1 (d, $J_{Y\text{-}C}$ = 37.5 Hz, -*C*H$_2$Si(CH$_3$)$_3$), 48.1, 44.1, 36.4, 30.1, 26.4, 25.3, 24.7, 4.7 (s, -Si(*C*H$_3$)$_3$). ^{89}Y NMR (24.5 MHz, C_6D_6, ppm, 298 K): δ 773.0. Anal. Calcd for $C_{60}H_{87}YN_6OSi$: C, 70.28; H, 8.55; N, 8.20. Found: C, 70.37; H, 8.34; N, 8.02.

Preparation of (κ^2-L^2)$_2$DyCH$_2$SiMe$_3$(THF) (3d). A similar procedure to that for the preparation of complex **3a** was used. Yellow crystals were obtained at room temperature by standing the

extraction for several days (204 mg, 62%). M.P. (sealed): 128 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3051(m), 2906(s), 2847(m), 2808(m), 2674(w), 2314(w), 1635(s), 1573(m), 1537(s), 1463(s), 1386(s), 1346(s), 1305(m), 1247(w), 1176(s), 1124(s), 1095(w), 1038(m), 1002(w), 925(w), 863(s), 811(m), 746(s). Anal. Calcd for $C_{60}H_{87}DyN_6OSi$: C, 65.58; H, 7.98; N, 7.65. Found: C, 65.81; H, 7.75; N, 7.56.

Preparation of (κ^2-L^2)$_2$GdCH$_2$SiMe$_3$(THF) (3e). A similar procedure to that for the preparation of complex **3a** was used. Yellow crystals were obtained at room temperature by standing the extraction for several days (167 mg, 51%). M.P. (sealed): 129 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3049(m), 2905(s), 2846(m), 2809(m), 2674(w), 2314(w), 1635(s), 1573(m), 1537(s), 1462(s), 1388(s), 1346(s), 1307(m), 1247(w), 1175(s), 1125(s), 1093(w), 1035(m), 1006(w), 923(w), 861(s), 812(m), 743(s). Anal. Calcd for $C_{60}H_{87}GdN_6OSi$: C, 65.89; H, 8.02; N, 7.68. Found: C, 65.71; H, 7.72; N, 7.69.

Preparation of 4a. To a mixture of **1a** (0.15 mmol, 136 mg) and 2-*N*,*N*-dimethylaminopyridine (0.15 mmol, 18 μL) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (6 mL) and THF (0.2 mL). Yellow crystals were obtained at room temperature by standing the extraction for several days (73 mg, 62%). M.P. (sealed): 179 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3051(m), 2907(s), 2848(m), 2809(w), 2675(w), 2379(w), 2312(w), 1925(w), 1633(s), 1592(s), 1570(m), 1538(m), 1498(m), 1461(s), 1445(w), 1379(w), 1355(m), 1308(m), 1251(m), 1180(m), 1123(m), 1097(w), 1062(m), 1039(w), 986(m), 922(m), 861(m), 799(m), 741(s). ^{1}H NMR (500 MHz, THF-d_8, ppm, 298 K): δ 8.31 (s, 2H, -C*H*=N-), 7.29-7.27 (m, 2H, Ph-*H*), 7.25-7.24 (m, 2H, Ph-*H*), 7.03-7.00 (m, 4H, Ph-*H*), 6.95-6.87 (m, 8H, Ph-*H*), 6.48-6.46 (m, 2H, Ph-*H*), 5.68 (d, *J* = 5.0 Hz, 2H, Py-*H*), 5.58 (t, *J* = 10.0 Hz, 2H, Py-*H*), 3.87-3.83 (m, 4H, -CH_2-), 3.62-3.60 (m, 8H, THF), 3.31-3.25 (m, 4H, -CH(CH_3)$_2$), 2.34-2.30 (m, 8H, -CH_2-), 2.15-2.10 (m, 4H, -CH_2-), 1.98 (s, 6H, -NCH_3), 1.78-1.76 (m, 8H, THF), 1.61-1.58 (m, 8H, -CH_2-), 1.49 (d, *J* = 5.0 Hz, 12H, -CH(CH_3)$_2$), 1.45-1.43 (m, 4H, -CH_2-), 1.16-1.15 (m, 2H, -C*H*-Lu), 0.84 (d, *J* = 5.0 Hz, 12H, -CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (125 MHz, THF-d_8, ppm, 298 K): δ 171.9 (imine *C*), 161.4, 160.4, 149.9, 144.3, 142.6, 141.3, 139.5, 138.0, 129.8, 125.0, 124.3, 122.3, 120.5, 119.9, 113.8, 108.6, 105.8, 103.7, 100.1, 67.6, 67.3, 55.9, 55.0, 40.4, 32.4, 29.5, 28.3, 26.4, 26.2, 25.8, 25.2, 25.0, 24.9, 24.7, 24.5, 24.4, 24.0. Anal. Calcd for $C_{78}H_{104}Lu_2N_{10}O_2$: C, 59.91; H, 6.70; N, 8.96. Found: C, 59.73; H, 6.44; N, 8.85.

Preparation of 4b. A similar procedure to that for the preparation of complex **4a** was used. Yellow crystals were obtained at room temperature by standing the extraction for several days (80 mg, 68%). M.P. (sealed): 182 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3050(m), 2908(s), 2848(m), 2809(w), 2675(w), 2378(w), 2312(w), 1926(w), 1632(s), 1592(s), 1570(m), 1538(m), 1497(m), 1461(s), 1446(w), 1379(w), 1355(m), 1308(m), 1251(m), 1180(m), 1125(m), 1098(w), 1062(m), 1039(w), 985(m), 921(m), 861(m), 798(m), 740(s). Anal. Calcd for $C_{78}H_{104}Yb_2N_{10}O_2$: C, 60.06; H, 6.72; N, 8.98. Found: C, 60.32; H, 6.71; N, 9.01.

Preparation of 4c. A similar procedure to that for the preparation of complex **4a** was used. Yellow crystals were obtained at room temperature by standing the extraction for several days (77 mg, 66%). M.P. (sealed): 185 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3051(m), 2908(s), 2848(m), 2808(w), 2674(w), 2379(w), 2310(w), 1924(w), 1633(s), 1592(s), 1571(m), 1539(m), 1498(m), 1462(s), 1445(w), 1378(w), 1355(m), 1308(m), 1250(m), 1180(m), 1123(m), 1097(w), 1062(m), 1039(w), 988(m), 921(m), 860(m), 798(m), 742(s). Anal. Calcd for $C_{78}H_{104}Er_2N_{10}O_2$: C, 60.51; H, 6.77; N, 9.05. Found: C, 60.37; H, 6.61; N, 8.87.

Preparation of 4d. A similar procedure to that for the preparation of complex **4a** was used. Yellow

crystals were obtained at room temperature by standing the extraction for several days (74 mg, 71%). M.P. (sealed): 178 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3050(m), 2906(s), 2848(m), 2810(w), 2675(w), 2379(w), 2310(w), 1925(w), 1632(s), 1592(s), 1571(m), 1537(m), 1498(m), 1460(s), 1445(w), 1379(w), 1355(m), 1308(m), 1251(m), 1180(m), 1123(m), 1097(w), 1062(m), 1039(w), 986(m), 923(m), 862(m), 798(m), 740(s). ^{1}H NMR (500 MHz, THF-d_8, ppm, 298 K): δ 8.49 (s, 2H, -C*H*=N-), 8.48 (br, 2H), 7.44-7.42 (m, 2H), 7.23-7.12 (m, 14H), 7.02-6.99 (m, 4H), 4.34-4.31 (m, 4H, -CH_2-), 3.67-3.65 (m, 8H, THF), 3.22-3.16 (m, 4H, -C*H*(CH_3)$_2$), 2.70 (s, 6H, -NCH_3), 2.69-2.66 (m, 4H, -CH_2-), 2.50 (br, 8H, -CH_2-), 1.83-1.80 (m, 8H, THF), 1.63-1.58 (m, 8H, -CH_2-), 1.48-1.47 (m, 4H, -CH_2-), 1.36 (br, 2H, -C*H*-), 1.20 (d, J = 10.0 Hz, 24H, -CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (125 MHz, THF-d_8, ppm, 298 K): δ 156.4 (imine *C*), 152.1, 142.7, 138.1, 137.1, 126.9, 123.1, 122.7, 122.1, 122.0, 121.2, 111.3, 109.1, 67.3, 58.4, 55.4, 41.7, 28.1, 26.5, 25.8, 25.2 (d, $J_{Y\text{-}C}$ = 25.0 Hz, -*C*H-), 23.3, 9.7 (N*C*H$_3$). ^{89}Y NMR (24.5 MHz, THF-d_8, ppm, 298 K): δ 880.7. Anal. Calcd for $C_{78}H_{104}Y_2N_{10}O_2$: C, 67.32; H, 7.53; N, 10.07. Found: C, 67.14; H, 7.67; N, 10.18.

Preparation of 5a. To a mixture of **2a** (0.15 mmol, 163 mg) and 2-*N*,*N*-dimethylaminopyridine (0.3 mmol, 36 μL) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (6 mL) and THF (0.2 mL). Black crystals were obtained at room temperature by standing the extraction for several days (106 mg, 62%). M.P. (sealed): 172 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3054(m), 2956(m), 2936(w), 2863(m), 2806(m), 2771(m), 2693(w), 2379(w), 2312(w), 1856(w), 1785(w), 1624(s), 1533(m), 1463(s), 1444(m), 1391(s), 1354(m), 1327(m), 1243(m), 1163(s), 1127(m), 1102(m), 1041(m), 1007(w), 954(w), 931(w), 912(w), 854(s), 769(m), 744(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.45 (s, 2H, -C*H*=N-), 7.33 (d, J = 5.0 Hz, 2H, Py-*H*), 7.27-7.26 (m, 2H, Ph-*H*), 7.14-7.11 (m, 2H, Ph-*H*), 7.06-6.97 (m, 8H, Ph-*H*), 6.76-6.73 (m, 1H, Ph-*H*), 6.62-6.60 (m, 1H, Ph-*H*), 5.63 (d, J = 10.0 Hz, 1H, Py-*H*), 5.59 (t, J = 7.5 Hz, 1H, Py-*H*), 4.06-4.02 (m, 2H, -CH_2-), 3.59-3.56 (m, 2H, -CH_2-), 3.49-3.43 (m, 4H, -C*H*(CH_3)$_2$), 2.96 (br, 4H, -CH_2-), 2.23-2.22 (m, 11H, -CH_2- & -NCH_3), 1.57 (d, J = 10.0 Hz, 6H, -CH(CH_3)$_2$), 1.55-1.52 (m, 8H, -CH_2-), 1.49 (d, J = 10.0 Hz, 6H, -CH(CH_3)$_2$), 1.33-1.29 (m, 4H, -CH_2-), 1.29-1.28 (m, 2H, -CH_2-Lu), 1.09-1.08 (m, 2H, -CH_2-Lu), 1.06 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), 1.01 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 171.0 (imine *C*), 161.7, 160.3, 150.1, 144.4, 142.8, 139.7, 138.3, 130.0, 125.3, 124.6, 122.7, 120.9, 120.3, 114.1, 109.0, 106.1, 103.9, 100.3, 56.0, 55.1, 40.6, 33.0, 29.8, 28.5, 26.6, 26.5, 25.3, 24.8, 24.5. Anal. Calcd for $C_{64}H_{83}LuN_8$: C, 67.47; H, 7.34; N, 9.83. Found: C, 67.77; H, 7.68; N, 9.79.

Preparation of 5b. A similar procedure to that for the preparation of complex **5a** was used. Black crystals were obtained at room temperature by standing the extraction for several days (107 mg, 63%). M.P. (sealed): 175 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3055(m), 2956(m), 2935(w), 2862(m), 2806(m), 2770(m), 2693(w), 2379(w), 2313(w), 1856(w), 1785(w), 1625(s), 1534(m), 1463(s), 1445(m), 1390(s), 1354(m), 1327(m), 1242(m), 1163(s), 1127(m), 1102(m), 1042(m), 1007(w), 954(w), 930(w), 912(w), 855(s), 769(m), 743(s). Anal. Calcd for $C_{64}H_{83}YbN_8$: C, 67.58; H, 7.36; N, 9.85. Found: C, 67.90; H, 7.68; N, 9.91.

Preparation of 5c. A similar procedure to that for the preparation of complex **5a** was used. Black crystals were obtained at room temperature by standing the extraction for several days (110 mg, 65%). M.P. (sealed): 176 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3054(m), 2955(m), 2935(w), 2863(m), 2806(m), 2770(m), 2693(w), 2378(w), 2312(w), 1857(w), 1785(w), 1624(s), 1533(m), 1462(s), 1444(m), 1391(s), 1355(m), 1327(m), 1243(m), 1165(s), 1128(m), 1102(m), 1041(m), 1008(w), 954(w), 931(w), 913(w), 854(s), 769(m), 744(s). Anal. Calcd for $C_{64}H_{83}ErN_8$: C, 67.93;

H, 7.39; N, 9.90. Found: C, 68.00; H, 7.40; N, 9.89.

Preparation of 5d. A similar procedure to that for the preparation of complex **5a** was used. Black crystals were obtained at room temperature by standing the extraction for several days (109 mg, 69%). M.P. (sealed): 177 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3056(m), 2956(m), 2936(w), 2863(m), 2807(m), 2771(m), 2694(w), 2379(w), 2312(w), 1856(w), 1785(w), 1624(s), 1534(m), 1463(s), 1444(m), 1390(s), 1354(m), 1328(m), 1248(m), 1163(s), 1126(m), 1101(m), 1040(m), 1008(w), 954(w), 930(w), 912(w), 854(s), 769(m), 743(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.43 (s, 2H, -C*H*=N-), 7.30 (d, *J* = 10.0 Hz, 2H, Py-*H*), 7.27-7.20 (m, 2H, Ph-*H*), 7.13-7.12 (m, 2H, Ph-*H*), 7.05-6.93 (m, 8H, Ph-*H*), 6.77-6.73 (m, 1H, Ph-*H*), 6.57-6.56 (m, 1H, Ph-*H*), 5.66 (d, *J* = 10.0 Hz, 1H, Py-*H*), 5.57 (t, *J* = 7.5 Hz, 1H, Py-*H*), 3.99 (br, 2H, -CH_2-), 3.60-3.57 (m, 6H, -CH_2- & -C*H*$(CH_3)_2$), 3.00-2.96 (m, 4H, -CH_2-), 2.27-2.16 (m, 11H, -CH_2- & -NCH_3), 1.58-1.47 (m, 20H, -CH_2- & -CH(CH_3)$_2$), 1.33-1.30 (m, 4H, -CH_2-), 1.29-1.28 (m, 2H, -CH_2-Y), 1.23-1.21 (m, 2H, -CH_2-Y), 1.06-1.02 (m, 12H, -CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 171.4 (imine *C*), 160.0, 159.1, 149.3, 144.0, 139.4, 138.4, 129.7, 124.9, 124.6, 124.2, 122.6, 120.4, 113.6, 108.4, 105.7, 103.3, 99.1, 55.5, 55.4 (d, $J_{Y\text{-}C}$ = 25.0 Hz, -*C*H_2-), 54.8, 40.5, 32.7, 29.5, 28.3, 26.2, 24.9, 24.5, 24.2. Anal. Calcd for $C_{64}H_{83}YN_8$: C, 72.98; H, 7.94; N, 10.64. Found: C, 72.87; H, 7.98; N, 10.68.

Preparation of 6a. To a mixture of **2a** (0.15 mmol, 163 mg) and 2-*N*-methylaminopyridine (0.15 mmol, 16 μL) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (6 mL) and toluene (0.2 mL). Yellow crystals were obtained at room temperature by standing the extraction for several days (130 mg, 78%). M.P. (sealed): 169 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3053(m), 2956(w), 2934(s), 2861(m), 2799(m), 2379(w), 2308(w), 1921(w), 1854(w), 1622(s), 1541(m), 1510(m), 1463(s), 1424(s), 1379(m), 1324(m), 1238(m), 1191(m), 1157(m), 1124(m), 1057(s), 986(m), 928(s), 858(w), 836(w), 743(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.69 (s, 2H, -C*H*=N-), 7.53 (d, *J* = 5.0 Hz, 2H, Py-*H*), 7.27-7.25 (m, 2H, Ph-*H*), 7.21-7.20 (m, 2H, Ph-*H*), 7.14-7.10 (m, 8H, Ph-*H*), 6.94-6.93 (m, 2H, Ph-*H*), 5.91 (d, *J* = 10.0 Hz, 1H, Py-*H*), 5.69 (t, *J* = 7.5 Hz, 1H, Py-*H*), 3.74-3.67 (m, 4H, -CH_2-), 3.26-3.21 (m, 2H, -C*H*$(CH_3)_2$), 2.85-2.80 (m, 2H, -C*H*$(CH_3)_2$), 2.68 (s, 3H, -NCH_3), 2.40-2.34 (m, 2H, -CH_2-), 2.28-2.23 (m, 2H, -CH_2-), 2.11-2.10 (m, 8H, -CH_2-), 1.44-1.40 (m, 14H, -CH_2- & -CH(CH_3)$_2$), 1.29 (d, *J* = 5.0 Hz, 6H, -CH(CH_3)$_2$), 1.26-1.23 (m, 4H, -CH_2-), 1.09 (d, *J* = 5.0 Hz, 6H, -CH(CH_3)$_2$), 0.34 (d, *J* = 5.0 Hz, 6H, -CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 216.5 (s, 2-indolyl-C_{sp2}), 171.3 (imine *C*), 168.7, 148.6, 145.5, 143.4, 142.6, 141.6, 140.3, 130.6, 126.2, 123.7, 123.5, 122.4, 121.4, 121.1, 116.1, 110.7, 106.7, 103.7, 59.9, 55.2, 46.7, 34.3, 30.1, 28.3, 26.4, 25.8, 24.8, 23.6, 21.1. Anal. Calcd for $C_{62}H_{79}LuN_8$: C, 67.01; H, 7.17; N, 10.08. Found: C, 67.15; H, 7.46; N, 9.72.

Preparation of 6b. A similar procedure to that for the preparation of complex **6a** was used. Yellow crystals were obtained at room temperature by standing the extraction for several days (126 mg, 76%). M.P. (sealed): 172 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3052(m), 2957(w), 2934(s), 2861(m), 2799(m), 2378(w), 2308(w), 1921(w), 1855(w), 1621(s), 1541(m), 1510(m), 1463(s), 1424(s), 1378(m), 1324(m), 1238(m), 1191(m), 1156(m), 1124(m), 1057(s), 987(m), 928(s), 858(w), 836(w), 742(s). Anal. Calcd for $C_{62}H_{79}YbN_8$: C, 67.12; H, 7.18; N, 10.10. Found: C, 66.93; H, 7.46; N, 10.40.

Preparation of 6c. A similar procedure to that for the preparation of complex **6a** was used. Yellow crystals were obtained at room temperature by standing the extraction for several days (119 mg, 72%). M.P. (sealed): 175 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3054(m), 2956(w), 2934(s),

2861(m), 2799(m), 2379(w), 2308(w), 1921(w), 1854(w), 1622(s), 1541(m), 1511(m), 1462(s), 1424(s), 1378(m), 1325(m), 1238(m), 1192(m), 1157(m), 1123(m), 1057(s), 986(m), 927(s), 858(w), 835(w), 742(s). Anal. Calcd for $C_{62}H_{79}ErN_8$: C, 67.48; H, 7.22; N, 10.15. Found: C, 67.13; H, 7.57; N, 9.88.

Preparation of 6d. A similar procedure to that for the preparation of complex **6a** was used. Yellow crystals were obtained at room temperature by standing the extraction for several days (115 mg, 75%). M.P. (sealed): 170 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3053(m), 2956(w), 2934(s), 2861(m), 2799(m), 2379(w), 2308(w), 1921(w), 1854(w), 1622(s), 1541(m), 1510(m), 1462(s), 1425(s), 1378(m), 1323(m), 1238(m), 1190(m), 1158(m), 1124(m), 1058(s), 986(m), 929(s), 858(w), 836(w), 743(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.62 (s, 2H, -C*H*=N-), 7.51 (d, J = 10.0 Hz, 2H, Py-*H*), 7.26-7.23 (m, 4H, Ph-*H*), 7.14-7.09 (m, 8H, Ph-*H*), 6.97-6.95 (m, 2H, Ph-*H*), 5.94 (d, J = 10.0 Hz, 1H, Py-*H*), 5.72 (t, J = 7.5 Hz, 1H, Py-*H*), 3.75-3.58 (m, 4H, -CH_2-), 3.22-3.17 (m, 2H, -C*H*(CH_3)$_2$), 2.85-2.79 (m, 2H, -C*H*(CH_3)$_2$), 2.68 (s, 3H, -NCH_3), 2.45-2.39 (m, 2H, -CH_2-), 2.31-2.25 (m, 2H, -CH_2-), 2.13-2.09 (m, 8H, -CH_2-), 1.46-1.36 (m, 14H, -CH_2- & -CH(CH_3)$_2$), 1.28 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), 1.11 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), 0.97-0.93 (m, 4H, -CH_2-), 0.36 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 206.0 (d, $J_{Y\text{-}C}$ = 50.0 Hz, 2-indolyl-C_{sp2}), 170.7 (imine *C*), 167.1, 146.9, 144.2, 141.8, 140.9, 139.8, 138.9, 129.3, 124.7, 122.3, 120.0, 119.8, 114.8, 109.3, 105.2, 102.2, 58.4, 53.7, 45.7, 32.9, 28.7, 27.2, 25.0, 24.9, 24.1, 23.4, 22.3, 19.8. Anal. Calcd for $C_{62}H_{79}YN_8$: C, 72.63; H, 7.77; N, 10.93. Found: C, 72.66; H, 8.05; N, 10.88.

Preparation of 7a. To a mixture of **3b** (0.15 mmol, 173 mg) and 2-*N*,*N*-dimethylaminopyridine (0.15 mmol, 18 μL) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (6 mL) and THF (0.2 mL). Black crystals were obtained at room temperature by standing the extraction for several days (106 mg, 62%). M.P. (sealed): 179 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3049(m), 2937(s), 2860(m), 2796(m), 2766(w), 2379(w), 2310(w), 1921(w), 1620(s), 1518(m), 1462(m), 1426(s), 1378(m), 1328(m), 1293(m), 1260(m), 1237(m), 1191(m), 1156(m), 1122(m), 1058(s), 987(w), 928(m), 862(m), 838(m), 739(s). Anal. Calcd for $C_{63}H_{85}ErN_8$: C, 66.51; H, 7.53; N, 9.85. Found: C, 66.85; H, 7.65; N, 10.03.

Preparation of 7b. A similar procedure to that for the preparation of complex **7a** was used. Black crystals were obtained at room temperature by standing the extraction for several days (94 mg, 59%). M.P. (sealed): 175 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3048(m), 2936(s), 2860(m), 2795(m), 2766(w), 2379(w), 2312(w), 1921(w), 1620(s), 1518(m), 1463(m), 1425(s), 1378(m), 1328(m), 1293(m), 1261(m), 1237(m), 1190(m), 1156(m), 1123(m), 1058(s), 988(w), 928(m), 863(m), 838(m), 740(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.95 (s, 1H, -C*H*=N-), 7.75 (d, J = 10.0 Hz, 1H, Py-*H*), 7.56-7.54 (m, 1H, Py-*H*), 7.42-7.41 (m, 1H, Py-*H*), 7.31-7.24 (m, 4H, Ph-*H*), 7.05-7.00 (m, 4H, Ph-*H*), 6.69 (br, 1H, -C=C*H*-NR-), 3.80 (br, 8H, THF & -CH_2-), 2.75-2.63 (m, 4H, -CH_2-), 2.32-2.26 (m, 8H, -CH_2-), 2.13-2.11 (m, 6H, Ad-*H*), 2.04 (br, 4H, -CH_2-), 1.95 (br, 6H, -N(CH_3)$_2$), 1.70-1.62 (m, 4H, -CH_2-), 1.56-1.53 (m, 12H, Ad-*H*), 1.46 (br, 4H, THF), 1.40-1.34 (m, 12H, Ad-*H*), 1.27-1.20 (m, 4H, -CH_2-). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 202.2 (d, $J_{Y\text{-}C}$ = 50.0 Hz, 2-indolyl-C_{sp2}), 164.8 (imine *C*), 160.5, 149.3, 140.3, 130.7, 122.8, 121.9, 120.6, 120.5, 119.6, 116.2, 115.3, 111.7, 110.1, 84.0, 70.4, 59.3, 57.6, 55.1, 51.0, 48.5, 44.6, 44.0, 37.1, 36.4, 30.0, 26.4, 26.1, 25.1, 24.7, 24.4. Anal. Calcd for $C_{63}H_{85}YN_8$: C, 71.43; H, 8.09; N, 10.58. Found: C, 71.08; H, 7.90; N, 10.76.

Preparation of 8a. To a mixture of **2c** (0.15 mmol, 173 mg) and 2-phenylpyridine (0.15 mmol,

22 μL) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (6 mL) and THF (0.2 mL). Black crystals were obtained at room temperature by standing the extraction for several days (122 mg, 71%). M.P. (sealed): 162 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3056(m), 2955(s), 2931(s), 2861(m), 2806(m), 2772(m), 2695(w), 2375(w), 2308(w), 1625(s), 1585(s), 1535(m), 1463(s), 1444(s), 1392(s), 1354(m), 1326(m), 1243(w), 1163(s), 1125(m), 1103(w), 1042(w), 1008(w), 956(w), 932(w), 912(s), 854(m), 790(m), 743(s). Anal. Calcd for $C_{67}H_{80}ErN_7$: C, 69.94; H, 7.01; N, 8.52. Found: C, 70.14; H, 7.32; N, 8.25.

Preparation of 8b. A similar procedure to that for the preparation of complex **8a** was used. Black crystals were obtained at room temperature by standing the extraction for several days (91 mg, 57%). M.P. (sealed): 171 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3055(m), 2957(s), 2931(s), 2863(m), 2804(m), 2772(m), 2694(w), 2376(w), 2308(w), 1626(s), 1585(s), 1535(m), 1463(s), 1444(s), 1391(s), 1354(m), 1325(m), 1242(w), 1162(s), 1125(m), 1102(w), 1042(w), 1006(w), 956(w), 932(w), 913(s), 855(m), 791(m), 743(s). ^{1}H NMR (500 MHz, THF-d_8, ppm, 298 K): δ 8.54 (s, 2H, -C*H*=N-), 7.89-7.84 (m, 2H, Py-*H*), 7.56-7.55 (m, 1H, Ph-*H*), 7.51-7.50 (m, 1H, Ph-*H*), 7.44-7.43 (m, 1H, Ph-*H*), 7.30-7.28 (m, 1H, Ph-*H*), 7.23-7.21 (m, 2H, Ph-*H*), 7.05-7.04 (m, 2H, Ph-*H*), 7.01-6.99 (m, 2H, Ph-*H*), 6.82-6.80 (m, 2H, Ph-*H*), 6.73-6.72 (m, 4H, Ph-*H*), 6.66-6.64 (m, 2H, Ph-*H*), 6.40-6.37 (m, 1H, Py-*H*), 6.33-6.32 (m, 1H, Py-*H*), 4.85-4.79 (m, 2H, -CH_2-), 4.54-4.49 (m, 2H, -CH_2-), 4.12-4.07 (m, 2H, -C*H*$(CH_3)_2$), 3.53-3.47 (m, 2H, -C*H*$(CH_3)_2$), 3.03-2.94 (m, 4H, -CH_2-), 2.82-2.74 (m, 4H, -CH_2-), 2.68-2.56 (m, 4H, -CH_2-), 1.52-1.38 (m, 8H, -CH_2-), 1.37 (d, *J* = 5.0 Hz, 3H, -CH(CH_3)$_2$), 1.27 (d, *J* = 5.0 Hz, 3H, -CH(CH_3)$_2$), 1.25 (d, *J* = 5.0 Hz, 3H, -CH(CH_3)$_2$), 1.05 (d, *J* = 5.0 Hz, 3H, -CH(CH_3)$_2$), 0.93 (d, *J* = 10.0 Hz, 3H, -CH(CH_3)$_2$), 0.59 (d, *J* = 5.0 Hz, 3H, -CH(CH_3)$_2$), 0.20 (d, *J* = 5.0 Hz, 3H, -CH(CH_3)$_2$), 0.09 (d, *J* = 5.0 Hz, 3H, -CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (125 MHz, THF-d_8, ppm, 298 K): δ 203.2 (d, $J_{Y\text{-}C}$ = 37.5 Hz, 2-indolyl-C_{sp2}), 192.0 (d, $J_{Y\text{-}C}$ = 37.5 Hz, phenyl-C_{sp2}), 170.1 (imine *C*), 162.6, 156.7, 151.4, 150.5, 149.7, 147.6, 146.8, 145.8, 142.6, 141.5, 141.4, 141.1, 140.1, 137.3, 131.9, 131.1, 129.4, 128.6, 126.5, 125.0, 124.9, 124.6, 124.5, 124.1, 123.1, 122.9, 122.7, 122.1, 120.8, 120.7, 118.8, 117.4, 116.7, 114.2, 111.4, 106.3, 103.7, 71.4, 59.6, 56.3, 55.6, 55.0, 54.8, 50.3, 43.3, 29.1, 28.5, 28.1, 26.9, 26.5, 25.6, 25.5, 23.9, 22.0, 19.7. ^{89}Y NMR (24.5 MHz, C_6D_6, ppm, 298 K): δ 501.0. Anal. Calcd for $C_{67}H_{80}YN_7$: C, 75.05; H, 7.52; N, 9.14. Found: C, 74.94; H, 7.89; N, 9.15.

Preparation of 9. A similar procedure to that for the preparation of complex **8a** was used. Black crystals were obtained at room temperature by standing the extraction for several days (124 mg, 68%). M.P. (sealed): 168 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3053(m), 2956(s), 2930(s), 2862(m), 2806(m), 2770(m), 2695(w), 2375(w), 2308(w), 1625(s), 1585(s), 1536(m), 1464(s), 1444(s), 1392(s), 1354(m), 1326(m), 1242(w), 1163(s), 1126(m), 1103(w), 1042(w), 1007(w), 956(w), 930(w), 913(s), 855(m), 789(m), 743(s). Anal. Calcd for $C_{67}H_{80}DyN_7$: C, 70.01; H, 7.28; N, 8.05. Found: C, 69.80; H, 7.41; N, 8.00.

Preparation of 10a. To a mixture of **2c** (0.15 mmol, 173 mg) and DMAP (0.3 mmol, 37 mg) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (6 mL) and THF (0.2 mL). Black crystals were obtained at room temperature by standing the extraction for several days (104 mg, 56%). M.P. (sealed): 156 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3051(w), 2906(s), 2846(m), 2808(w), 2676(w), 2380(w), 2312(w), 1635(s), 1538(m), 1461(m), 1449(m), 1386(m), 1358(m), 1307(w), 1226(w), 1177(m), 1123(m), 1095(w), 1038(w), 992(m), 921(w), 858(m), 807(m), 742(s). Anal. Calcd for $C_{70}H_{91}ErN_{10}$:

C, 67.81; H, 7.40; N, 11.30. Found: C, 68.05; H, 7.56; N, 11.20.

Preparation of 10b. A similar procedure to that for the preparation of complex **10a** was used. Black crystals were obtained at room temperature by standing the extraction for several days (85 mg, 49%). M.P. (sealed): 136 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3052(w), 2905(s), 2847(m), 2809(w), 2675(w), 2380(w), 2312(w), 1635(s), 1538(m), 1461(m), 1448(m), 1385(m), 1358(m), 1307(w), 1226(w), 1176(m), 1123(m), 1095(w), 1037(w), 991(m), 921(w), 858(m), 806(m), 742(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.84 (s, 1H, -C*H*=N-), 7.81 (br, 2H), 7.76-7.74 (m, 1H, Py-*H*), 7.65-7.63 (m, 1H, Py-*H*), 7.55-7.53 (m, 1H, Py-*H*), 7.26-7.22 (m, 4H), 7.13-7.11 (m, 2H), 7.06-7.05 (m, 2H), 7.02-6.97 (m, 4H), 6.45 (s, 1H, -C=C*H*-NR-), 5.71 (br, 1H, Py-*H*), 5.56 (br, 1H, Py-*H*), 4.69 (br, 1H, Py-*H*), 4.57 (br, 1H, Py-*H*), 3.33-3.30 (m, 2H, -CH_2-), 2.84-2.79 (m, 2H, -CH_2-), 2.70-2.63 (m, 2H, -C*H*$(CH_3)_2$), 2.55-2.48 (m, 2H, -C*H*$(CH_3)_2$), 2.41 (s, 6H, -N(CH_3)$_2$), 2.30 (br, 4H, -CH_2-), 2.11 (s, 6H, -N(CH_3)$_2$), 1.88-1.83 (m, 8H, -CH_2-), 1.64-1.58 (m, 4H, -CH_2-), 1.52-1.41 (m, 8H, -CH_2-), 1.29 (d, J = 5.0 Hz, 3H, -CH(CH_3)$_2$), 1.23 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), 1.15 (d, J = 5.0 Hz, 6H, -CH(CH_3)$_2$), 0.95 (d, J = 5.0 Hz, 3H, -CH(CH_3)$_2$), 0.66 (d, J = 5.0 Hz, 3H, -CH(CH_3)$_2$), 0.61 (d, J = 5.0 Hz, 3H, -CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 204.3 (d, $J_{Y\text{-}C}$ = 37.5 Hz, 2-indolyl-C$_{sp2}$), 167.2 (imine *C*), 159.4, 156.2, 154.7, 154.4, 151.8, 150.8, 150.5, 148.8, 148.5, 147.7, 145.2, 144.7, 143.7, 138.4, 137.9, 134.2, 129.3, 125.7, 124.0, 123.6, 123.4, 122.1, 119.1, 117.6, 116.9, 115.8, 113.8, 109.8, 108.1, 105.6, 104.9, 104.5, 102.3, 101.8, 100.8, 89.2, 71.4, 59.9, 58.3, 55.7, 55.3, 54.9, 44.5, 38.8, 38.1, 38.0, 28.6, 26.7, 26.6, 26.4, 25.5, 24.7, 24.6, 23.8, 21.4. Anal. Calcd for $C_{70}H_{91}YN_{10}$: C, 72.39; H, 7.90; N, 12.06. Found: C, 72.70; H, 8.05; N, 11.87.

Preparation of 10c. A similar procedure to that for the preparation of complex **10a** was used. Black crystals were obtained at room temperature by standing the extraction for several days (122 mg, 66%). M.P. (sealed): 159 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3051(w), 2906(s), 2846(m), 2808(w), 2676(w), 2382(w), 2310(w), 1634(s), 1538(m), 1462(m), 1448(m), 1385(m), 1357(m), 1307(w), 1226(w), 1175(m), 1123(m), 1093(w), 1038(w), 991(m), 920(w), 858(m), 808(m), 741(s). Anal. Calcd for $C_{70}H_{91}DyN_{10}$: C, 68.07; H, 7.43; N, 11.34. Found: C, 67.99; H, 7.57; N, 11.46.

Preparation of 11. To a mixture of **3d** (0.15 mmol, 164 mg) and 4-*N*,*N*-dimethylaminopyridine (DMAP) (0.3 mmol, 37 mg) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (6 mL) and THF (0.2 mL). Black crystals were obtained at room temperature by standing the extraction for several days (122 mg, 69%). M.P. (sealed): 156 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3055(m), 2957(s), 2933(s), 2863(m), 2806(m), 2126(w), 1922(w), 1626(s), 1535(m), 1463(s), 1442(s), 1386(s), 1356(m), 1260(w), 1225(s), 1164(s), 1125(m), 1104(w), 1042(m), 990(s), 950(m), 855(s), 806(s), 745(s). Anal. Calcd for $C_{66}H_{87}DyN_{10}$: C, 67.01; H, 7.41; N, 11.84. Found: C, 67.23; H, 7.75; N, 12.00.

Preparation of 12a. To a mixture of **2b** (0.15 mmol, 163 mg) and 2,2'-bipyridine (0.15 mmol, 24 mg) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (6 mL) and THF (0.2 mL). Black crystals were obtained at room temperature by standing the extraction for several days (115 mg, 66%). M.P. (sealed): 155 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3057(m), 2957(s), 2934(s), 2863(m), 2804(w), 2379(w), 2311(w), 1627(s), 1583(m), 1538(m), 1463(s), 1390(s), 1356(m), 1325(m), 1248(m), 1165(s), 1125(m), 1103(m), 1040(w), 1008(w), 931(w), 913(s), 854(m), 789(m), 746(s). Anal. Calcd for $C_{66}H_{80}YbN_8$: C, 68.43; H, 6.96; N, 9.67. Found: C, 68.61; H, 6.61; N, 9.72.

Preparation of 12b. A similar procedure to that for the preparation of complex **12a** was used. Black crystals were obtained at room temperature by standing the extraction for several days (100 mg, 58%). M.P. (sealed): 158 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3056(m), 2958(s), 2933(s), 2863(m), 2805(w), 2379(w), 2312(w), 1625(s), 1583(m), 1537(m), 1463(s), 1391(s), 1355(m), 1325(m), 1247(m), 1165(s), 1126(m), 1103(m), 1041(w), 1008(w), 930(w), 913(s), 854(m), 788(m), 745(s). Anal. Calcd for $C_{66}H_{80}ErN_8$: C, 68.77; H, 7.00; N, 9.72. Found: C, 68.65; H, 7.36; N, 9.75.

Preparation of 12c. A similar procedure to that for the preparation of complex **12a** was used. Black crystals were obtained at room temperature by standing the extraction for several days (98 mg, 61%). M.P. (sealed): 168 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3057(m), 2957(s), 2932(s), 2864(m), 2806(w), 2378(w), 2311(w), 1626(s), 1582(m), 1538(m), 1462(s), 1390(s), 1356(m), 1325(m), 1246(m), 1164(s), 1125(m), 1104(m), 1040(w), 1009(w), 931(w), 912(s), 854(m), 787(m), 744(s). ^{1}H NMR (500 MHz, THF-d_8, ppm, 298 K): δ 8.58 (br, 1H, Py-*H*), 8.45-8.44 (m, 2H, -C*H*=N-), 8.25 (s, 1H, Py-*H*), 7.79-7.76 (m, 1H, Py-*H*), 7.72 (s, 1H, Py-*H*), 7.45-7.43 (m, 1H, Ph-*H*), 7.27 (br, 1H, Ph-*H*), 7.14-7.11 (m, 4H, Ph-*H*), 7.06-7.05 (m, 4H, Ph-*H*), 6.95-6.92 (m, 4H, Ph-*H*), 6.85 (br, 1H, Py-*H*), 4.29-4.26 (m, 4H, -CH_2-), 3.14-3.08 (m, 4H, -C*H*$(CH_3)_2$-), 2.69-2.66 (m, 4H, -CH_2-), 2.42 (br, 8H, -CH_2-), 1.54-1.51 (m, 8H, -CH_2-), 1.40 (br, 4H, -CH_2-), 1.12 (d, 24H, -CH(CH_3)$_2$-). ^{13}C{^{1}H} NMR (125 MHz, THF-d_8, ppm, 298 K): δ 157.1, 156.8, 152.1, 148.8, 143.5, 140.9, 138.5, 135.7, 127.1, 126.6, 123.9, 123.5, 123.3, 123.1, 121.8, 115.7, 110.4, 108.3, 68.0, 59.2, 56.0, 55.6, 45.2, 30.5, 28.7, 27.1, 26.4, 25.8, 23.9, 21.7. Anal. Calcd for $C_{66}H_{80}YN_8$: C, 73.79; H, 7.51; N, 10.43. Found: C, 73.91; H, 7.75; N, 10.58.

Preparation of 12d. A similar procedure to that for the preparation of complex **12a** was used. Black crystals were obtained at room temperature by standing the extraction for several days (119 mg, 69%). M.P. (sealed): 162 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3057(m), 2956(s), 2932(s), 2863(m), 2804(w), 2378(w), 2311(w), 1627(s), 1582(m), 1536(m), 1462(s), 1390(s), 1356(m), 1326(m), 1248(m), 1165(s), 1125(m), 1102(m), 1040(w), 1008(w), 931(w), 913(s), 854(m), 788(m), 745(s). Anal. Calcd for $C_{66}H_{80}DyN_8$: C, 69.06; H, 7.02; N, 9.76. Found: C, 68.85; H, 7.01; N, 9.63.

Preparation of 13. To a mixture of **3b** (0.15 mmol, 173 mg) and 2,2'-bipyridine (0.15 mmol, 24 mg) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature for 2 h. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (6 mL) and THF (0.2 mL). Black crystals were obtained at room temperature by standing the extraction for several days (87 mg, 53%). M.P. (sealed): 167 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3057(m), 2958(s), 2931(s), 2863(m), 2804(w), 2380(w), 2312(w), 1642(s), 1615(s), 1556(m), 1515(m), 1490(w), 1463(w), 1438(m), 1382(w), 1354(w), 1320(m), 1273(m), 1178(m), 1121(m), 1041(w), 1030(w), 936(w), 858(s), 741(s). Anal. Calcd for $C_{62}H_{76}ErN_8$: C, 67.66; H, 6.96; N, 10.18. Found: C, 67.68; H, 7.19; N, 10.51.

Preparation of 14a. To a mixture of **12a** (0.15 mmol, 174 mg) and $Ph_2C{=}N_2$ (0.45 mmol, 87 mg) was added 3 mL toluene, the resulted mixture was allowed to be stirred at room temperature overnight. After the reaction was completed, the solvent was evaporated under reduced pressure. The residue was extracted with a mixture of *n*-hexane (4 mL) and PhCl (0.2 mL). Yellow crystals were obtained at room temperature by standing the extraction for several days (127 mg, 54%). M.P. (sealed): 171 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3052(m), 2955(w), 2934(s), 2860(m), 2797(w), 2379(w), 2308(w), 1621(s), 1541(m), 1513(m), 1463(s), 1425(s), 1379(m), 1325(m), 1237(m), 1191(m), 1156(m), 1123(m), 1057(s), 927(m), 859(w), 836(w), 741(s). Anal. Calcd for $C_{95}H_{102}YbN_{11}$: C, 72.63; H, 6.54; N, 9.81. Found: C, 72.28; H, 6.79; N, 9.72.

Preparation of 14b. A similar procedure to that for the preparation of complex **14a** was used. Yellow crystals were obtained at room temperature by standing the extraction for several days (134

mg, 57%). M.P. (sealed): 172 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3051(m), 2956(w), 2933(s), 2860(m), 2797(w), 2379(w), 2307(w), 1620(s), 1542(m), 1514(m), 1463(s), 1426(s), 1378(m), 1325(m), 1236(m), 1190(m), 1156(m), 1124(m), 1057(s), 927(m), 858(w), 836(w), 740(s). Anal. Calcd for $C_{95}H_{102}ErN_{11}$: C, 72.90; H, 6.57; N, 9.84. Found: C, 72.57; H, 6.91; N, 9.75.

Preparation of 14c. A similar procedure to that for the preparation of complex **14a** was used. Yellow crystals were obtained at room temperature by standing the extraction for several days (114 mg, 51%). M.P. (sealed): 169 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): *v* 3052(m), 2956(w), 2934(s), 2860(m), 2798(w), 2378(w), 2307(w), 1620(s), 1541(m), 1513(m), 1463(s), 1425(s), 1379(m), 1326(m), 1237(m), 1192(m), 1156(m), 1123(m), 1056(s), 928(m), 858(w), 835(w), 740(s). ^{1}H NMR (500 MHz, C_6D_6, ppm, 298 K): δ 8.26 (m, 2H, -C*H*=N-), 7.42-7.40 (m, 2H, Ph-*H*), 7.34-7.31 (m, 3H, Ph-*H*), 7.25-7.21 (m, 8H, Ph-*H*), 7.11-7.09 (m, 6H, Ph-*H*), 7.02-6.96 (m, 10H, Ph-*H*), 6.92-6.89 (m, 2H, Ph-*H*), 6.82-6.78 (m, 10H, Ph-*H*), 6.64-6.61 (m, 3H, Ph-*H*), 4.23-4.18 (m, 2H, -CH_2-), 3.21-3.11 (m, 2H, -CH_2-), 3.10-3.02 (m, 4H, -C*H*$(CH_3)_2$), 1.79 (br, 8H, -CH_2-), 1.57-1.51 (m, 4H, -CH_2-), 1.45 (d, *J* = 5.0 Hz, 6H, -CH(CH_3)$_2$), 1.43 (d, *J* = 5.0 Hz, 6H, -CH(CH_3)$_2$), 1.32-1.24 (m, 12H, -CH_2-), 0.83 (d, *J* = 5.0 Hz, 6H, -CH(CH_3)$_2$), 0.45 (d, *J* = 10.0 Hz, 6H, -CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm, 298 K): δ 160.7 (imine *C*), 159.9, 157.3, 151.9, 143.8, 143.4, 142.9, 138.4, 137.2, 134.8, 130.4, 129.9, 129.0, 128.8, 128.4, 127.4, 126.5, 124.6, 124.4, 121.4, 121.2, 115.8, 109.9, 99.4, 56.0, 54.4, 40.6, 28.4, 28.0, 26.5, 25.8, 25.1, 24.7. Anal. Calcd for $C_{95}H_{102}YN_{11}$: C, 76.74; H, 6.92; N, 10.36. Found: C, 76.51; H, 6.90; N, 10.00.

3. ^{1}H, ^{13}C{^{1}H}, 2D HSQC, and ^{89}Y NMR Spectra of the Ligands and Complexes

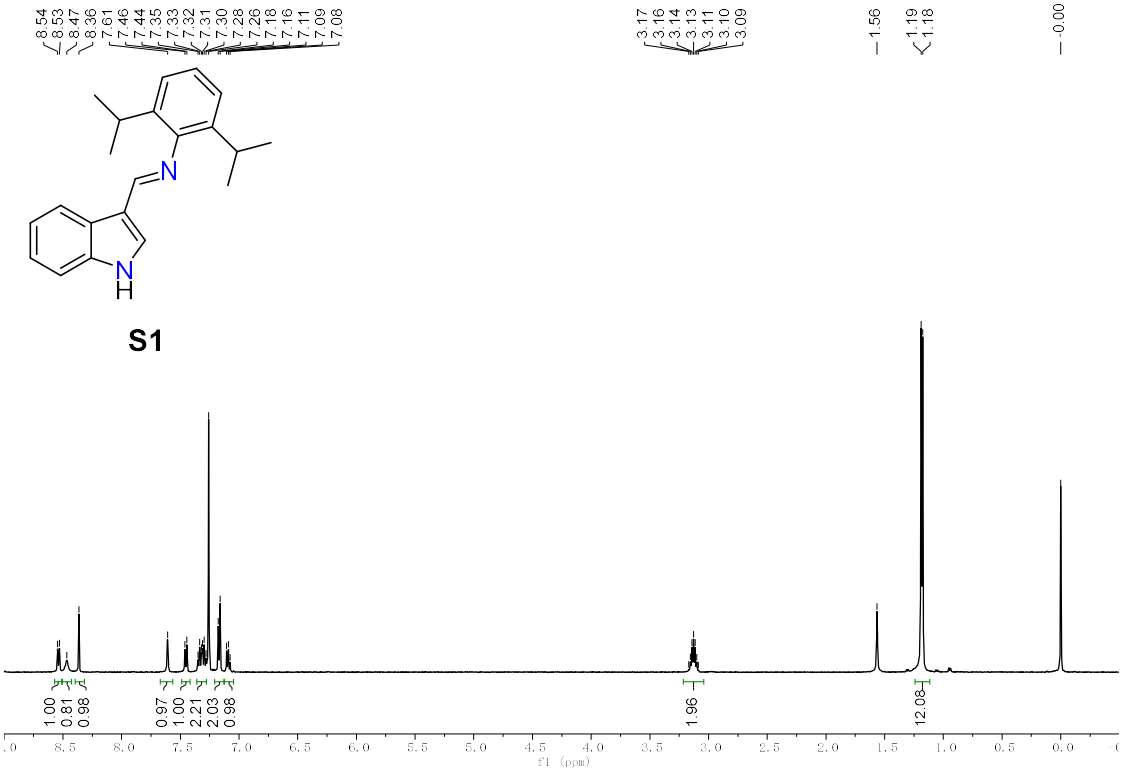


Fig. S1. ^{1}H NMR spectrum of **S1** (500 MHz, $CDCl_3$, 298 K)

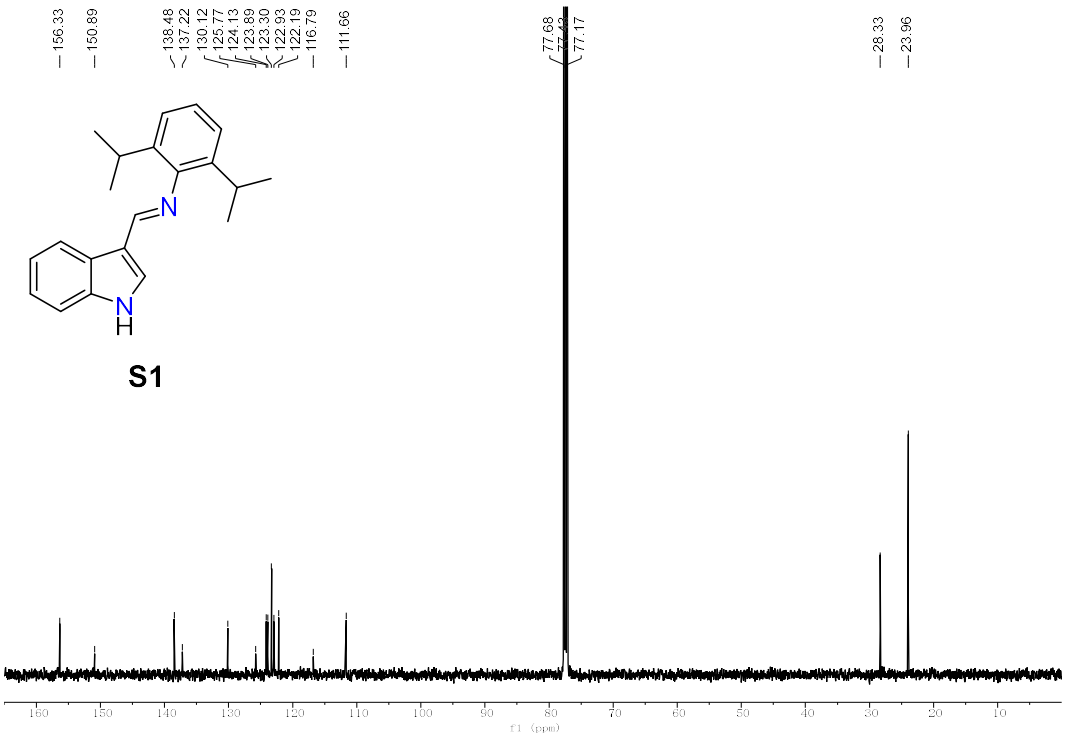


Fig. S2. $^{13}C\{^{1}H\}$ NMR spectrum of **S1** (125 MHz, $CDCl_3$, 298 K)

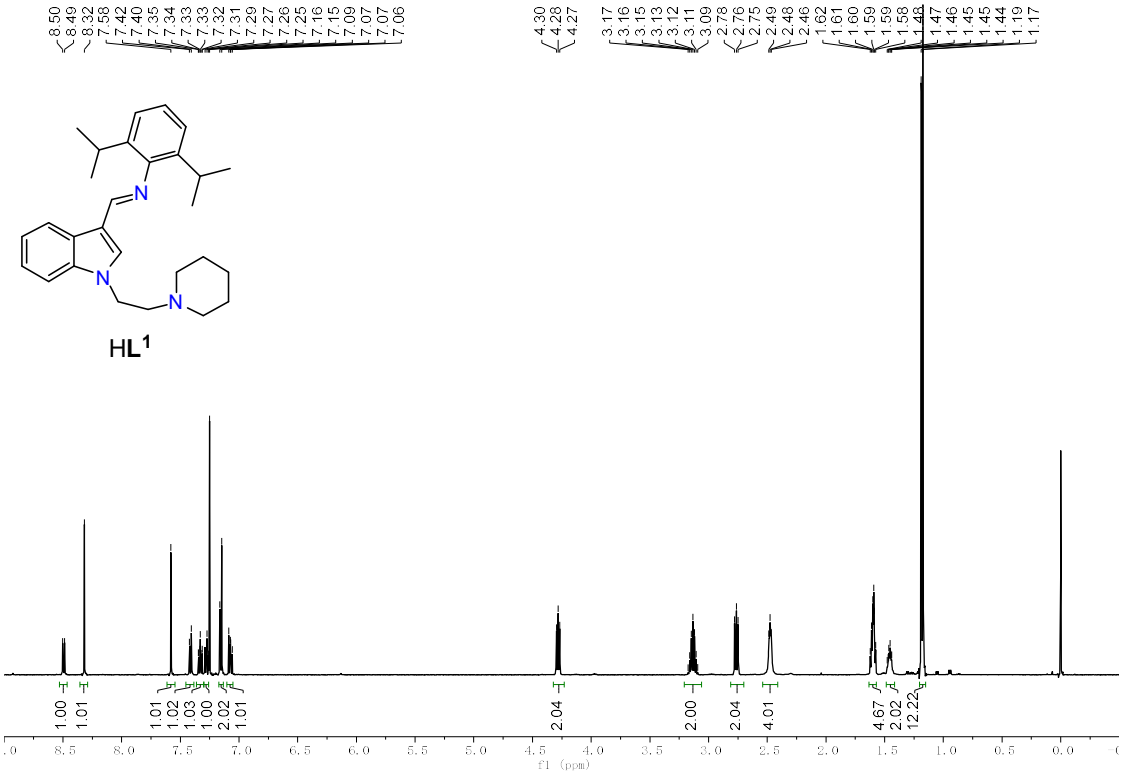


Fig. S3. ^{1}H NMR spectrum of H**L**^{1} (500 MHz, $CDCl_3$, 298 K)

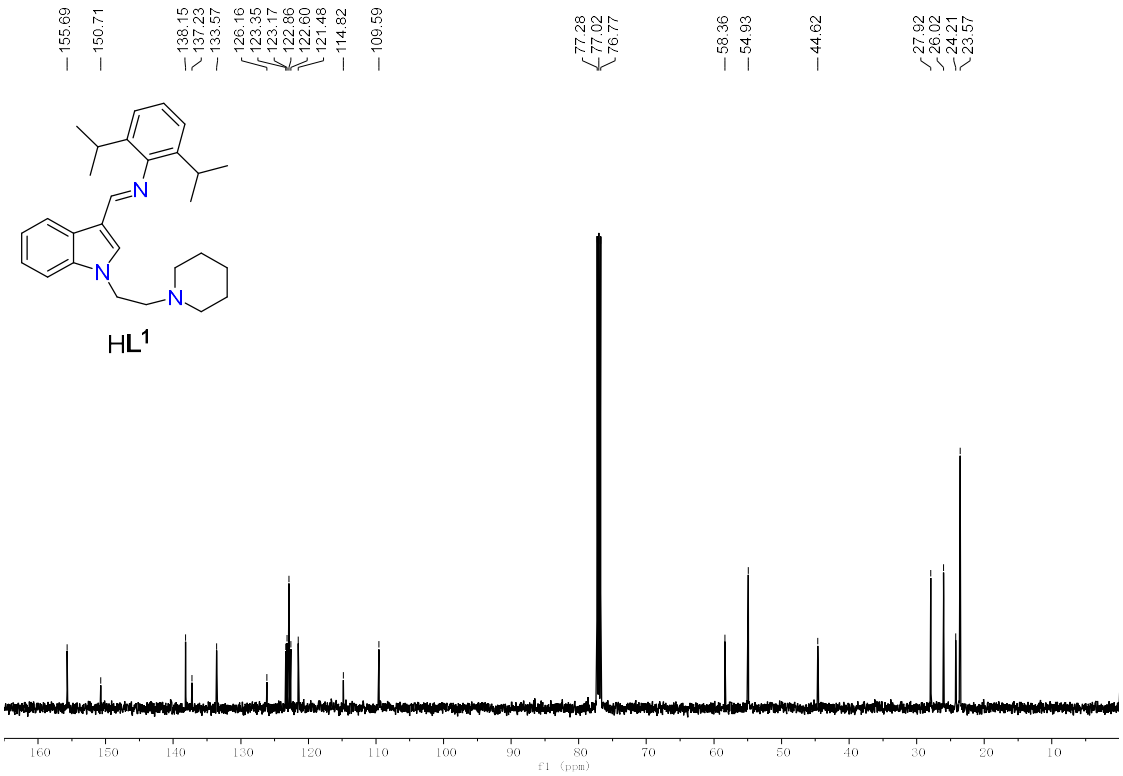


Fig. S4. $^{13}C\{^{1}H\}$ NMR spectrum of H**L**^{1} (125 MHz, $CDCl_3$, 298 K)

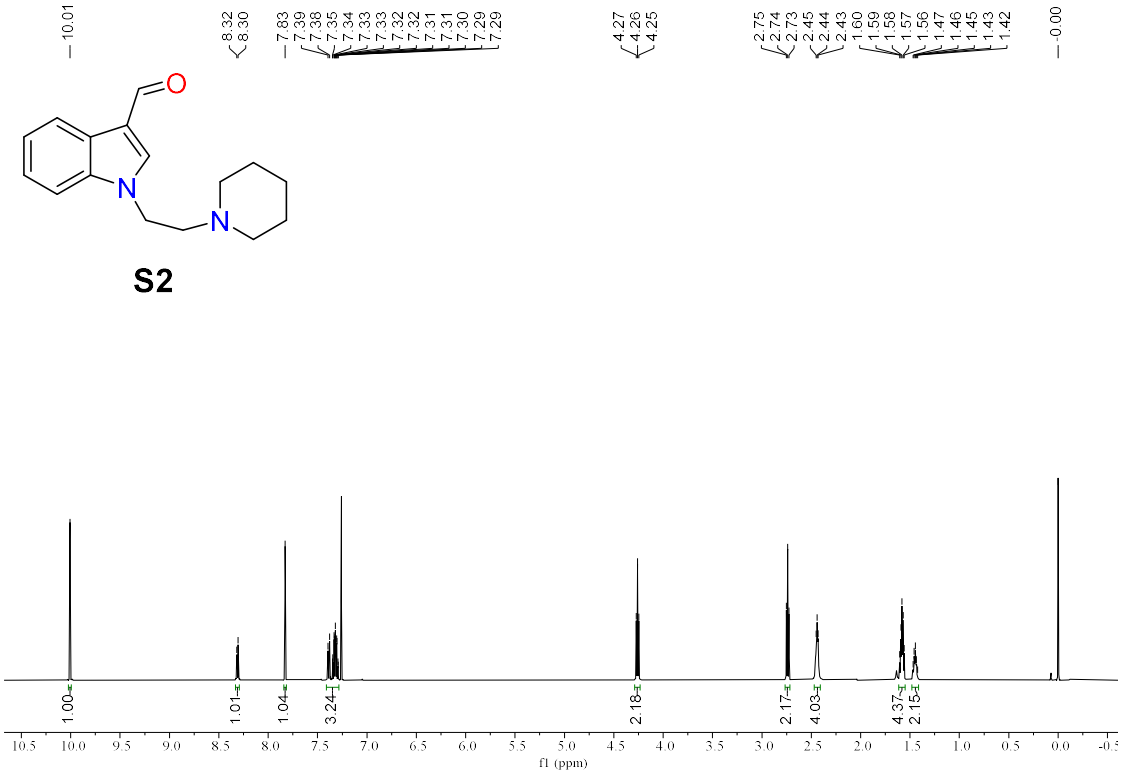


Fig. S5. ^{1}H NMR spectrum of **S2** (500 MHz, $CDCl_3$, 298 K)

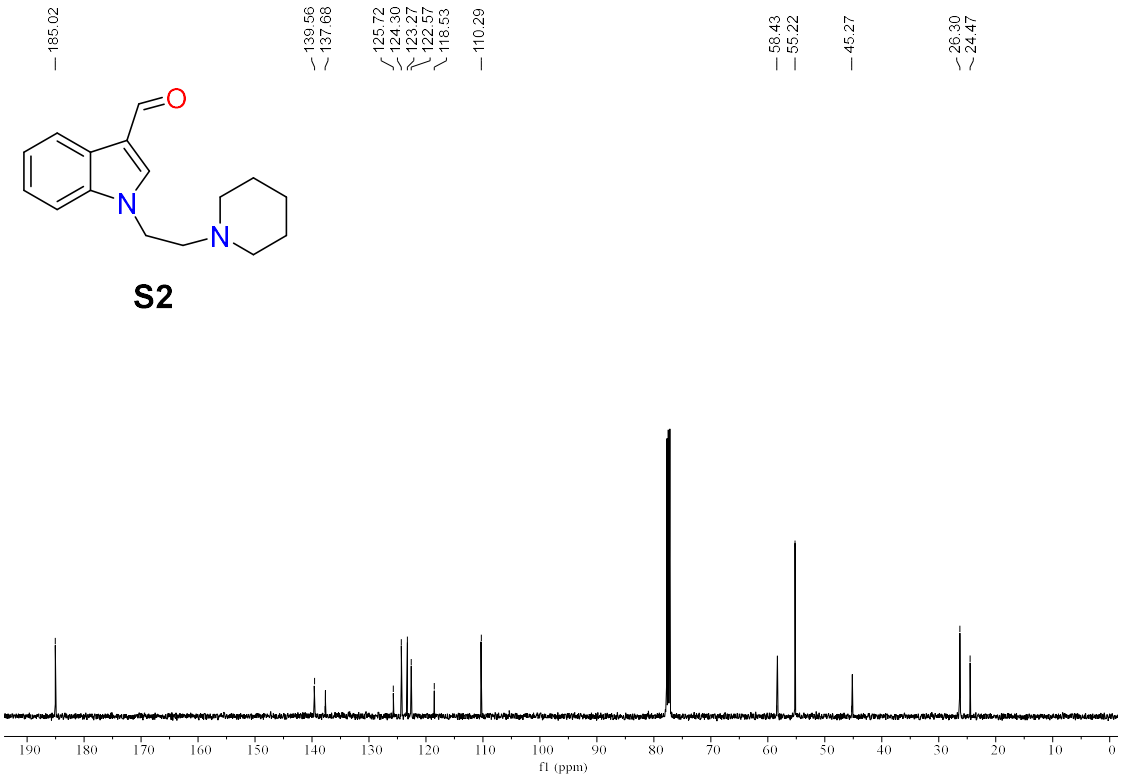


Fig. S6. $^{13}C\{^{1}H\}$ NMR spectrum of **S2** (125 MHz, $CDCl_3$, 298 K)

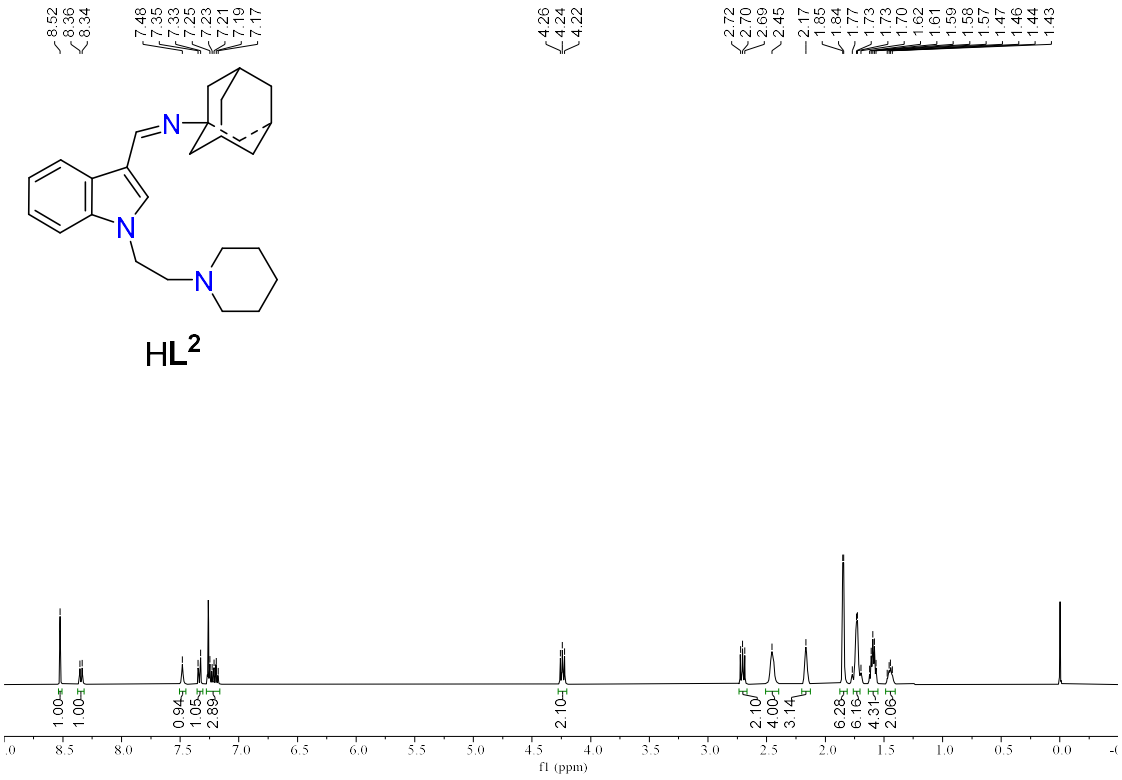


Fig. S7. ^{1}H NMR spectrum of H**L²** (500 MHz, $CDCl_3$, 298 K)

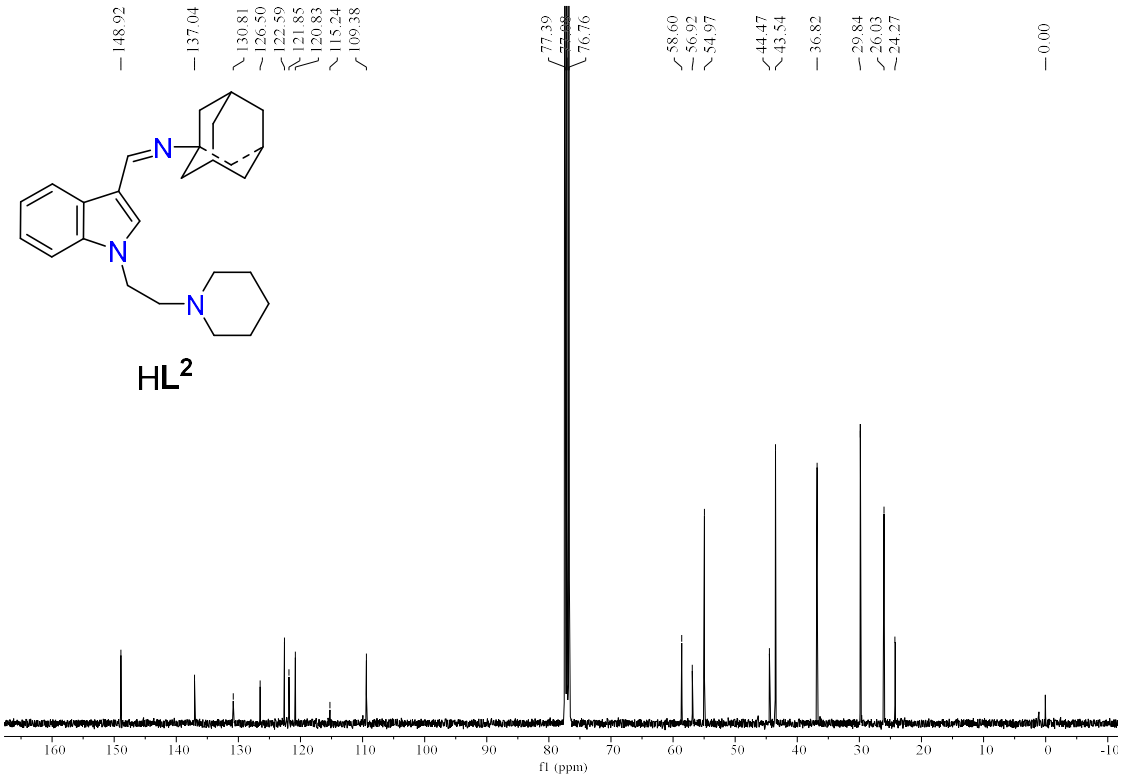


Fig. S8. $^{13}C\{^{1}H\}$ NMR spectrum of H**L**^{2} (125 MHz, $CDCl_3$, 298 K)

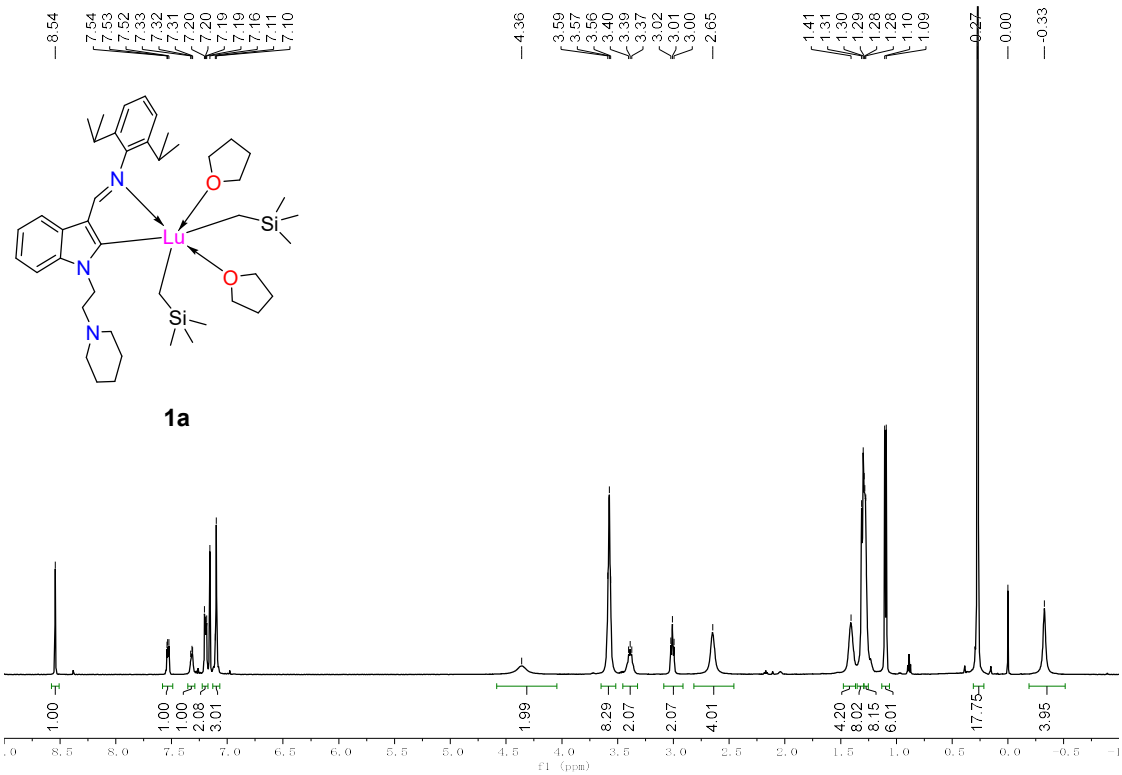


Fig. S9. ^{1}H NMR spectrum of **1a** (500 MHz, C_6D_6, 298 K)

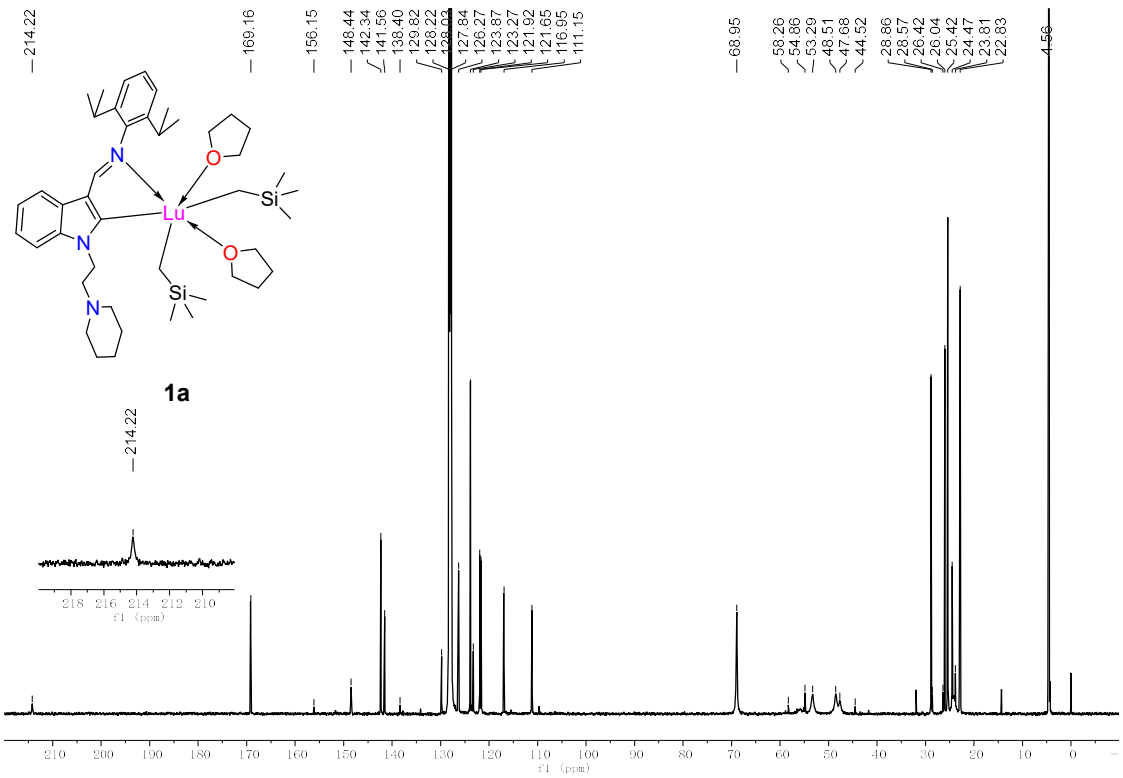


Fig. S10. $^{13}C\{^{1}H\}$ NMR spectrum of **1a** (125 MHz, C_6D_6, 298 K)

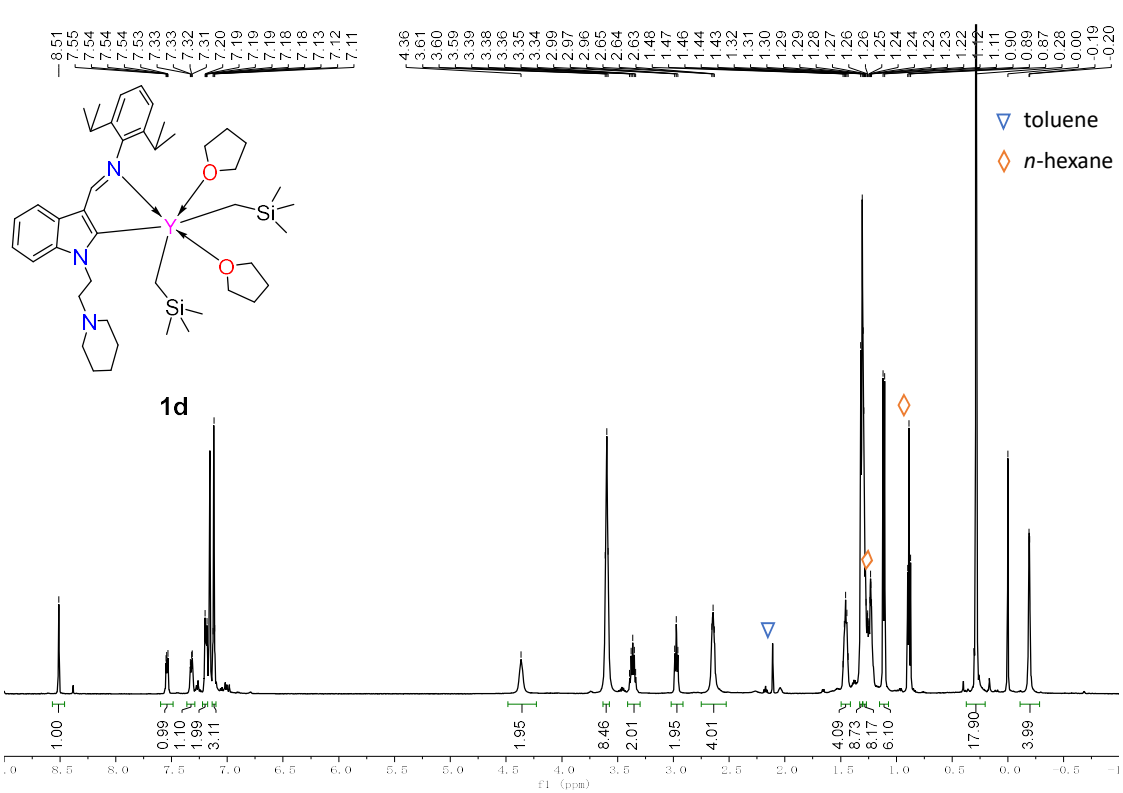


Fig. S11. ^{1}H NMR spectrum of **1d** (500 MHz, C_6D_6, 298 K)

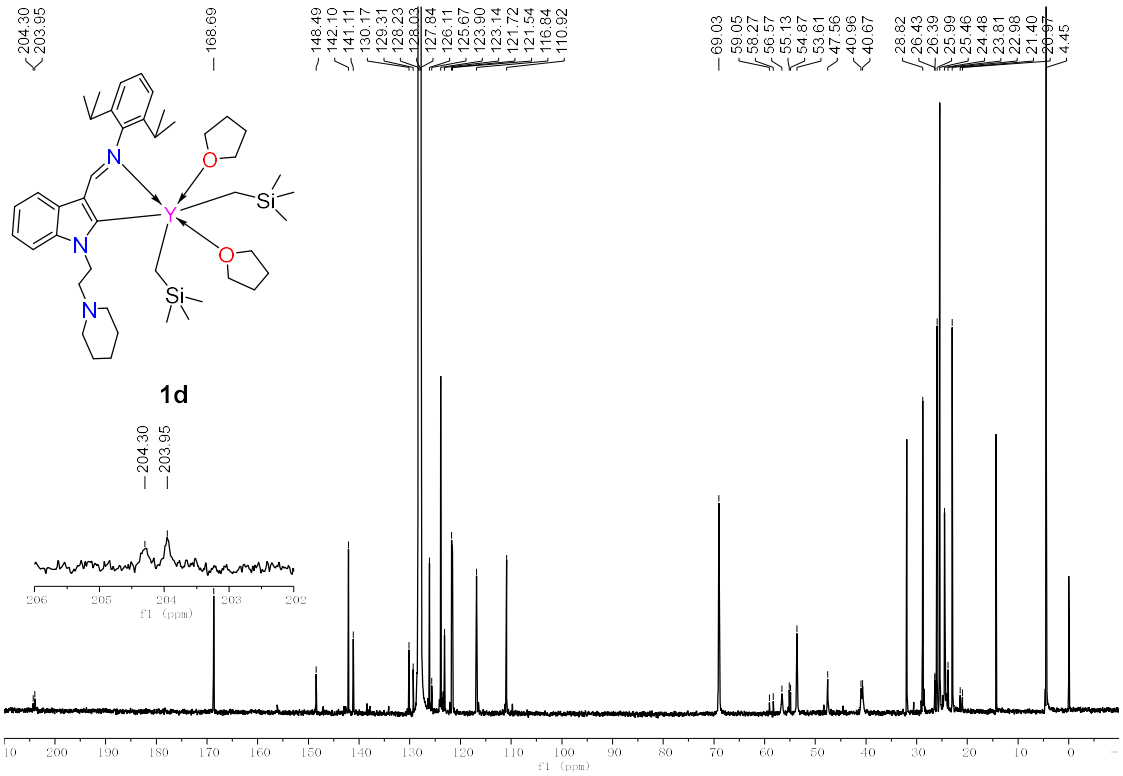


Fig. S12. $^{13}C\{^{1}H\}$ NMR spectrum of **1d** (125 MHz, C_6D_6, 298 K)

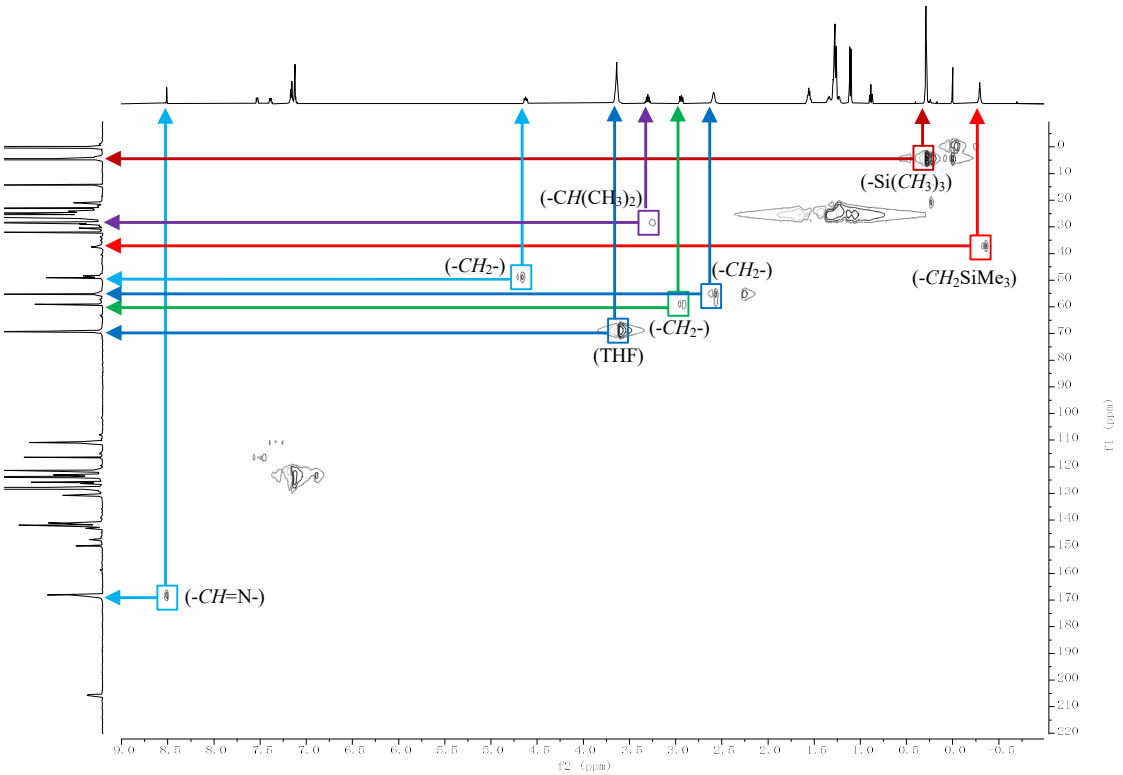


Fig. S13. 2D HSQC NMR spectrum of **1d** (C_6D_6, 298 K)

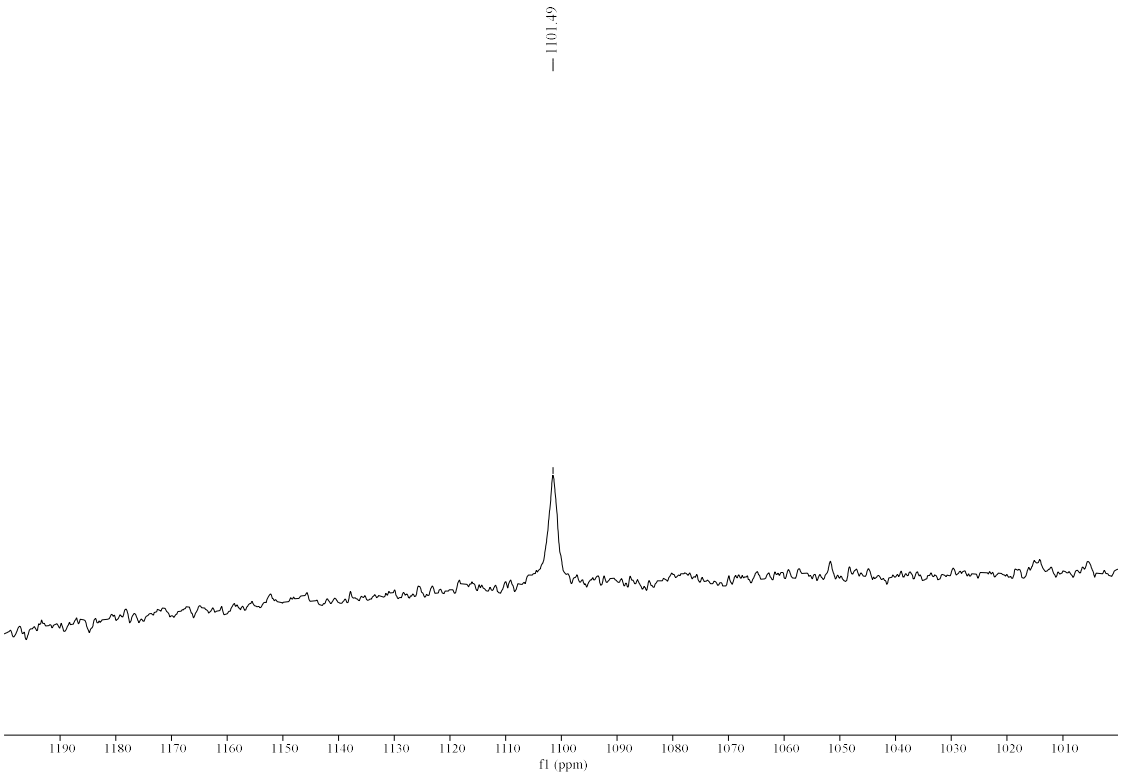


Fig. S14. ^{89}Y NMR spectrum of **1d** (24.5 MHz, C_6D_6, 298 K)

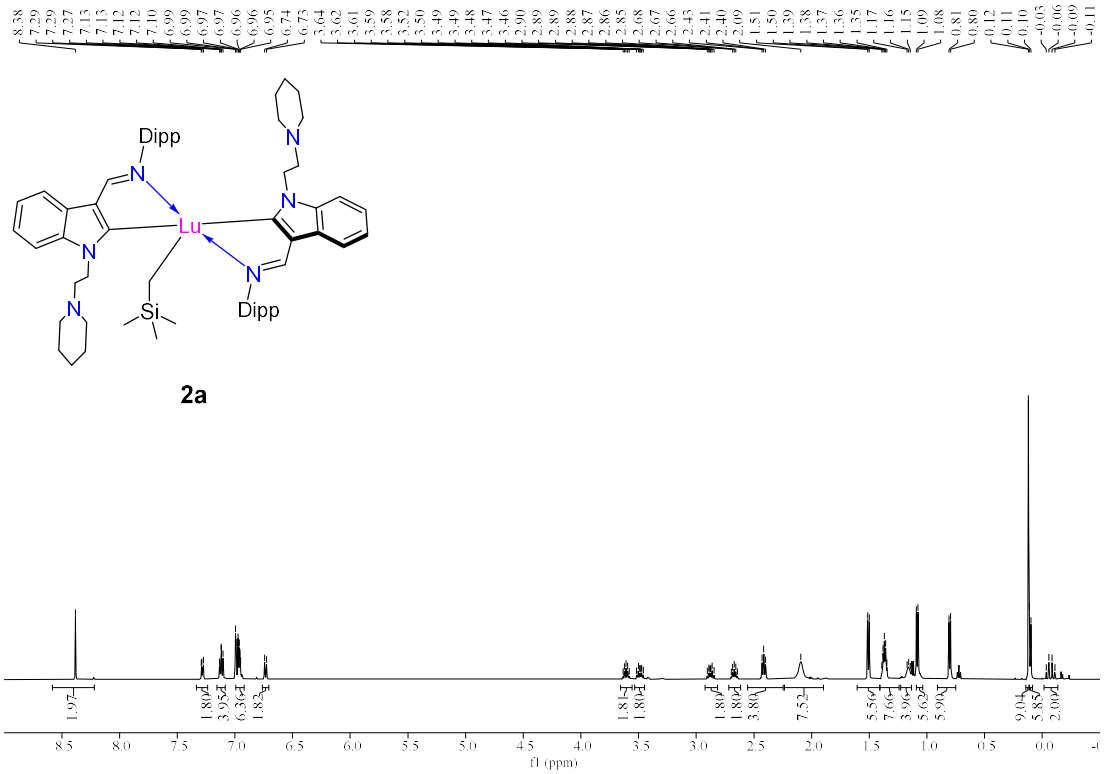


Fig. S15. ^{1}H NMR spectrum of **2a** (500 MHz, C_6D_6, 298 K)

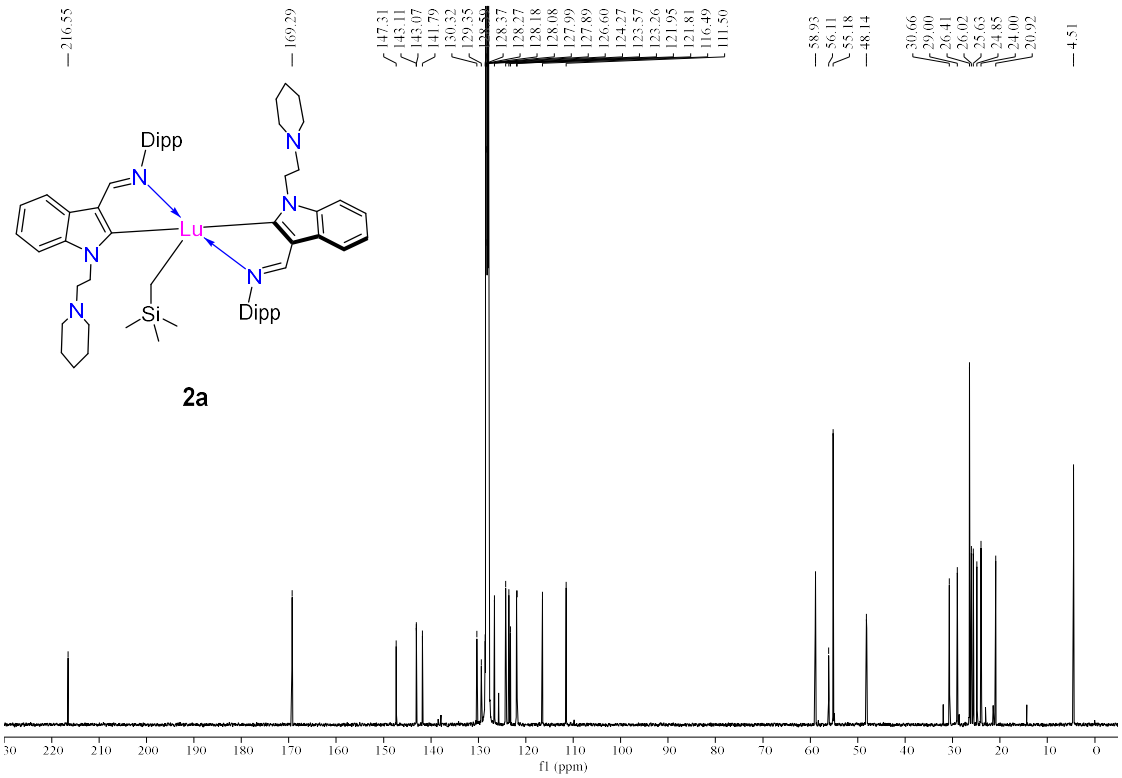


Fig. S16. $^{13}C\{^{1}H\}$ NMR spectrum of **2a** (125 MHz, C_6D_6, 298 K)

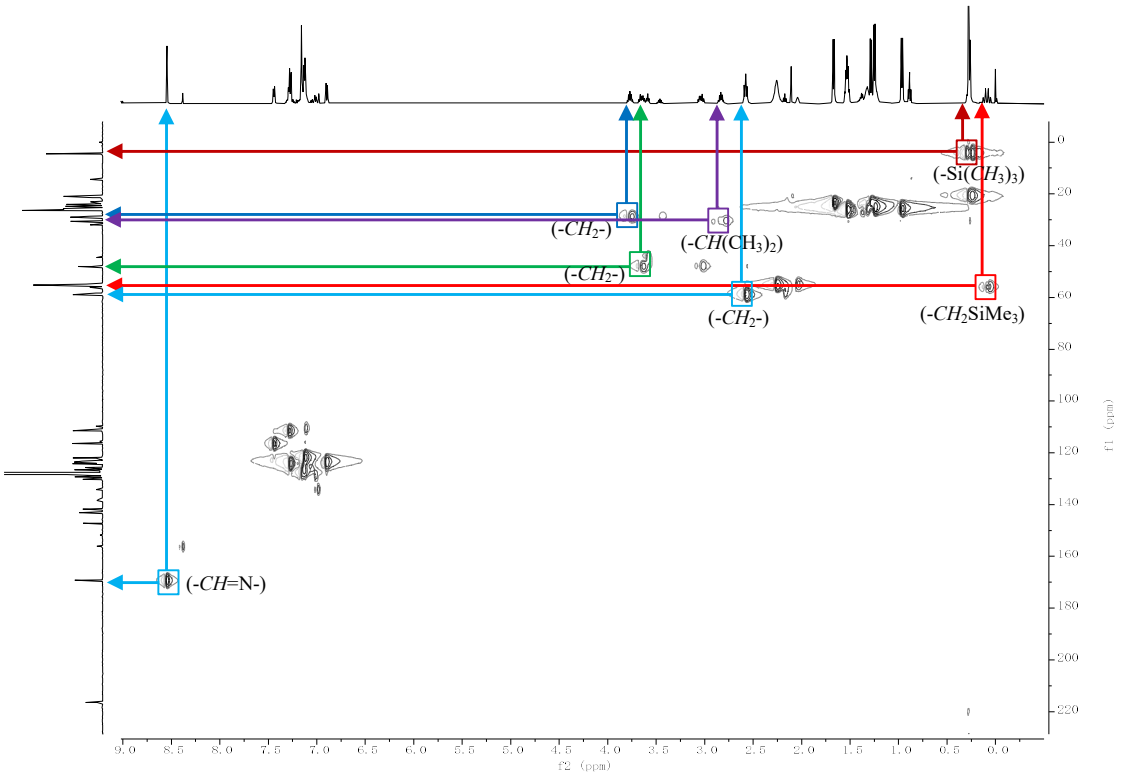


Fig. S17. 2D HSQC NMR spectrum of **2a** (C_6D_6, 298 K)

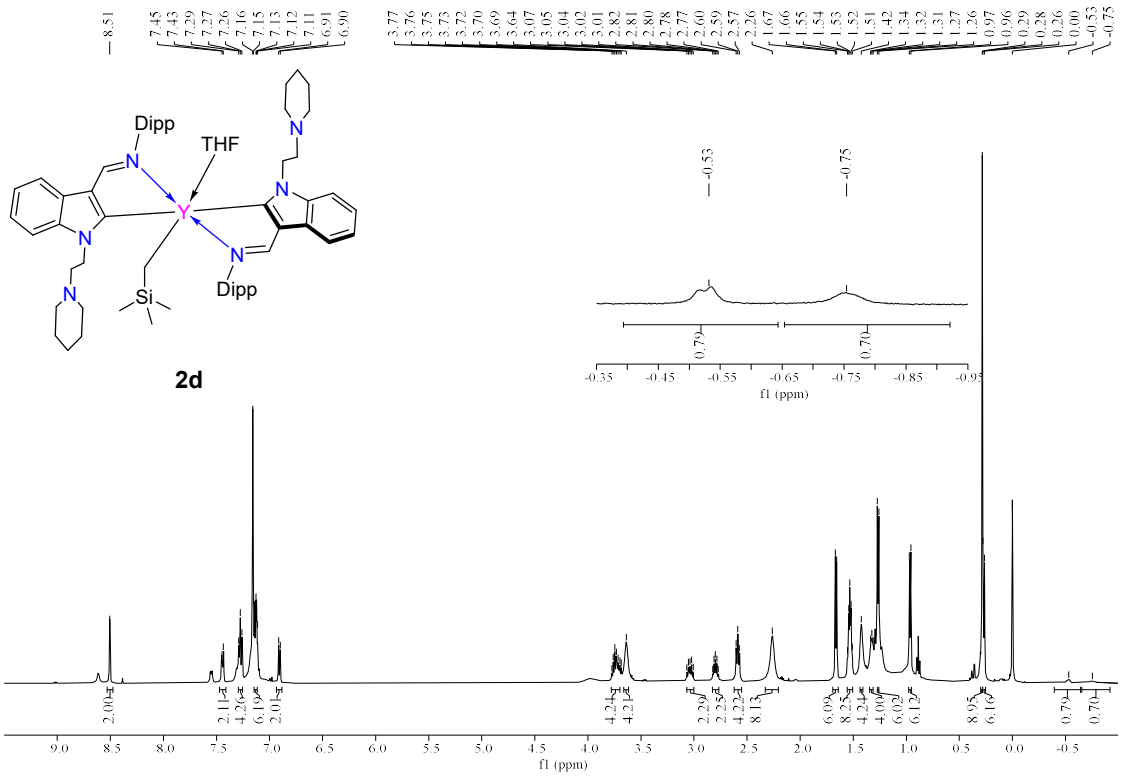


Fig. S18. ^{1}H NMR spectrum of **2d** (500 MHz, C_6D_6, 298 K)

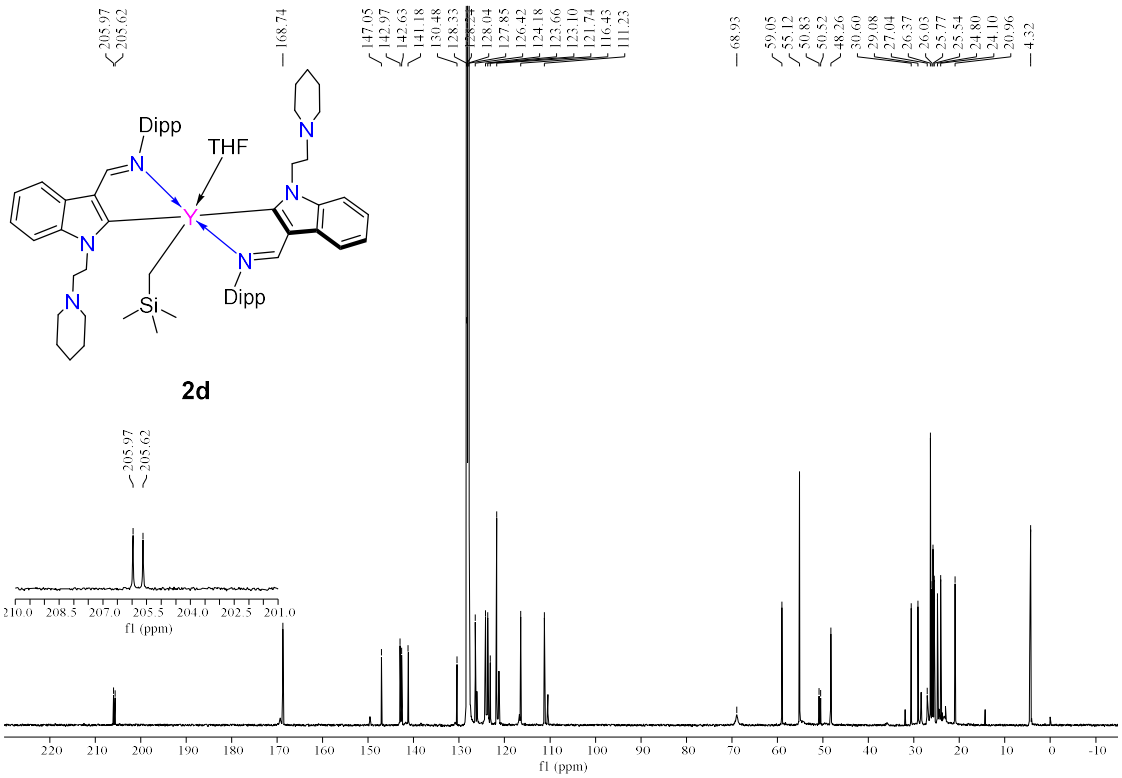


Fig. S19. ^{13}C{^{1}H} NMR spectrum of **2d** (125 MHz, C_6D_6, 298 K)

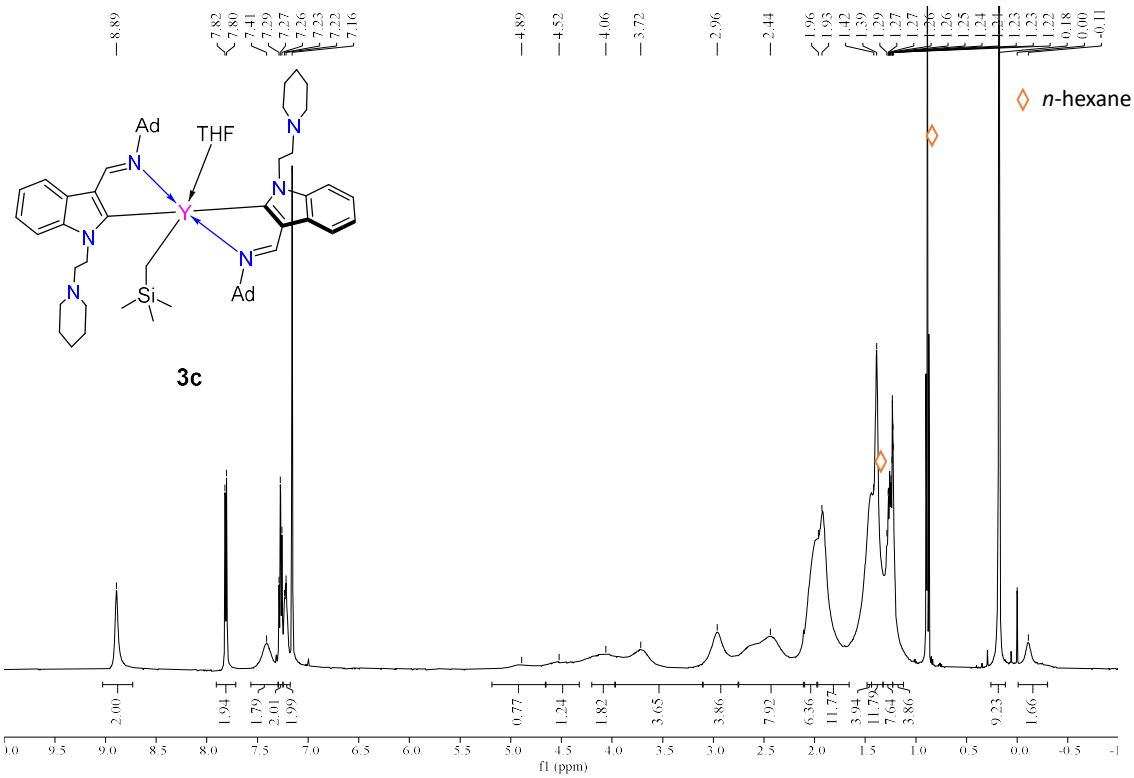


Fig. S20. ^{1}H NMR spectrum of **3c** (500 MHz, C_6D_6, 298 K)

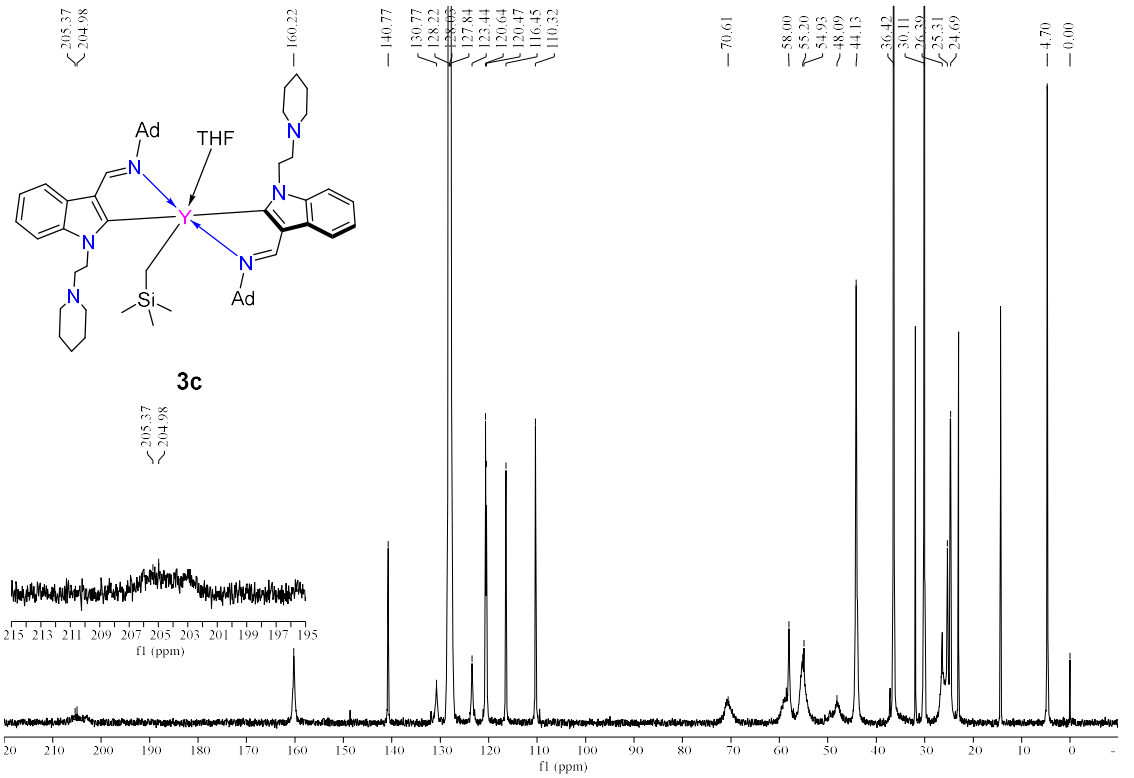


Fig. S21. ^{13}C{^{1}H} NMR spectrum of **3c** (125 MHz, C_6D_6, 298 K)

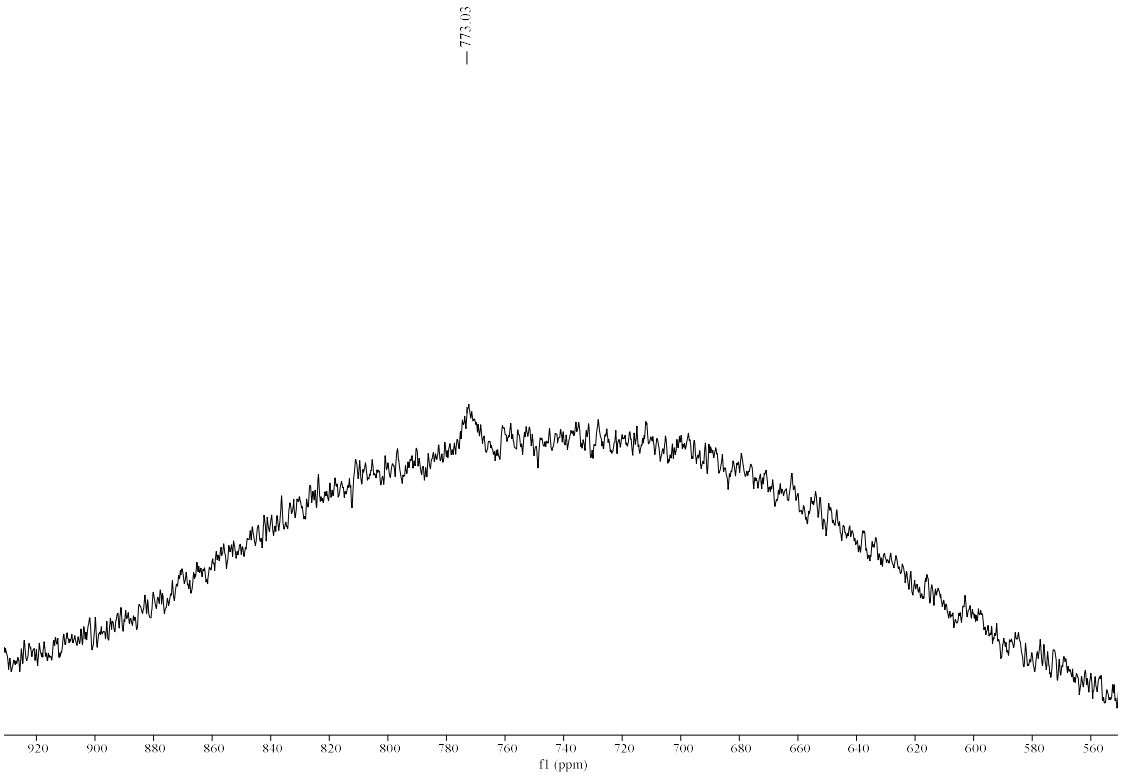


Fig. S22. ^{89}Y NMR spectrum of **3c** (24.5 MHz, C_6D_6, 298 K) (scanning for 4 hours)

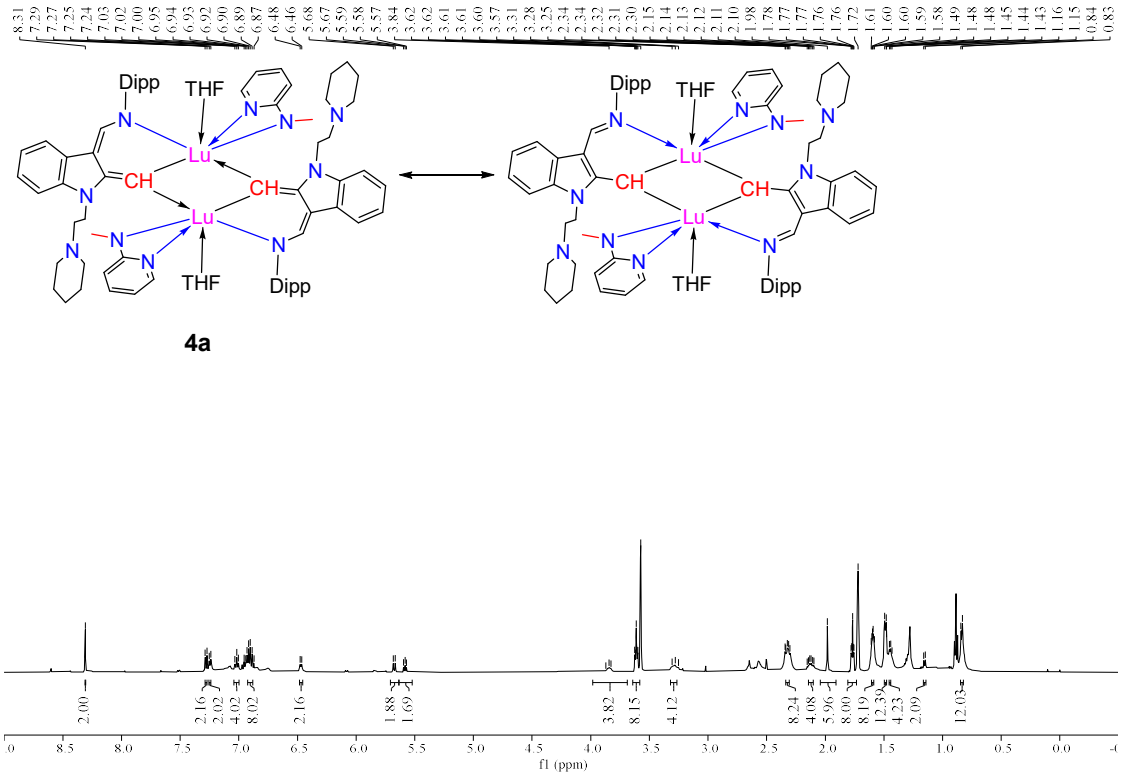


Fig. S23. ^{1}H NMR spectrum of **4a** (500 MHz, THF-d_8, 298 K)

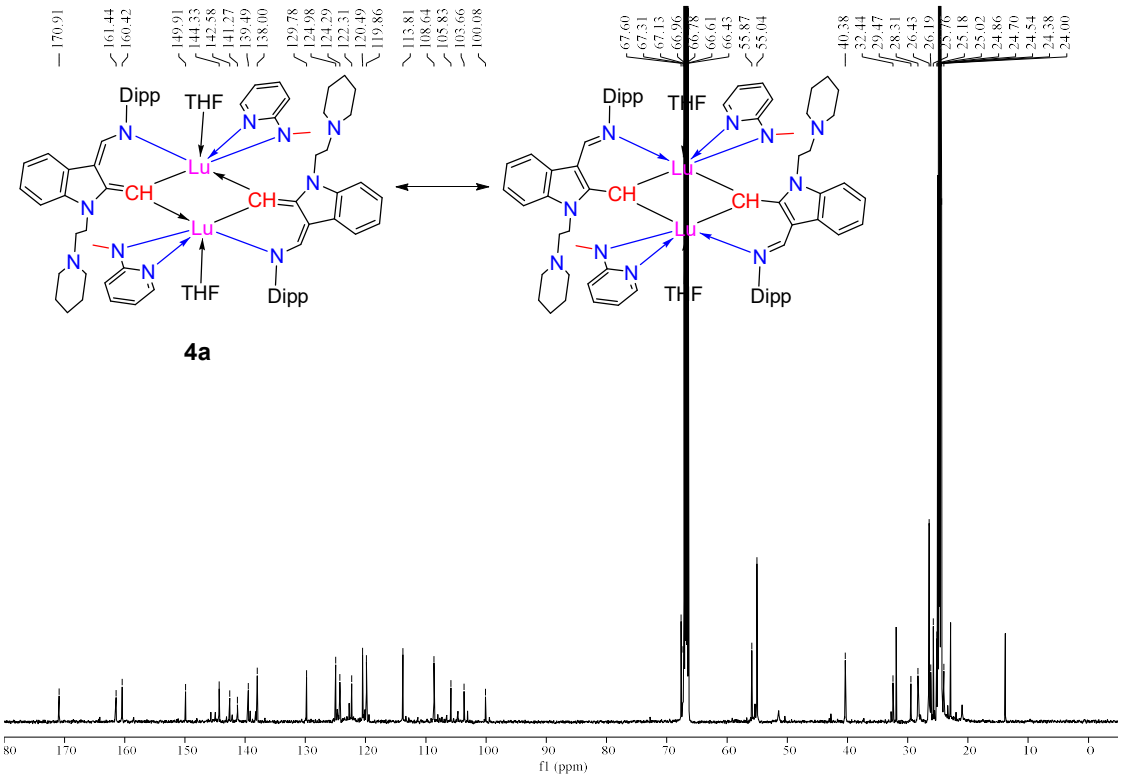


Fig. S24. $^{13}C\{^{1}H\}$ NMR spectrum of **4a** (125 MHz, THF-d_8, 298 K)

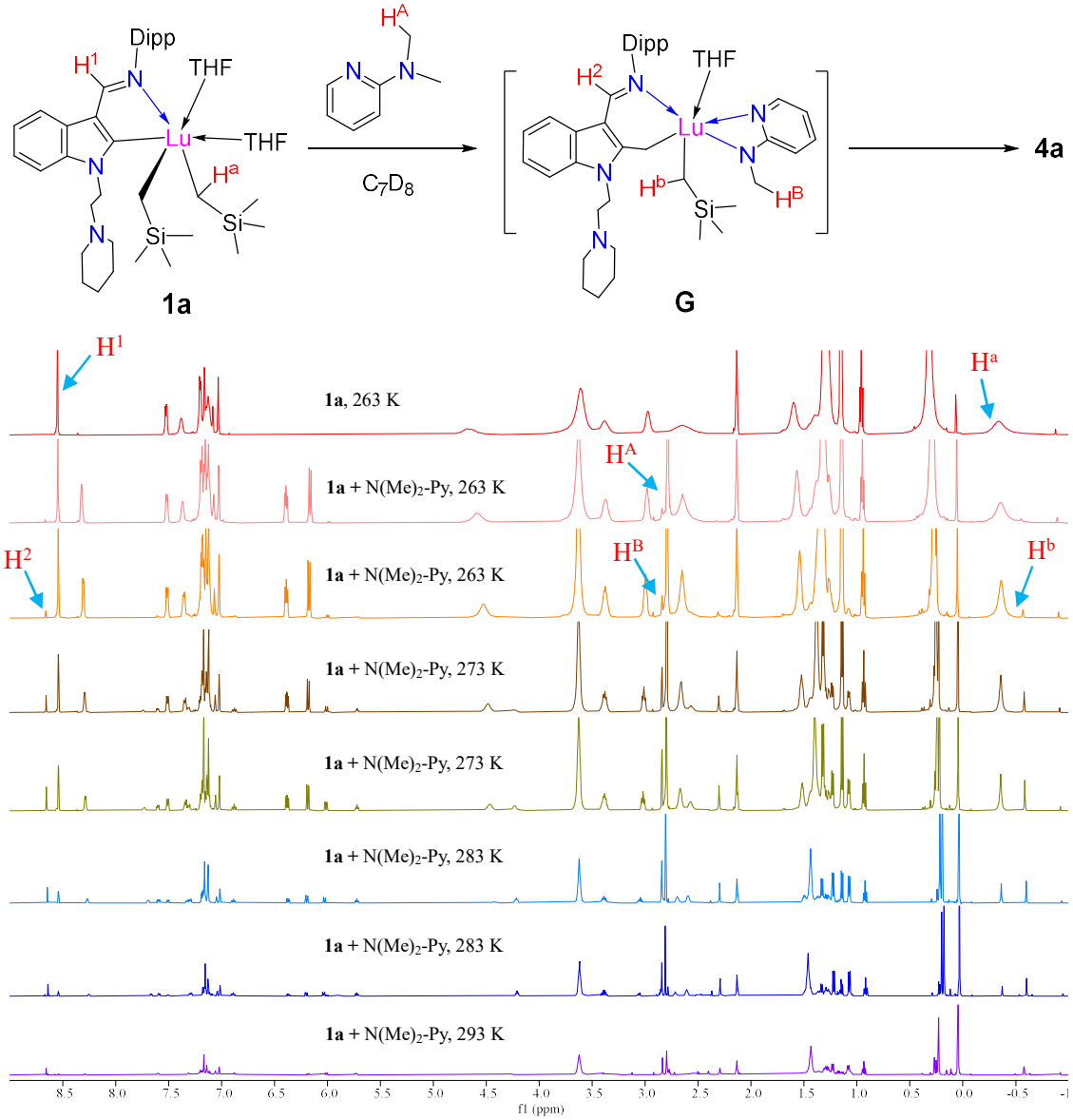


Fig. S25. VT-NMR (C_7D_8) spectrum of **1a** with 2-*N,N*-dimethylaminopyridine from 263 K to 293 K

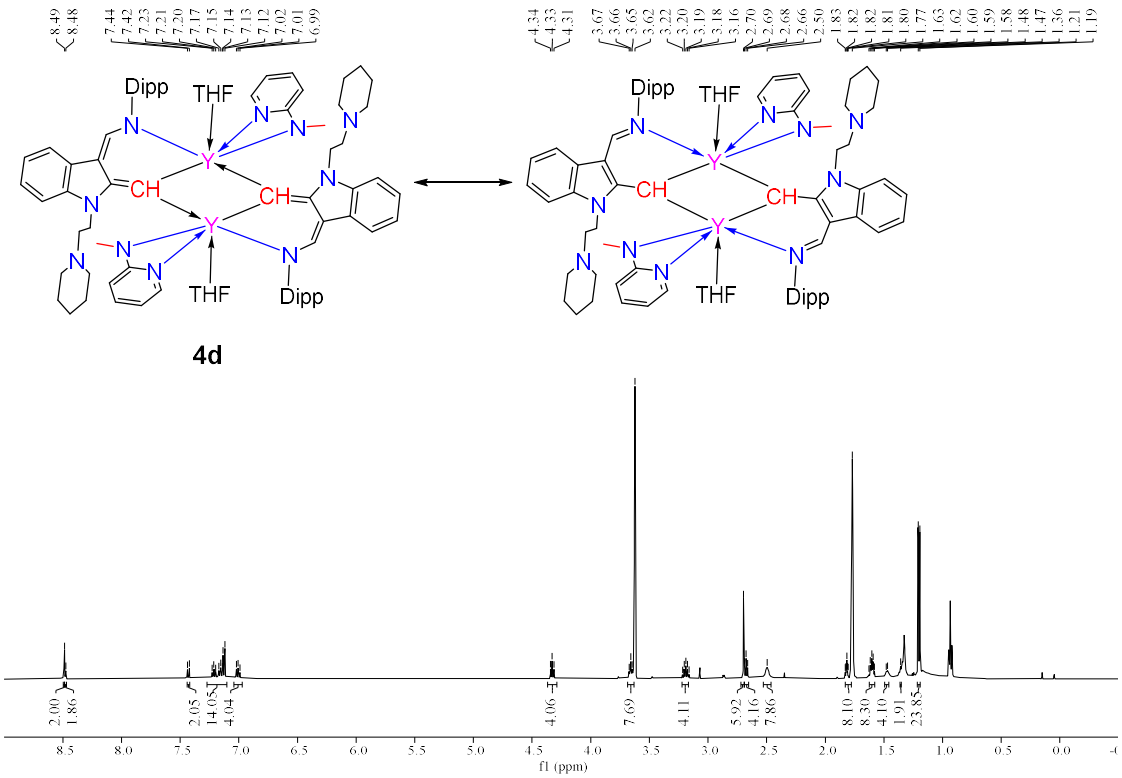


Fig. S26. ^{1}H NMR spectrum of **4d** (500 MHz, THF-d_8, 298 K)

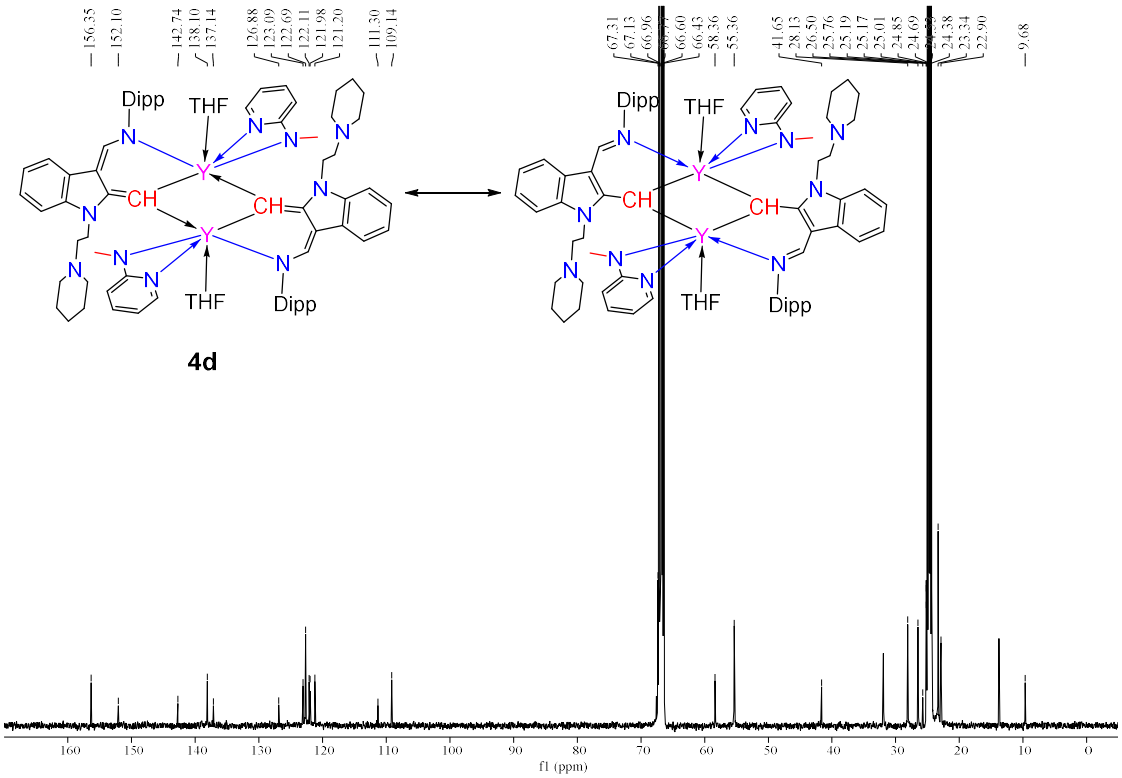


Fig. S27. ^{13}C{^{1}H} NMR spectrum of **4d** (125 MHz, THF-d_8, 298 K)

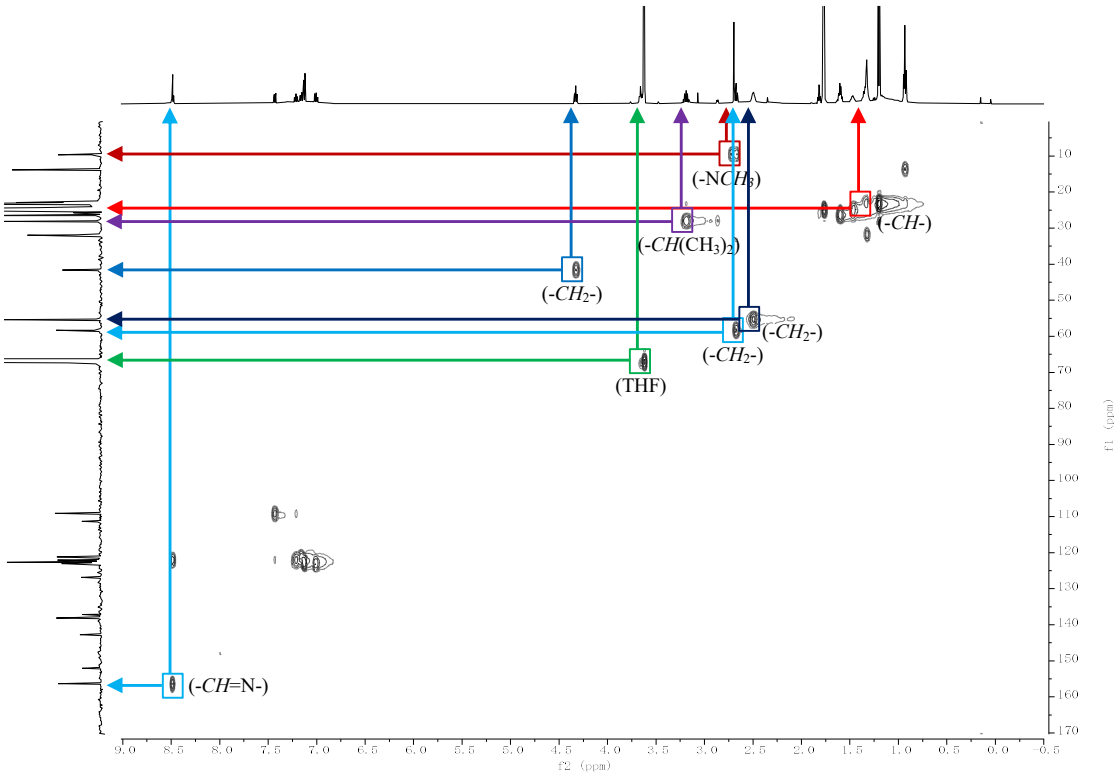


Fig. S28. 2D HSQC NMR spectrum of **4d** (THF-d_8, 298 K)

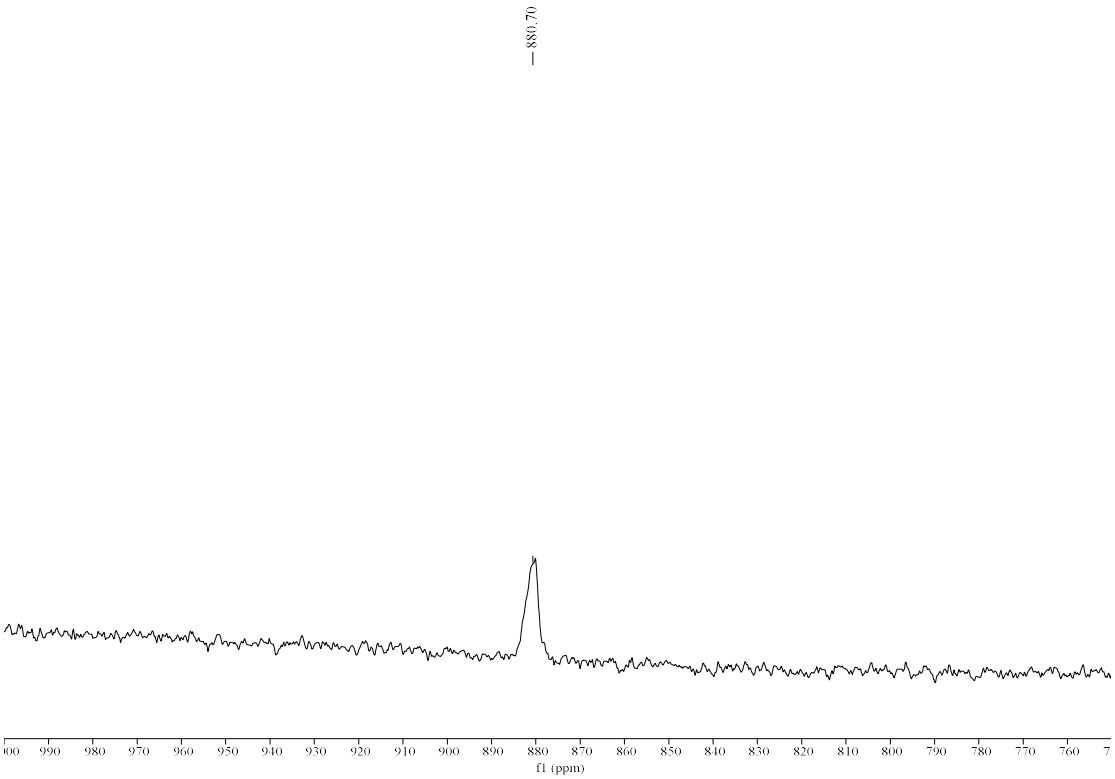


Fig. S29. ^{89}Y NMR spectrum of **4d** (24.5 MHz, THF-d_8, 298 K)

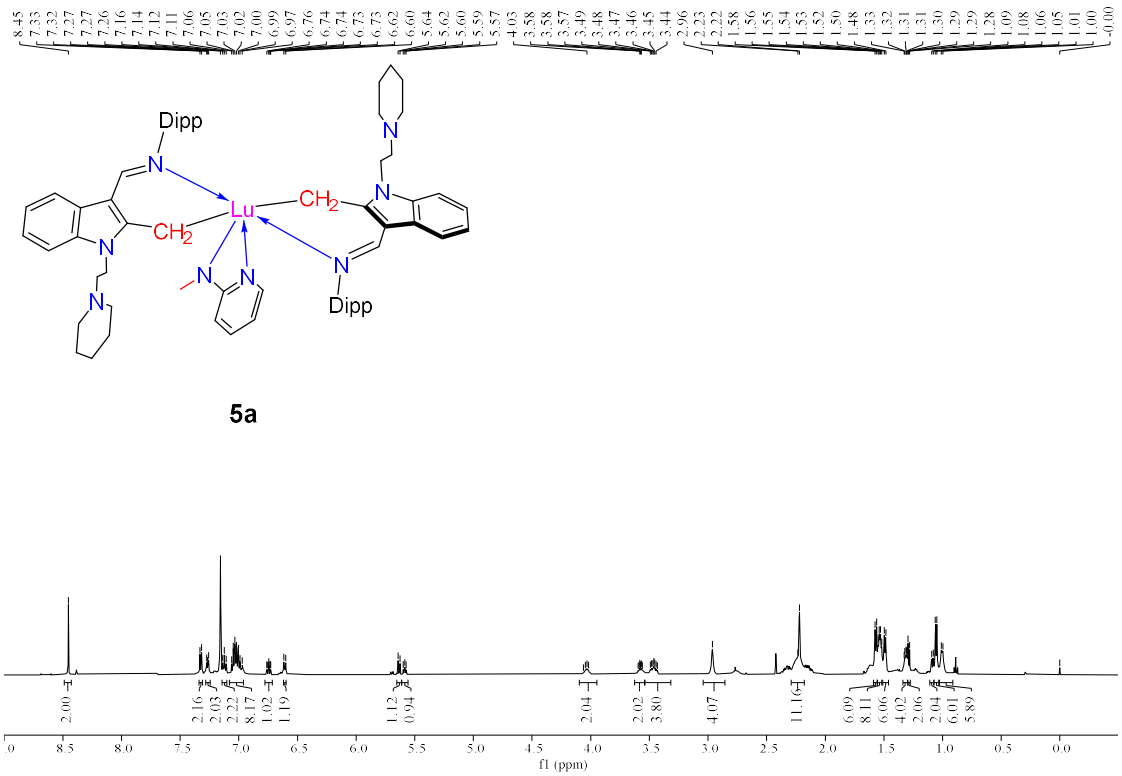


Fig. S30. ^{1}H NMR spectrum of **5a** (500 MHz, C_6D_6, 298 K)

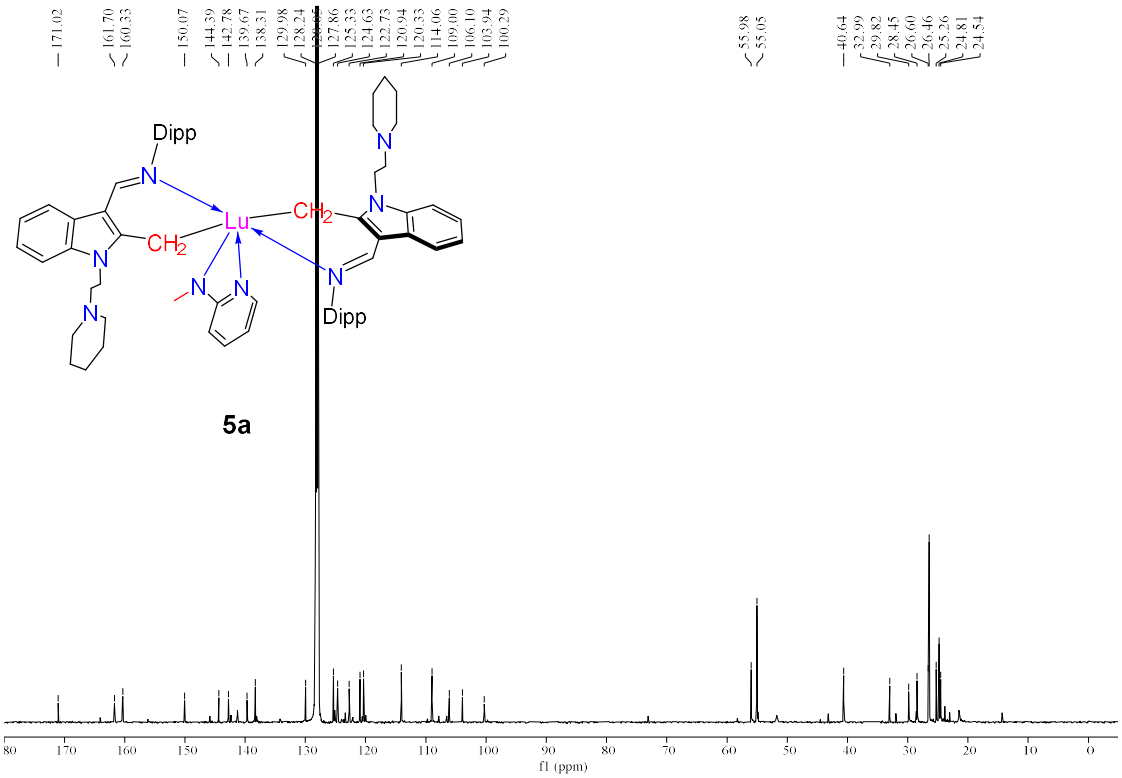


Fig. S31. ^{13}C{^{1}H} NMR spectrum of **5a** (125 MHz, C_6D_6, 298 K)

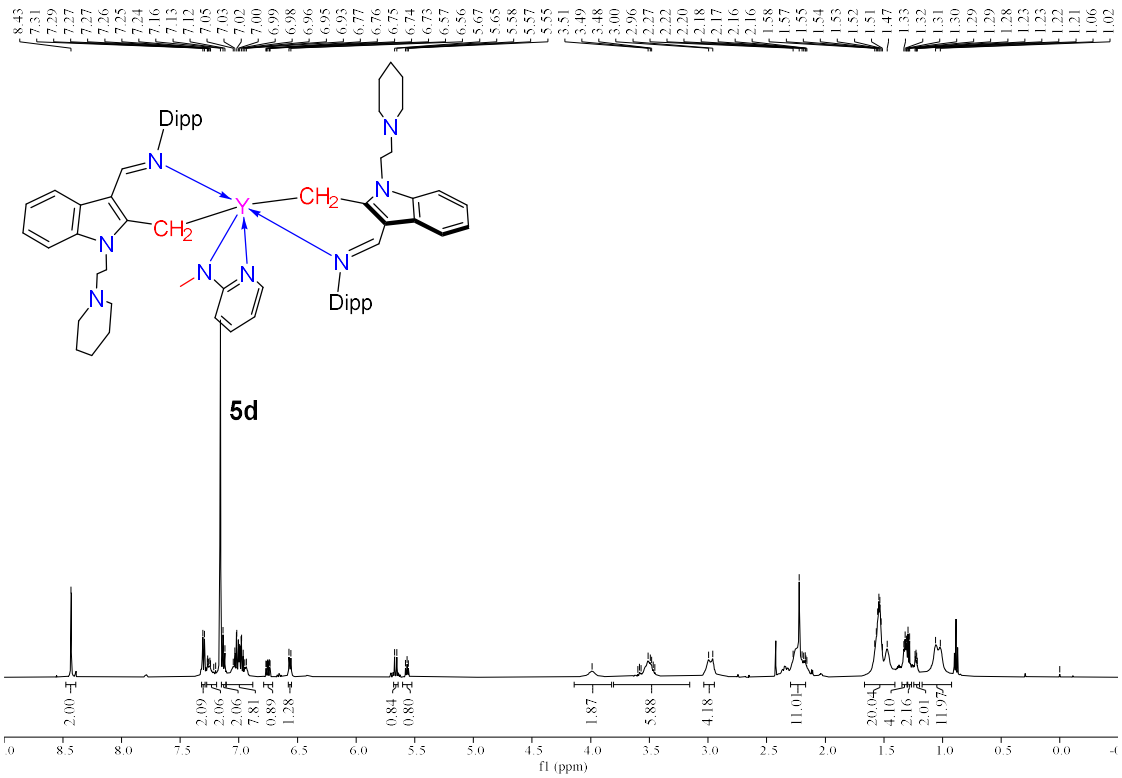


Fig. S32. ^{1}H NMR spectrum of **5d** (500 MHz, C_6D_6, 298 K)

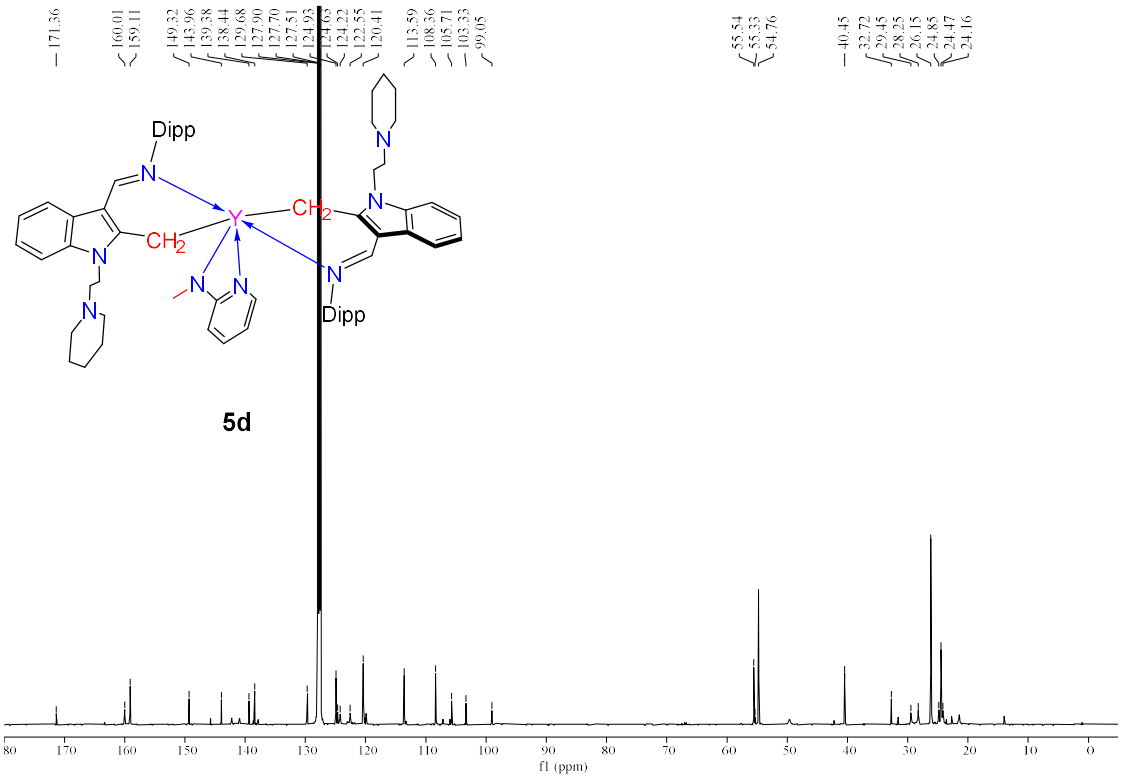


Fig. S33. ^{13}C{^{1}H} NMR spectrum of **5d** (125 MHz, C_6D_6, 298 K)

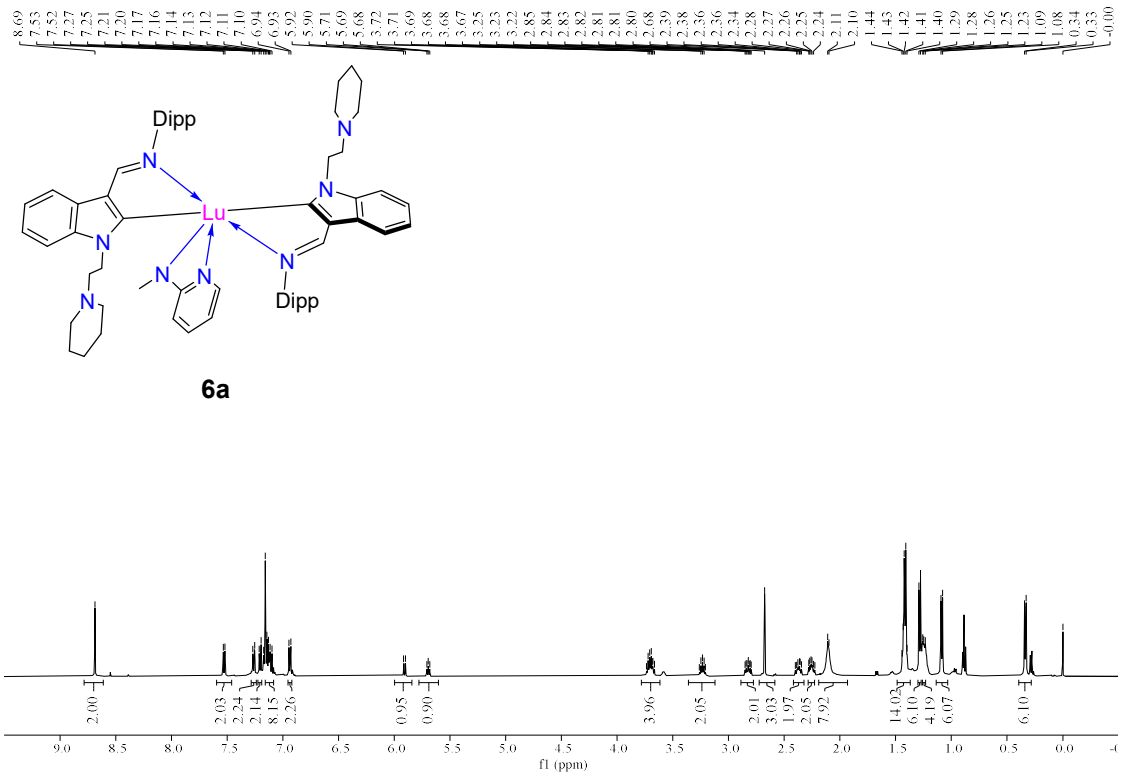


Fig. S34. ^{1}H NMR spectrum of **6a** (500 MHz, C_6D_6, 298 K)

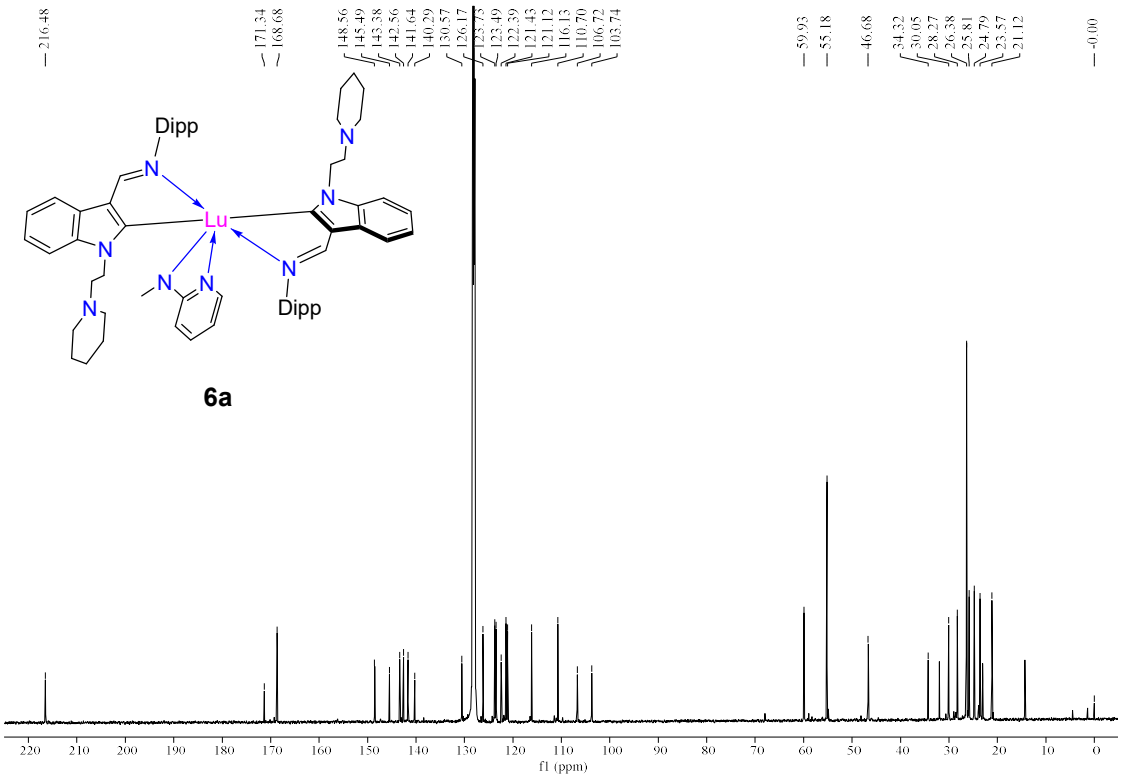


Fig. S35. ^{13}C{^{1}H} NMR spectrum of **6a** (125 MHz, C_6D_6, 298 K)

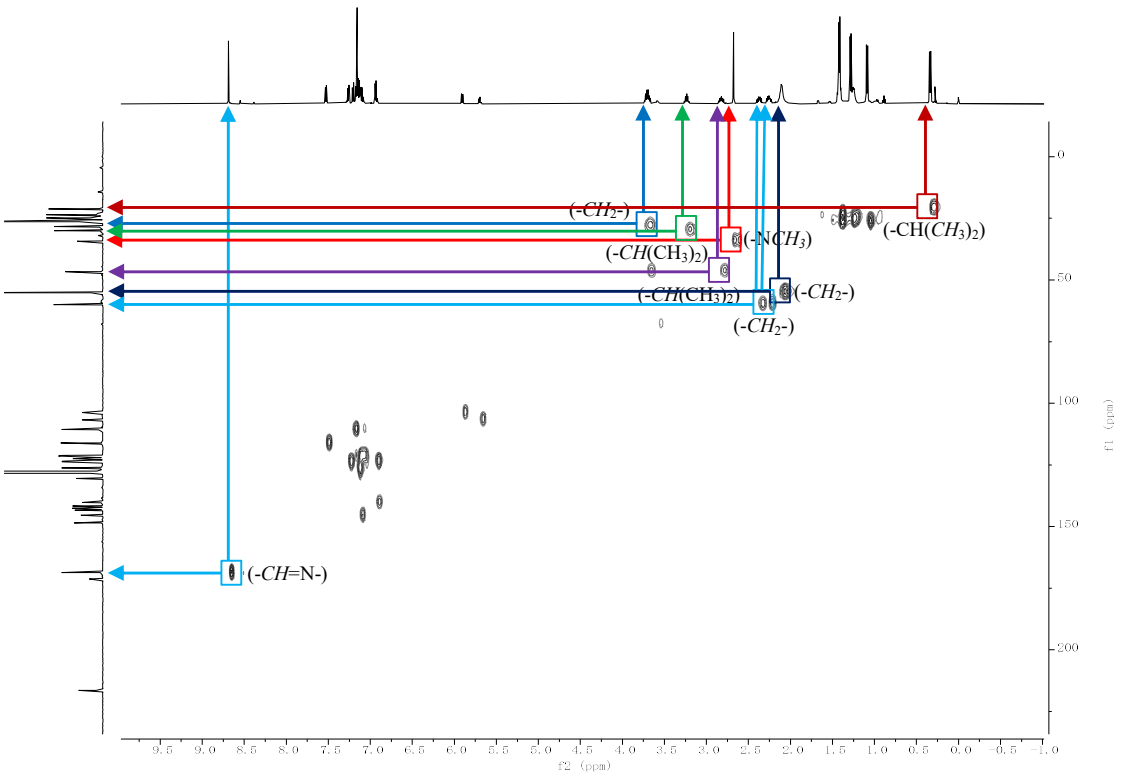


Fig. S36. 2D HSQC NMR spectrum of **6a** (C_6D_6, 298 K)

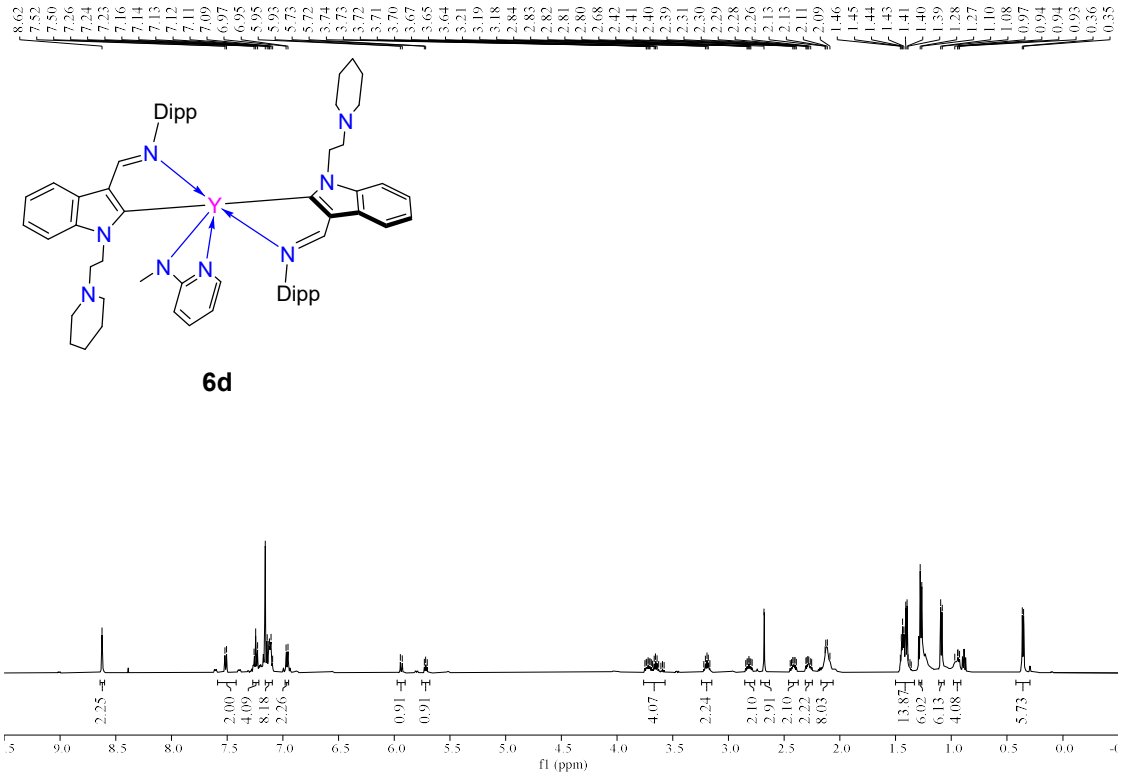


Fig. S37. ^{1}H NMR spectrum of **6d** (500 MHz, C_6D_6, 298 K)

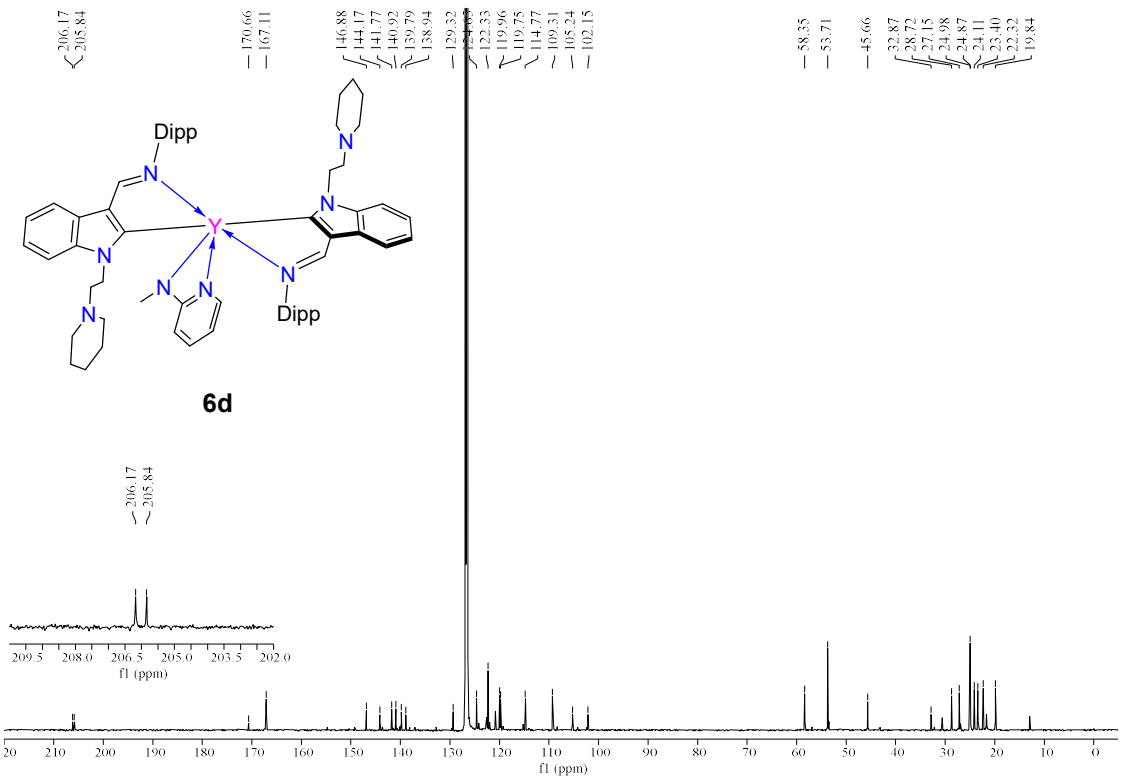


Fig. S38. $^{13}C\{^{1}H\}$ NMR spectrum of **6d** (125 MHz, C_6D_6, 298 K)

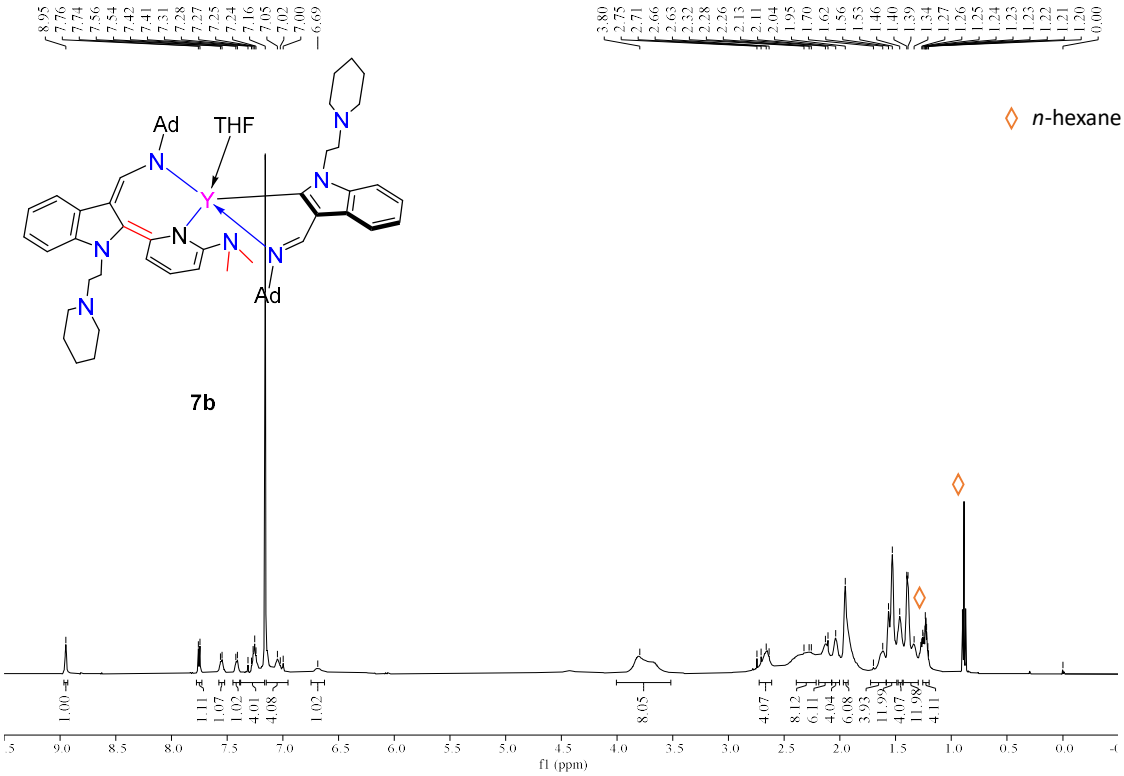


Fig. S39. ^{1}H NMR spectrum of **7b** (500 MHz, C_6D_6, 298 K)

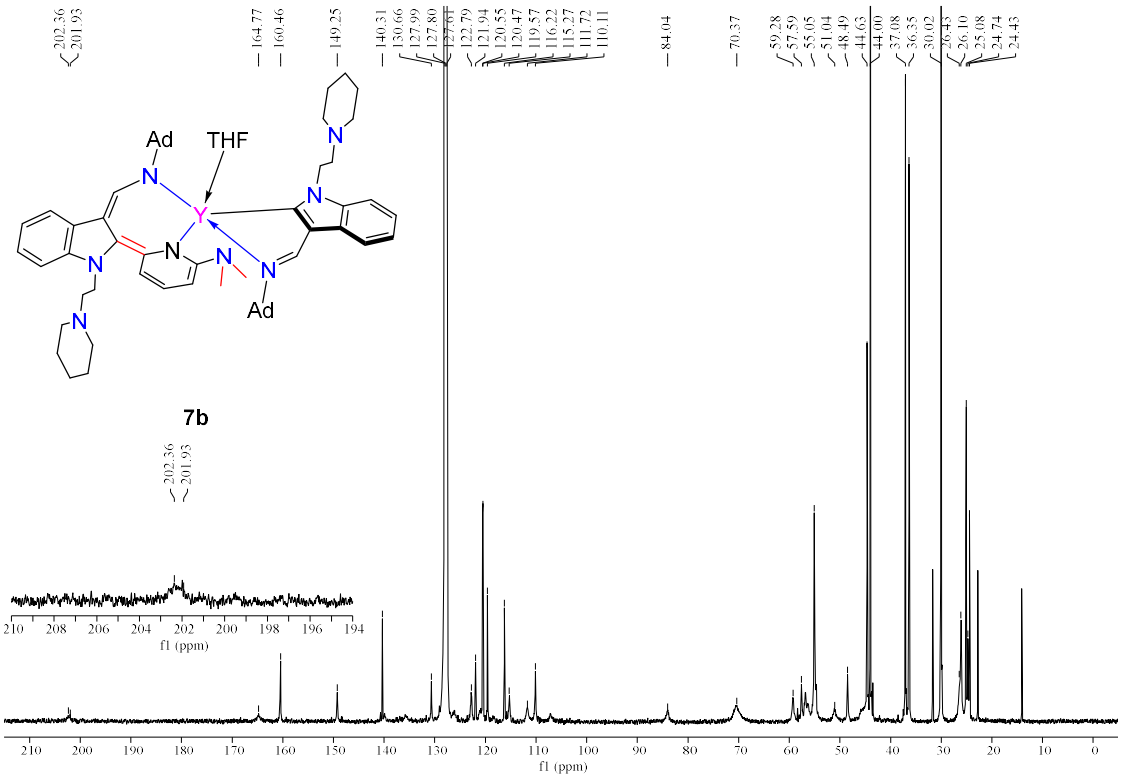


Fig. S40. $^{13}C\{^{1}H\}$ NMR spectrum of **7b** (125 MHz, C_6D_6, 298 K)

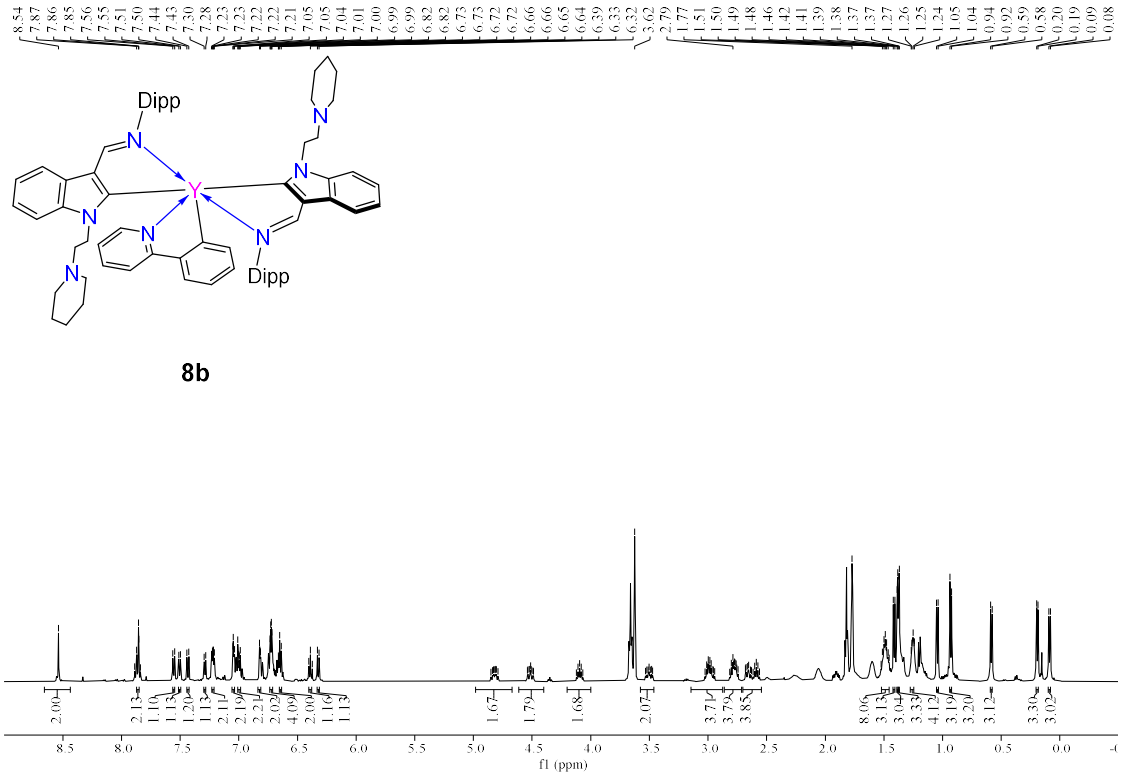


Fig. S41. ^{1}H NMR spectrum of **8b** (500 MHz, THF-d_8, 298 K)

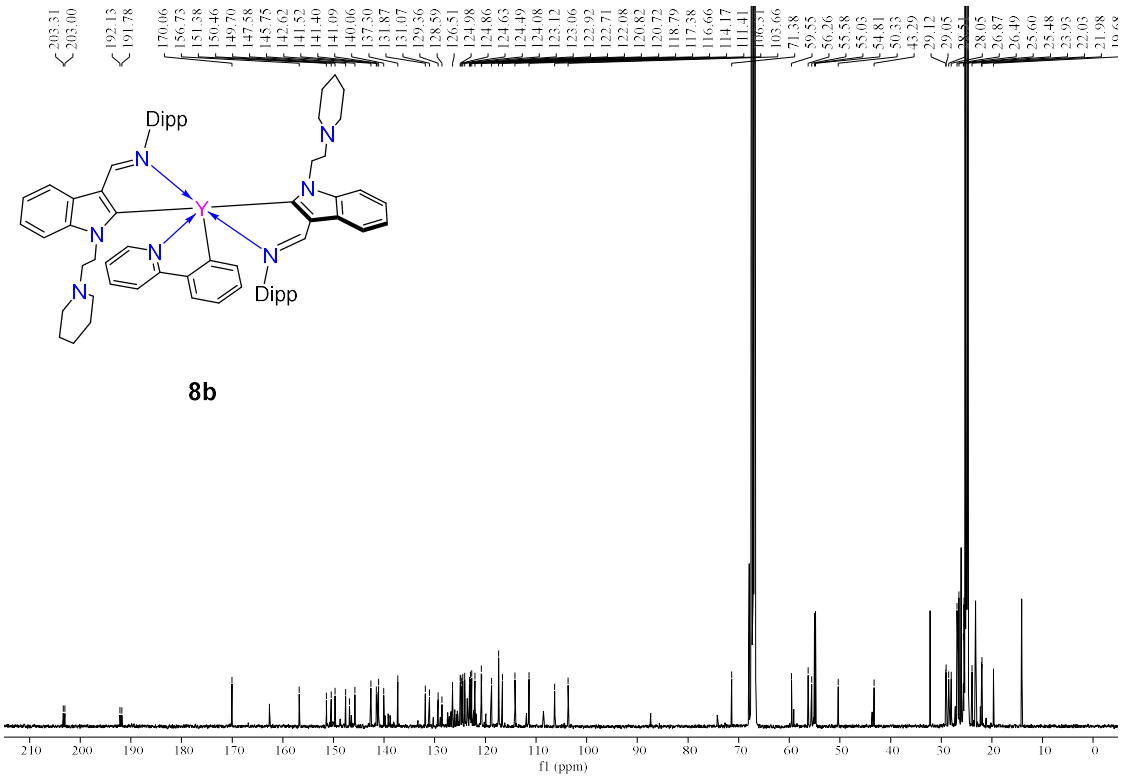


Fig. S42. $^{13}C\{^{1}H\}$ NMR spectrum of **8b** (125 MHz, THF-d_8, 298 K)

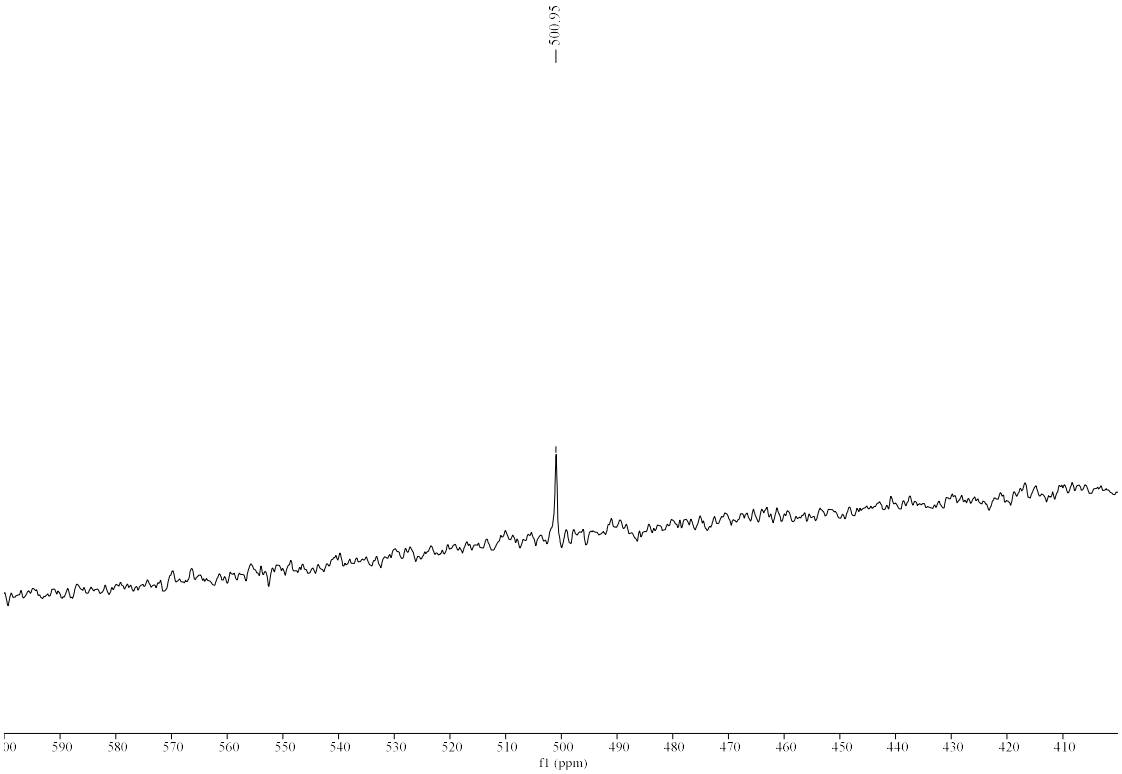


Fig. S43. ^{89}Y NMR spectrum of **8b** (24.5 MHz, C_6D_6, 298 K)

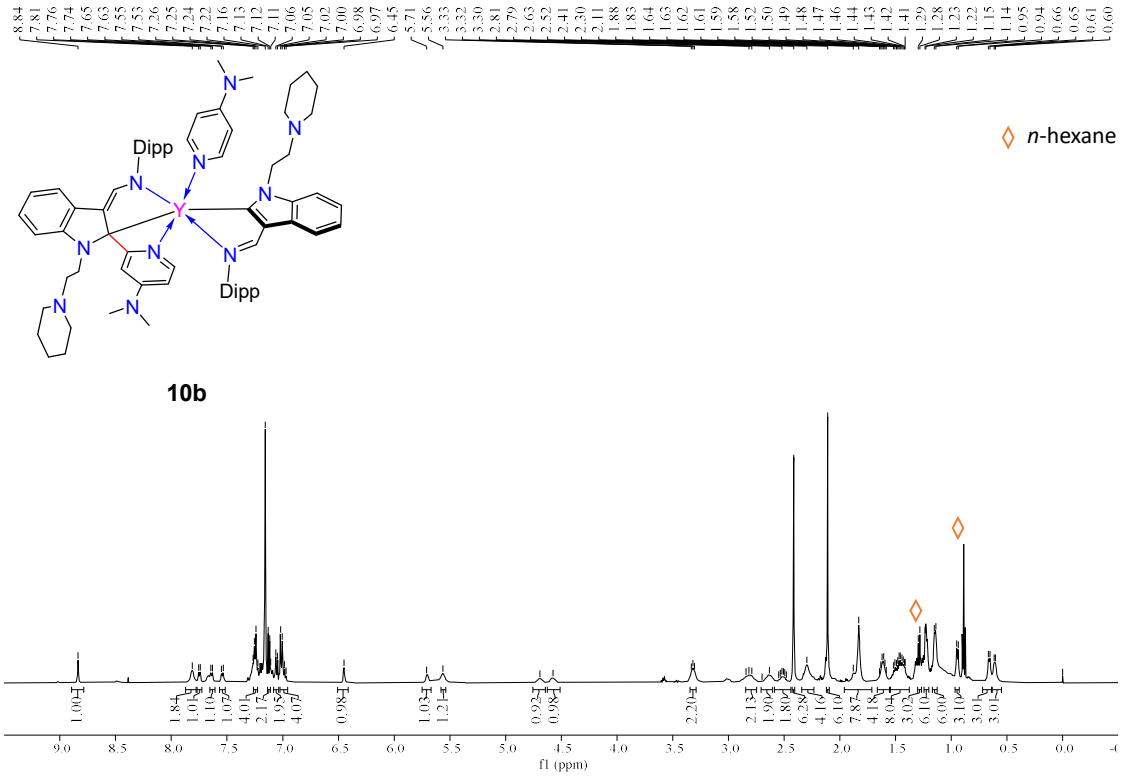


Fig. S44. ^{1}H NMR spectrum of **10b** (500 MHz, C_6D_6, 298 K)

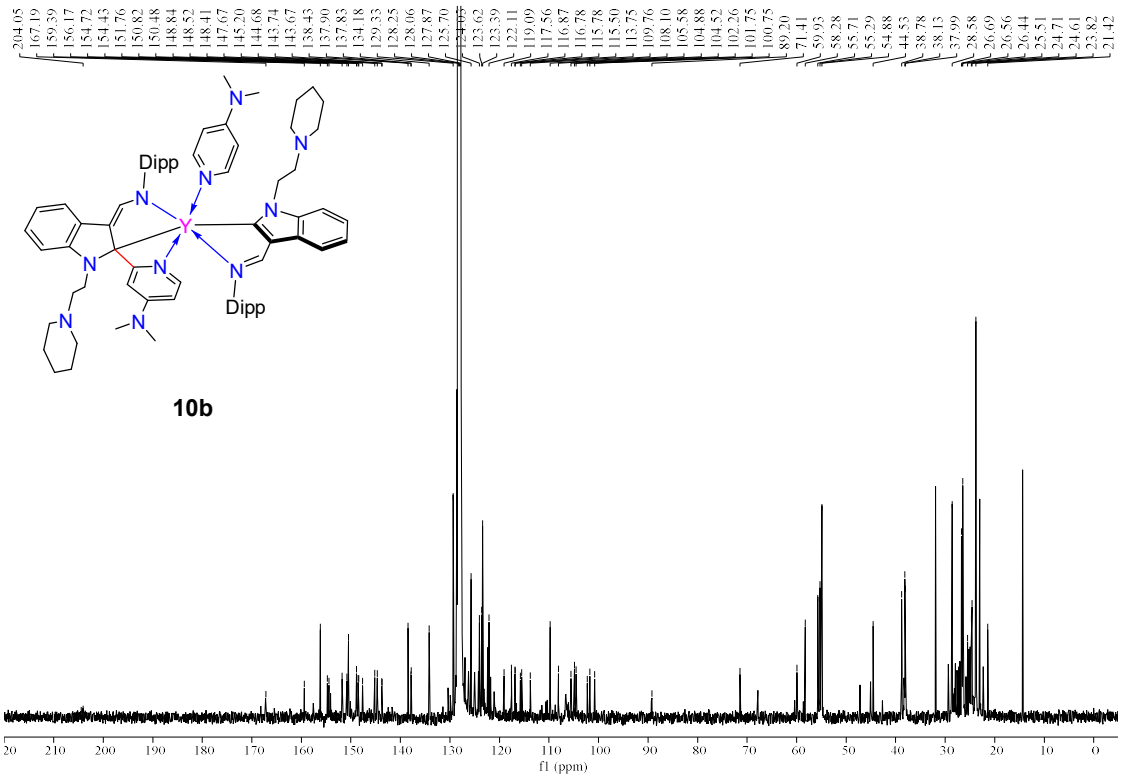


Fig. S45. ^{13}C{^{1}H} NMR spectrum of **10b** (125 MHz, C_6D_6, 298 K)

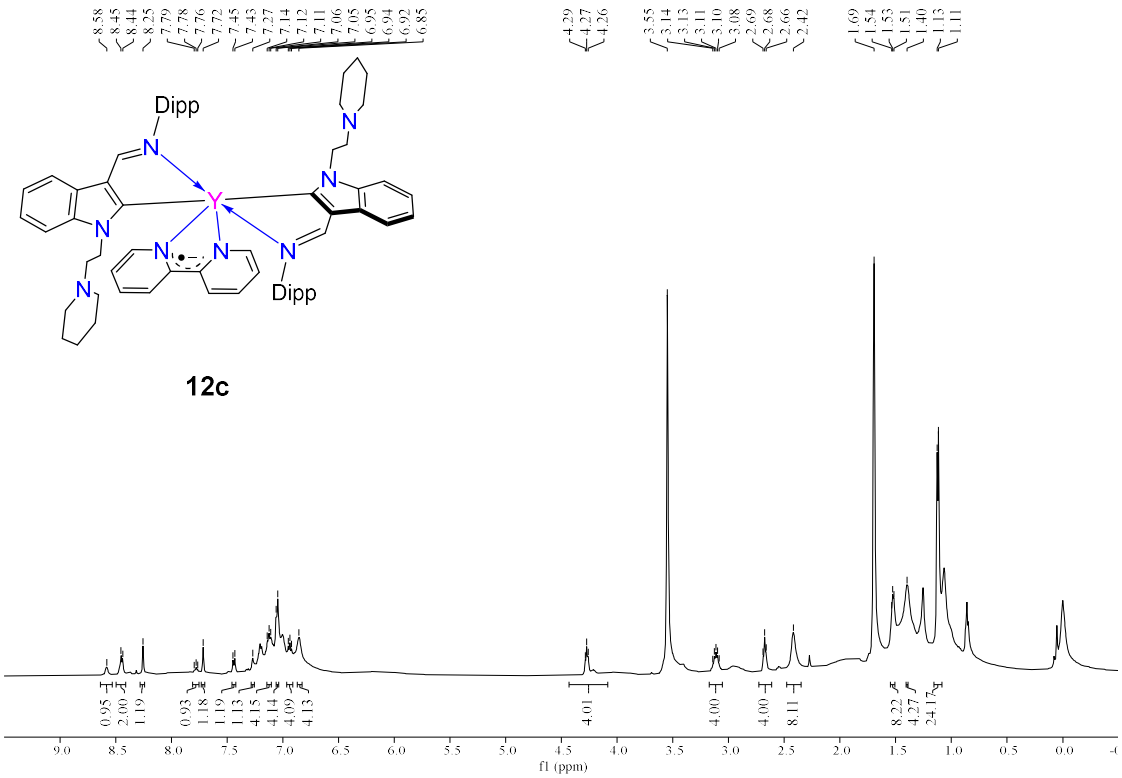


Fig. S46. ^{1}H NMR spectrum of **12c** (500 MHz, THF-d_8, 298 K)

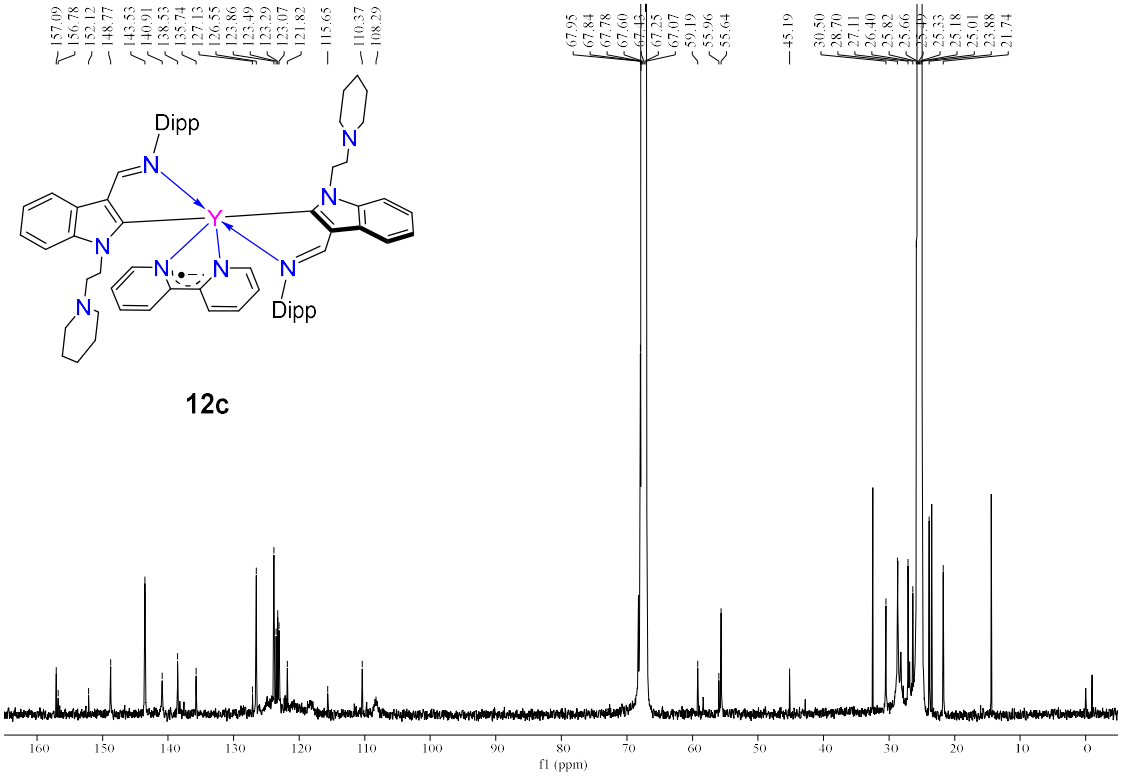


Fig. S47. ^{13}C{^{1}H} NMR spectrum of **12c** (125 MHz, THF-d_8, 298 K)

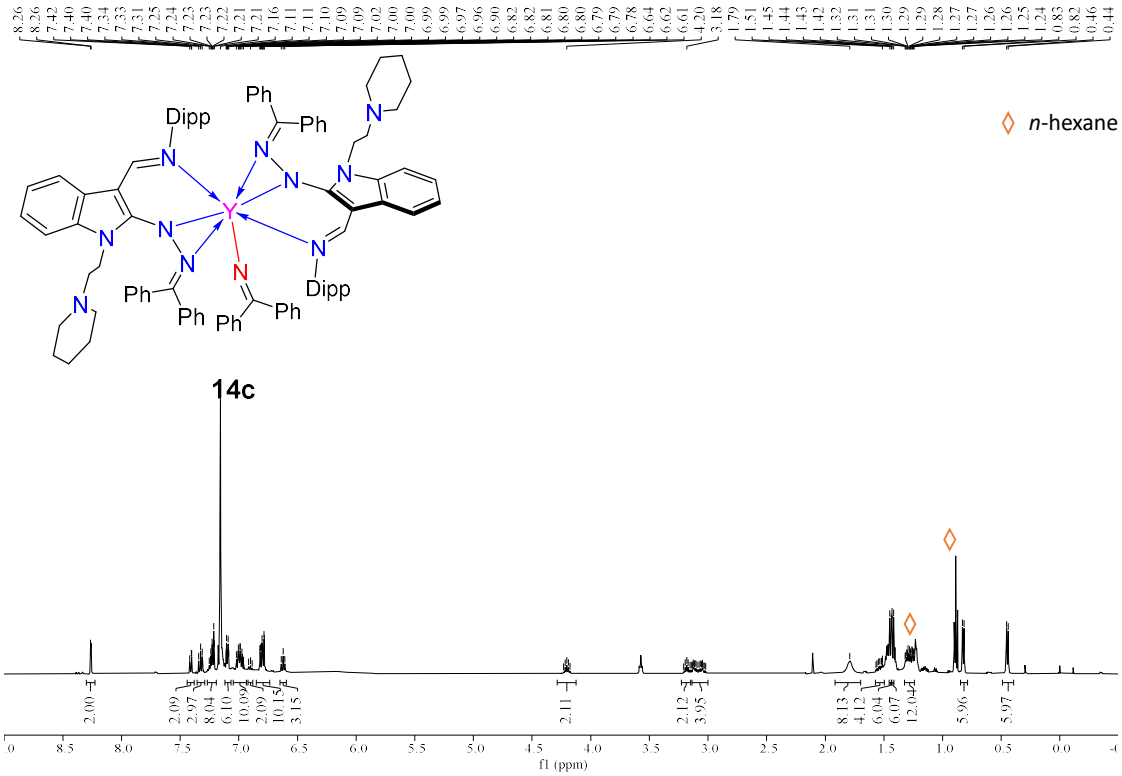


Fig. S48. ^{1}H NMR spectrum of **14c** (500 MHz, C_6D_6, 298 K)

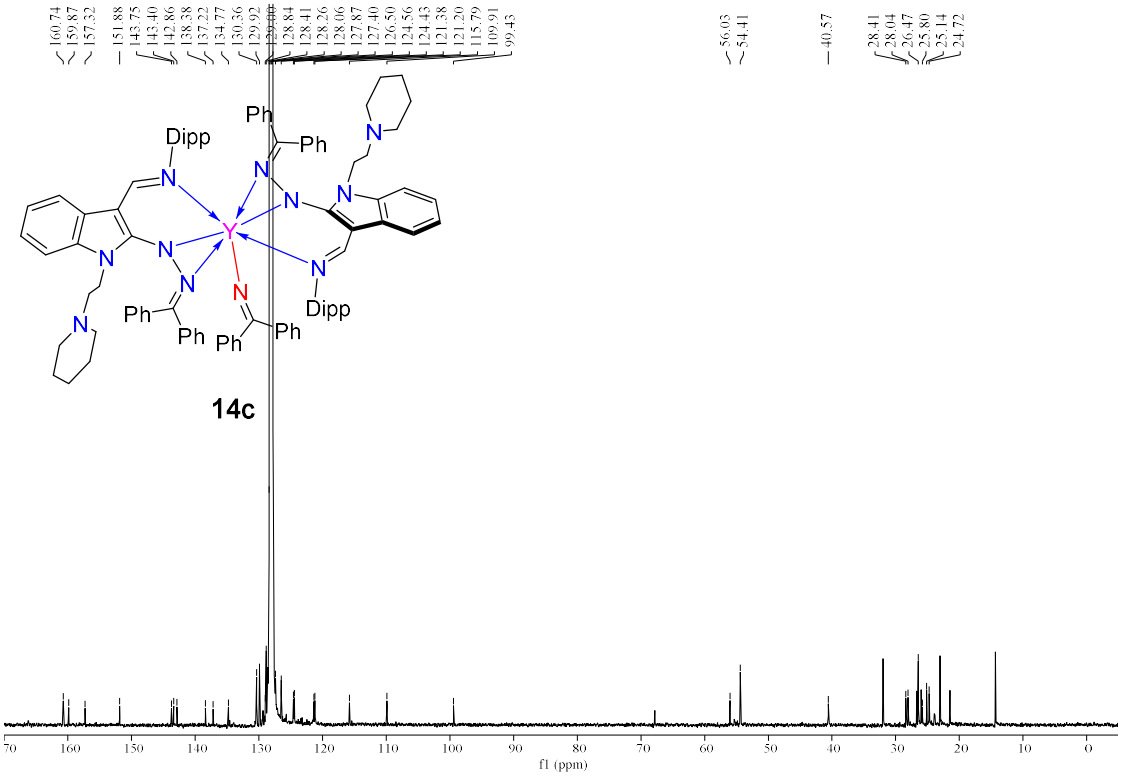


Fig. S49. ^{13}C{^{1}H} NMR spectrum of **14c** (125 MHz, C_6D_6, 298 K)

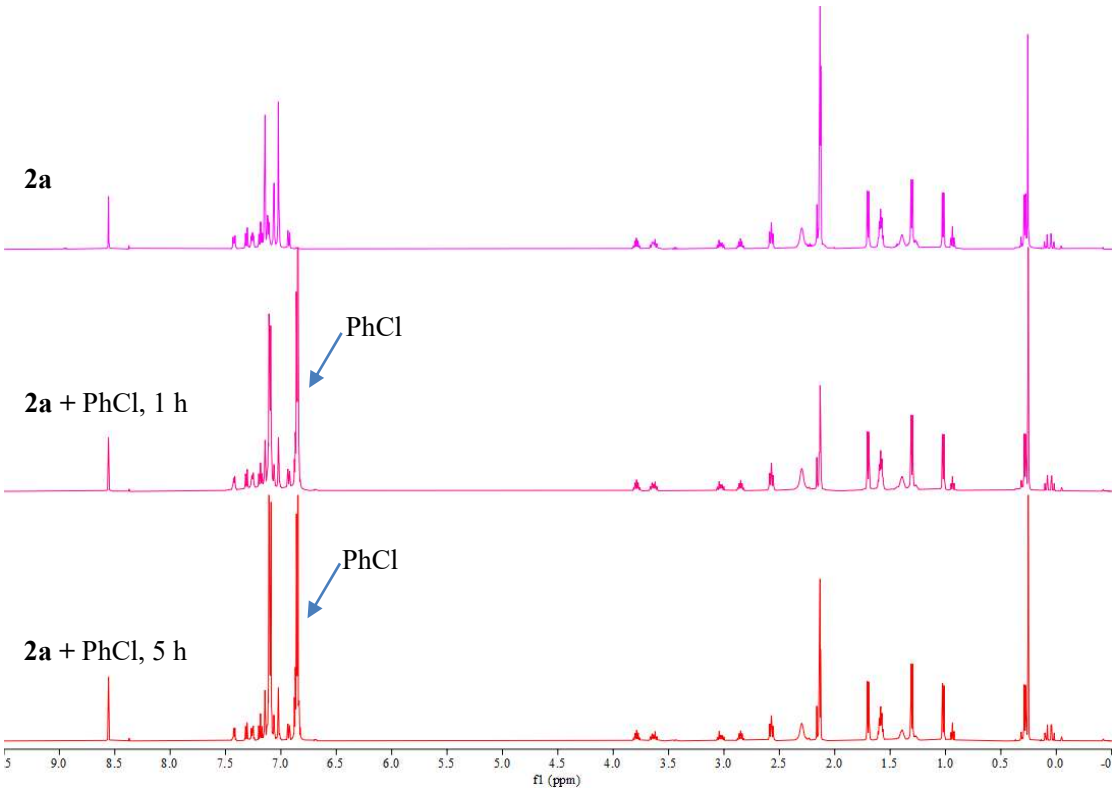


Fig. S50. The reaction of **2a** with PhCl monitored by ^{1}H NMR spectrum (500 MHz, C_7D_8, 298 K)

4. DFT Calculations

Computational details

The optimization of yttrium complexes was carried out by employing DFT hybrid functional (B3PW91)[11] along with small core pseudopotential Stuttgart basis set for yttrium, and silicon atoms with additional polarization functions for silicon atoms.[12] Pople basis sets (6-31G**) were employed for the rest of the atoms.[13] Frequency calculations were performed to locate minima for the optimized structures (maxima for TS structures). All the calculations were performed using Gaussian 09 suite of programs.[14]

Table S1. DFT computed natural charges for **1d**

Atom Label	Natural Charges
C1	-0.19823
C65	-1.66362
C80	-1.64763
N120	-0.60406
O122	-0.63627
O123	-0.61515
Y126	1.76870

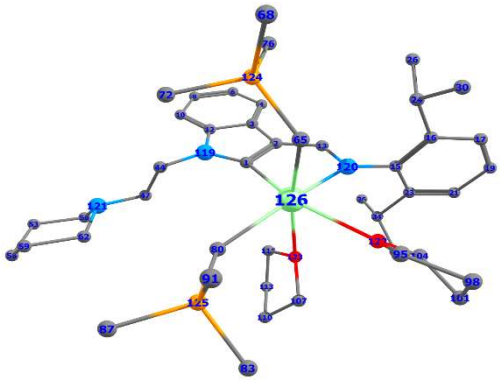


Table S2. DFT computed natural charges for **B**

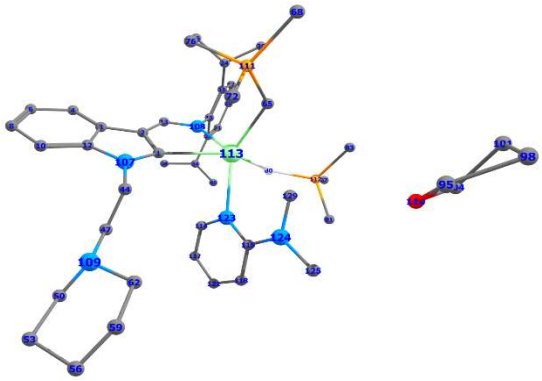
Atom Label	Natural Charges	
C1	-0.15301	
C65	-1.63233	
C80	-1.63411	
N108	-0.63435	
O110	-0.60922	
Y113	1.65191	
N123	-0.58339	

Table S3. DFT computed natural charges for **TS(B-C)**

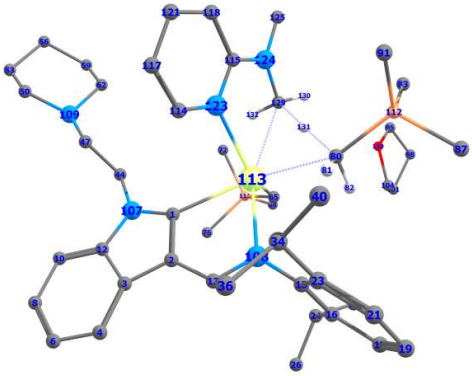
Atom Label	Natural Charges	
Y113	1.64070	
C80	-1.48911	
H131	0.24266	
C129	-0.66886	

Table S4. DFT computed Wiberg bond index for **TS(B-C)**

Atom Label	Wiberg bond index
Y113	0.0000
C80	0.2597
H131	0.0655
C129	0.1904

Table S5. DFT computed natural charges for **C**

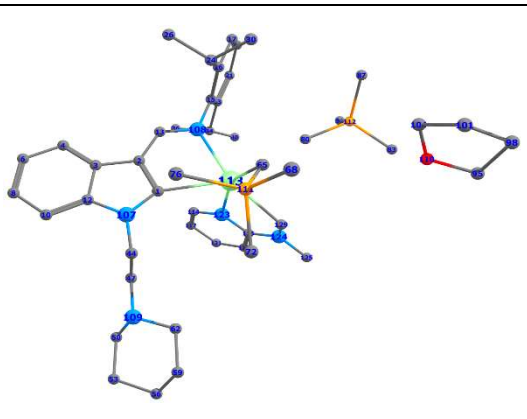
Atom Label	Natural Charges	
C1	-0.17668	
C65	-1.65738	
C80	-1.24387	
N108	-0.64407	
O110	-0.59366	
Y113	1.80566	
N123	-0.61825	
C129	-0.88502	

Table S6. DFT computed natural charges for **D**

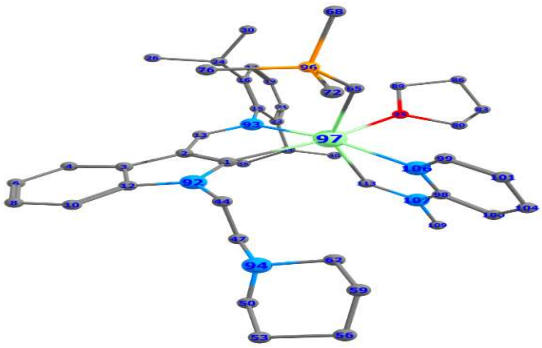
Atom Label	Natural Charges	
C1	-0.15925	
C65	-1.63333	
N93	-0.63973	
O95	-0.61545	
Y97	1.76058	
N106	-0.61844	
C113	-0.87897	

Table S7. DFT computed natural charges for **TS(D-E)**

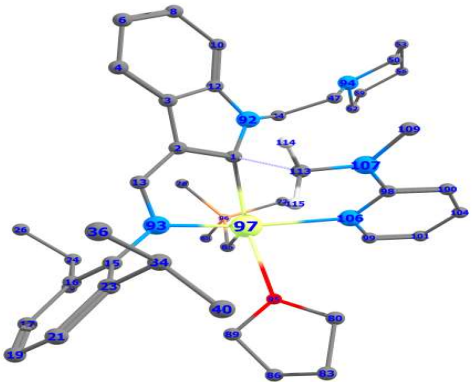
Atom Label	Natural Charges	
Y97	1.79592	
C1	-0.25395	
C113	-0.49957	
N107	-0.39461	

Table S8. DFT computed Wiberg bond index for **TS(D-E)**

Atom Label	Wiberg bond index
Y97	0.0000
C1	0.4060
C113	0.1530
N107	0.0143

Table S9. DFT computed natural charges for **TS(E-F)**

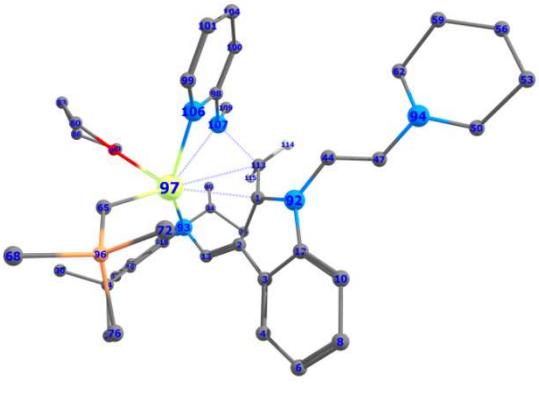
Atom Label	Natural Charges	
Y97	1.73303	
C1	-0.13528	
C113	-0.33082	
N107	-0.57631	

Table S10. DFT computed Wiberg bond index for **TS(E-F)**

Atom Label	Wiberg bond index
Y97	0.0000
C1	0.1942
C113	0.0708
N107	0.1586

Table S11. DFT computed natural charges for **TS(G-H)**

Atom Label	Natural Charges
Y97	1.81287
C65	-1.46132
C113	-0.94504
H114	0.25556

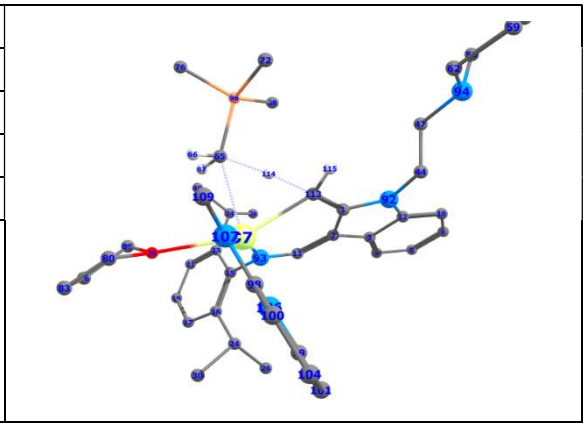


Table S12. DFT computed Wiberg bond index for **TS(G-H)**

Atom Label	Wiberg bond index
Y97	0.0000
C65	0.2475
C113	0.4063
H114	0.0616

Table S13. DFT computed natural charges for **H**

Atom Label	Natural Charges
Y81	1.72848
N78	-0.75622
N90	-0.63912
N91	-0.76698
C97	-0.87935

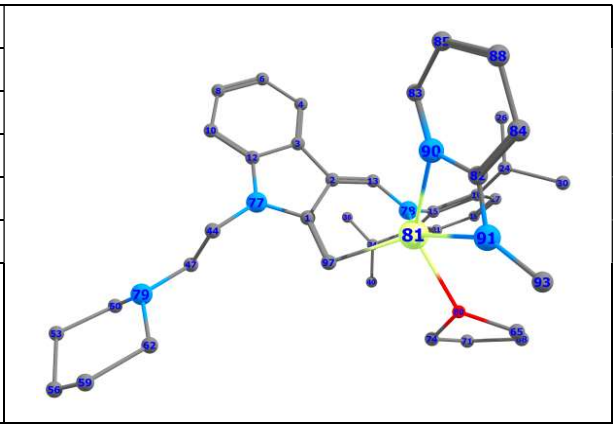


Table S14. DFT computed Wiberg bond index for **H**

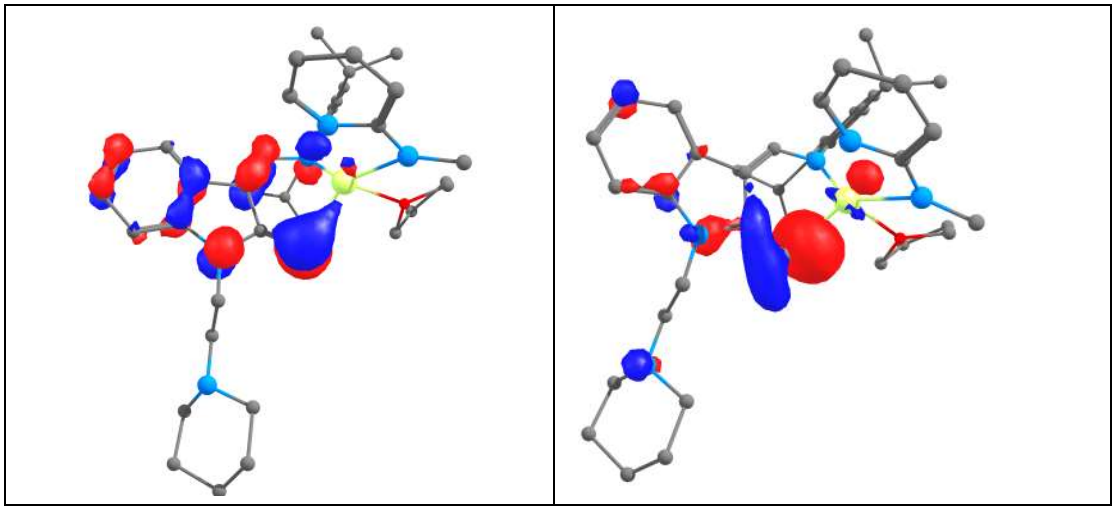
Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Y81	0.0000		
N78	0.3471		
N90	0.2536		
N91	0.3150		
C97	0.6703	C97	1.5994

C1	0.0929	C1	0.0000

Table S15. Second order perturbation analysis for **H**

Donor	Acceptor	E2 (kcal/mol)
BD (1) C1-C97 (53.58%) 0.7320*C1 s (42.14%) p 1.37 (57.84%) d 0.00 (0.03%) (46.42%) 0.6813*C97 s(37.26%) p 1.68 (62.68%) d 0.00 (0.06%)	LP* (1) Y81 s (40.92%) p 0.32 (13.16%) d 1.12 (45.92%)	7.45
BD (1) C1-C97 (53.58%) 0.7320*C1 s (42.14%) p 1.37 (57.84%) d 0.00 (0.03%) (46.42%) 0.6813*C97 s (37.26%) p 1.68 (62.68%) d 0.00 (0.06%)	LP* (7) Y81 s (3.11%) p 23.44 (72.85%) d 7.74 (24.05%)	7.48
BD (2) C1-C97 (47.41%) 0.6885*C1 s (0.04%) p 99.99 (99.91%) d 1.18 (0.05%) (52.59%) 0.7252*C97 s (0.02%) p 99.99 (99.89%) d 5.87 (0.09%)	LP* (4) Y81 s (3.72%) p 4.89 (18.21%) d 20.96 (78.07%)	11.13
BD (2) C1-C97 (47.41%) 0.6885*C1 s (0.04%) p 99.99 (99.91%) d 1.18 (0.05%) (52.59%) 0.7252*C97 s (0.02%) p 99.99 (99.89%) d 5.87 (0.09%)	BD* (2) C2-C13 (42.14%) 0.6492*C2 s (0.08%) p 99.99 (99.90%) d 0.23 (0.02%) (57.86%) -0.7607*C13 s (0.03%) p 99.99 (99.90%) d 2.33 (0.07%)	11.07
BD (1) C2-C13 (51.20%) 0.7156*C2 s (37.08%) p 1.70 (62.88%) d 0.00 (0.03%) (48.80%) 0.6985*C13 s (38.41%) p 1.60 (61.55%) d 0.00 (0.04%)	LP* (7) Y81 s (3.11%) p 23.44 (72.85%) d 7.74 (24.05%)	8.32
BD (2) C2-C13 (57.86%) 0.7607*C2 s (0.08%) p 99.99 (99.90%) d 0.23 (0.02%) (42.14%) 0.6492*C13 s (0.03%) p 99.99 (99.90%) d 2.33 (0.07%)	BD* (2) C1-C97 (52.59%) 0.7252*C1 s (0.04%) p 99.99 (99.91%) d 1.18 (0.05%) (47.41%) -0.6885*C97 s (0.02%) p 99.99 (99.89%) d 5.87 (0.09%)	15.93
LP (1) C97 s (30.28%) p 2.30 (69.70%) d 0.00 (0.02%)	LP* (1) Y81 s (40.92%) p 0.32 (13.16%) d 1.12 (45.92%)	111.28
LP (1) C97 s (30.28%) p 2.30 (69.70%) d 0.00 (0.02%)	LP* (4) Y81 s (3.72%) p 4.89 (18.21%) d 20.96 (78.07%)	7.33

Fig. S51. DFT computed MOs (left-HOMO and Right-HOMO-4) for **H**



Optimized coordinates

1d

C	4.393341000	6.275227000	-0.112615000
C	3.368531000	6.241177000	-1.089240000
C	3.596874000	7.284478000	-2.063392000
C	2.958470000	7.721599000	-3.231644000
H	2.051977000	7.237965000	-3.586792000
C	3.505843000	8.783562000	-3.942618000
H	3.019703000	9.127841000	-4.851355000
C	4.683320000	9.415267000	-3.510267000
H	5.094701000	10.236678000	-4.090113000
C	5.334484000	9.002939000	-2.351931000
H	6.249760000	9.488798000	-2.026812000
C	4.775321000	7.940707000	-1.638901000
C	2.303512000	5.301215000	-1.082630000
H	1.577164000	5.366548000	-1.902494000
C	0.987350000	3.536659000	-0.311947000
C	1.079075000	2.325578000	-1.035572000
C	-0.050323000	1.502039000	-1.109065000
H	0.007402000	0.574398000	-1.672218000
C	-1.245236000	1.850738000	-0.492779000
H	-2.111370000	1.198571000	-0.566761000
C	-1.326988000	3.048173000	0.209772000
H	-2.265756000	3.324176000	0.681559000
C	-0.227869000	3.904506000	0.316923000
C	2.344456000	1.925167000	-1.776576000
H	3.157334000	2.564903000	-1.419663000
C	2.184647000	2.173022000	-3.284824000
H	1.364899000	1.572602000	-3.695974000
H	3.101027000	1.906061000	-3.821697000
H	1.964980000	3.223969000	-3.496665000

C	2.755541000	0.471849000	-1.509677000
H	2.848963000	0.274009000	-0.437115000
H	3.724004000	0.262539000	-1.975302000
H	2.035215000	-0.243433000	-1.921977000
C	-0.356486000	5.220840000	1.067529000
H	0.651633000	5.495909000	1.394239000
C	-0.879088000	6.333476000	0.144514000
H	-0.223433000	6.486527000	-0.716797000
H	-0.955551000	7.285229000	0.683129000
H	-1.875123000	6.081483000	-0.236595000
C	-1.237343000	5.129060000	2.320174000
H	-2.293892000	4.979944000	2.072315000
H	-1.175355000	6.061458000	2.891733000
H	-0.932917000	4.307325000	2.976481000
C	6.375469000	7.764169000	0.271329000
H	7.209795000	7.927865000	-0.420118000
H	6.654695000	6.957893000	0.951038000
C	6.107254000	9.068036000	1.036562000
H	5.671548000	9.791429000	0.339058000
H	5.339269000	8.882325000	1.814332000
C	7.177352000	11.069472000	1.861631000
H	6.423255000	11.253777000	2.656811000
H	6.808142000	11.560397000	0.953654000
C	8.509384000	11.685953000	2.282471000
H	9.211098000	11.608215000	1.442457000
H	8.367451000	12.752919000	2.491613000
C	9.083301000	10.962415000	3.500633000
H	8.435906000	11.147489000	4.369948000
H	10.073791000	11.356643000	3.755731000
C	9.148359000	9.459048000	3.233013000
H	9.463570000	8.914137000	4.130160000
H	9.888734000	9.253373000	2.449796000
C	7.791924000	8.931200000	2.773040000
H	7.867108000	7.863505000	2.547488000
H	7.059189000	9.029264000	3.603306000
C	5.622038000	2.639507000	0.284181000
H	6.197991000	2.213501000	1.128144000
H	4.961372000	1.825671000	-0.064126000
C	7.842408000	1.333023000	-1.519594000
H	8.374754000	0.942022000	-0.644936000
H	8.580519000	1.510089000	-2.310649000
H	7.160655000	0.548736000	-1.868336000
C	8.183196000	4.211865000	-0.541838000
H	7.719620000	5.190496000	-0.381855000

H	8.957186000	4.328861000	-1.308675000
H	8.676834000	3.915049000	0.390334000
C	6.063068000	3.547371000	-2.673943000
H	5.357297000	2.807453000	-3.067466000
H	6.810277000	3.737861000	-3.452619000
H	5.511089000	4.476086000	-2.496640000
C	5.938582000	4.936332000	3.056065000
H	6.738544000	5.127927000	2.310616000
H	5.638316000	5.937322000	3.417880000
C	5.683155000	3.688427000	5.936366000
H	5.257737000	4.603115000	6.365939000
H	6.244866000	3.187927000	6.733226000
H	4.851982000	3.031222000	5.656142000
C	8.244268000	5.148403000	5.198522000
H	8.993154000	5.381482000	4.433029000
H	8.756122000	4.633064000	6.019843000
H	7.862164000	6.099499000	5.586969000
C	7.645070000	2.458761000	3.897812000
H	6.913261000	1.740010000	3.516022000
H	8.186558000	1.984050000	4.723864000
H	8.364576000	2.647432000	3.093561000
C	3.844358000	1.292413000	3.010882000
H	4.544236000	1.625442000	3.782111000
H	4.410184000	0.900444000	2.162961000
C	2.799843000	0.320960000	3.556249000
H	2.481466000	-0.380169000	2.777570000
H	3.184529000	-0.260982000	4.397648000
C	1.641543000	1.246241000	3.937563000
H	1.830075000	1.725858000	4.904683000
H	0.677981000	0.732550000	3.988385000
C	1.692063000	2.267155000	2.814610000
H	1.214803000	1.893154000	1.902821000
H	1.265147000	3.240629000	3.061254000
C	2.687434000	5.469479000	4.355598000
H	3.539110000	4.836033000	4.611282000
H	1.754661000	4.941461000	4.592579000
C	2.729782000	6.842154000	5.016635000
H	3.766868000	7.161969000	5.162945000
H	2.229843000	6.849596000	5.988890000
C	2.043902000	7.722205000	3.969785000
H	0.955142000	7.612915000	4.027571000
H	2.285984000	8.783706000	4.068860000
C	2.576860000	7.129542000	2.674013000
H	1.915675000	7.252136000	1.813555000

H	3.560025000	7.538094000	2.416664000
N	5.210696000	7.313126000	-0.470040000
N	2.133285000	4.377540000	-0.172425000
N	7.321329000	9.643088000	1.587341000
O	3.103053000	2.463544000	2.562800000
O	2.720942000	5.711738000	2.930345000
Si	6.881758000	2.924773000	-1.072378000
Si	6.834330000	4.088479000	4.460338000
Y	4.284032000	4.297235000	1.395654000

B

C	-0.323317000	1.203192000	-1.617286000
C	-1.456230000	1.214790000	-2.468023000
C	-1.195597000	2.051654000	-3.617279000
C	-1.903098000	2.427497000	-4.765923000
H	-2.914583000	2.069513000	-4.940603000
C	-1.290375000	3.265871000	-5.691109000
H	-1.830956000	3.563202000	-6.585546000
C	0.019674000	3.730012000	-5.492797000
H	0.477070000	4.377686000	-6.235424000
C	0.744333000	3.370427000	-4.359897000
H	1.759813000	3.727147000	-4.213532000
C	0.119856000	2.535149000	-3.432463000
C	-2.636204000	0.490989000	-2.168711000
H	-3.494795000	0.605487000	-2.840178000
C	-4.052729000	-0.879653000	-0.910425000
C	-4.357575000	-2.144412000	-1.456851000
C	-5.629616000	-2.679635000	-1.227165000
H	-5.881905000	-3.647460000	-1.652180000
C	-6.577167000	-1.996046000	-0.476217000
H	-7.560825000	-2.427833000	-0.312166000
C	-6.259191000	-0.755261000	0.064415000
H	-7.002881000	-0.223190000	0.650981000
C	-5.002506000	-0.177238000	-0.133860000
C	-3.366999000	-2.909380000	-2.319578000
H	-2.389809000	-2.428407000	-2.209444000
C	-3.754903000	-2.824398000	-3.803697000
H	-4.738270000	-3.275509000	-3.978941000
H	-3.025668000	-3.353149000	-4.427327000
H	-3.801432000	-1.785869000	-4.146481000
C	-3.210970000	-4.371178000	-1.881012000
H	-2.944537000	-4.443934000	-0.822149000
H	-2.422672000	-4.859323000	-2.463950000
H	-4.131728000	-4.944553000	-2.034916000

C	-4.697527000	1.195851000	0.445476000
H	-3.607729000	1.310454000	0.442448000
C	-5.283547000	2.308544000	-0.437664000
H	-4.891511000	2.264597000	-1.458472000
H	-5.046192000	3.296832000	-0.027284000
H	-6.374366000	2.222115000	-0.497851000
C	-5.167922000	1.353200000	1.896184000
H	-6.260275000	1.345123000	1.977623000
H	-4.824282000	2.312081000	2.300234000
H	-4.772407000	0.553695000	2.528428000
C	1.912797000	2.333738000	-1.707626000
H	2.653716000	2.248849000	-2.511599000
H	2.148340000	1.583800000	-0.950532000
C	1.970584000	3.754808000	-1.129581000
H	1.462897000	4.425143000	-1.831595000
H	1.391493000	3.786907000	-0.186616000
C	3.357035000	5.682442000	-0.751735000
H	2.841736000	5.959397000	0.192640000
H	2.799331000	6.157138000	-1.567523000
C	4.786769000	6.215521000	-0.717138000
H	5.248152000	6.049280000	-1.698752000
H	4.767999000	7.298055000	-0.544756000
C	5.603560000	5.504996000	0.361738000
H	5.206970000	5.772098000	1.351867000
H	6.648598000	5.835140000	0.340750000
C	5.508312000	3.991748000	0.172098000
H	6.013017000	3.462063000	0.988932000
H	6.009714000	3.704457000	-0.760660000
C	4.050435000	3.541887000	0.100790000
H	4.012028000	2.464539000	-0.090340000
H	3.561830000	3.710761000	1.084341000
C	0.283416000	-2.612520000	-0.600972000
H	0.789890000	-3.108148000	0.245760000
H	-0.613311000	-3.232806000	-0.785039000
C	1.921125000	-4.631702000	-2.377990000
H	2.468202000	-5.018411000	-1.510467000
H	2.567195000	-4.737259000	-3.257412000
H	1.045352000	-5.273422000	-2.525852000
C	2.999312000	-1.807340000	-1.907338000
H	2.784840000	-0.734452000	-1.847857000
H	3.663899000	-1.964451000	-2.764242000
H	3.548554000	-2.096665000	-1.003987000
C	0.525952000	-2.231030000	-3.688053000
H	-0.366029000	-2.833485000	-3.892072000

H	1.190544000	-2.320838000	-4.554692000
H	0.212685000	-1.184782000	-3.607974000
C	-2.034272000	-1.040441000	2.128316000
H	-2.344081000	-0.058336000	2.529038000
H	-2.939164000	-1.455420000	1.646371000
C	-1.026266000	-3.836460000	3.098535000
H	-1.721427000	-4.338675000	2.416194000
H	-0.884070000	-4.488123000	3.968308000
H	-0.066945000	-3.749783000	2.576815000
C	-3.279158000	-2.471626000	4.644383000
H	-3.703451000	-1.537427000	5.029731000
H	-3.072951000	-3.125283000	5.500265000
H	-4.048411000	-2.954110000	4.030853000
C	-0.454593000	-1.324283000	4.805077000
H	0.522428000	-1.171225000	4.334852000
H	-0.305156000	-1.945627000	5.695392000
H	-0.818732000	-0.345858000	5.138704000
C	5.613466000	-3.532655000	2.186410000
H	6.455620000	-2.868821000	2.414661000
H	5.394297000	-3.449881000	1.113531000
C	5.873082000	-4.984327000	2.593838000
H	6.309695000	-5.574652000	1.783903000
H	6.556438000	-5.027942000	3.449386000
C	4.476220000	-5.454318000	3.008125000
H	4.487954000	-6.317276000	3.679291000
H	3.879783000	-5.714158000	2.126566000
C	3.923716000	-4.197756000	3.669747000
H	2.832013000	-4.129244000	3.642309000
H	4.248061000	-4.129284000	4.719451000
N	0.597575000	2.008492000	-2.228113000
N	-2.762470000	-0.296668000	-1.127464000
N	3.332822000	4.237755000	-0.963540000
O	4.462537000	-3.100883000	2.925152000
Si	1.390273000	-2.817716000	-2.098439000
Si	-1.708396000	-2.129909000	3.610197000
Y	-0.673648000	-0.563209000	0.182909000
C	-0.395271000	2.259395000	1.622644000
C	1.441399000	1.226240000	2.590549000
H	-1.167110000	2.207531000	0.855630000
C	-0.308902000	3.370655000	2.438050000
C	1.607421000	2.337078000	3.458429000
H	-1.016745000	4.185027000	2.337685000
H	2.412014000	2.347906000	4.181748000
C	0.727083000	3.395163000	3.379805000

H	0.845857000	4.243879000	4.047779000
N	0.435098000	1.200461000	1.682305000
N	2.288354000	0.162712000	2.638059000
C	3.358487000	0.111953000	3.619362000
H	3.893177000	-0.831722000	3.506157000
H	4.071818000	0.933555000	3.476438000
H	2.968407000	0.163908000	4.644213000
C	2.044062000	-0.981112000	1.787823000
H	2.816181000	-1.732871000	1.959146000
H	1.077128000	-1.451479000	2.022772000
H	2.080556000	-0.712748000	0.722463000

TS(B-C)

C	4.270156000	6.545924000	-1.265967000
C	2.994017000	6.447273000	-1.872833000
C	2.955294000	7.274448000	-3.058104000
C	2.006708000	7.567558000	-4.045813000
H	1.012825000	7.128216000	-4.013738000
C	2.354174000	8.430576000	-5.079424000
H	1.625545000	8.663728000	-5.850998000
C	3.634390000	9.003263000	-5.146299000
H	3.881143000	9.669484000	-5.968106000
C	4.594380000	8.729271000	-4.176613000
H	5.584941000	9.170901000	-4.235302000
C	4.236492000	7.866771000	-3.139396000
C	1.961200000	5.622286000	-1.361011000
H	1.007050000	5.609150000	-1.900454000
C	0.922179000	4.127538000	0.102997000
C	0.742097000	2.815523000	-0.384416000
C	-0.394347000	2.106336000	0.017716000
H	-0.552749000	1.099461000	-0.359739000
C	-1.326322000	2.665299000	0.882890000
H	-2.203794000	2.098512000	1.182249000
C	-1.130210000	3.955135000	1.363781000
H	-1.862735000	4.387995000	2.039171000
C	-0.011961000	4.706552000	0.991692000
C	1.720998000	2.177555000	-1.357574000
H	2.609044000	2.816254000	-1.400589000
C	1.131718000	2.120790000	-2.774990000
H	0.226915000	1.502846000	-2.800922000
H	1.853815000	1.691062000	-3.478060000
H	0.861276000	3.118131000	-3.136104000
C	2.180941000	0.787167000	-0.900925000
H	2.605306000	0.819981000	0.107144000

H	2.948682000	0.400927000	-1.580034000
H	1.356904000	0.065262000	-0.894968000
C	0.158262000	6.129583000	1.503534000
H	1.220492000	6.384394000	1.405271000
C	-0.636087000	7.124847000	0.642745000
H	-0.323789000	7.095813000	-0.405321000
H	-0.499949000	8.149442000	1.007271000
H	-1.706850000	6.894151000	0.676104000
C	-0.217785000	6.289078000	2.981291000
H	-1.295270000	6.177789000	3.143923000
H	0.058909000	7.288328000	3.334117000
H	0.294171000	5.552738000	3.607210000
C	6.351075000	7.829185000	-1.804957000
H	6.910563000	7.818861000	-2.747060000
H	6.799653000	7.083538000	-1.146412000
C	6.423504000	9.237276000	-1.199019000
H	5.803576000	9.900103000	-1.812943000
H	5.968349000	9.223991000	-0.189907000
C	7.785895000	11.221107000	-1.045874000
H	7.378017000	11.528839000	-0.059634000
H	7.125890000	11.648285000	-1.809874000
C	9.196842000	11.782014000	-1.202808000
H	9.543469000	11.575510000	-2.223166000
H	9.172525000	12.871253000	-1.080039000
C	10.150858000	11.140243000	-0.195712000
H	9.868555000	11.451291000	0.820425000
H	11.178080000	11.487130000	-0.357186000
C	10.070269000	9.617781000	-0.298657000
H	10.674212000	9.139694000	0.481496000
H	10.470623000	9.290715000	-1.266391000
C	8.624095000	9.139652000	-0.183047000
H	8.589038000	8.053270000	-0.311673000
H	8.244881000	9.355298000	0.839034000
C	5.627607000	3.102386000	-0.198102000
H	5.883019000	2.496994000	0.689426000
H	4.847796000	2.527750000	-0.733673000
C	7.862586000	1.380081000	-1.597909000
H	8.172983000	0.934850000	-0.646041000
H	8.737254000	1.407204000	-2.258283000
H	7.121246000	0.712692000	-2.051813000
C	8.535966000	4.174381000	-0.576159000
H	8.238207000	5.221862000	-0.450705000
H	9.421712000	4.156619000	-1.221273000
H	8.832175000	3.792330000	0.407588000

C	6.683334000	3.823356000	-3.029274000
H	5.934636000	3.192806000	-3.522386000
H	7.561445000	3.869129000	-3.683157000
H	6.261551000	4.830141000	-2.948801000
C	3.342533000	3.810290000	2.724729000
H	2.458221000	4.453005000	2.574901000
H	3.163804000	2.901808000	2.121596000
C	4.785546000	2.338223000	5.103750000
H	5.110911000	1.585878000	4.377465000
H	4.592200000	1.832099000	6.056574000
H	5.621691000	3.027008000	5.265301000
C	1.739989000	2.108691000	4.783392000
H	0.810195000	2.583929000	4.453553000
H	1.623728000	1.827006000	5.836243000
H	1.863306000	1.188362000	4.201743000
C	2.995633000	4.789282000	5.646530000
H	3.822384000	5.495665000	5.518929000
H	2.954911000	4.501321000	6.702858000
H	2.066807000	5.319061000	5.409917000
C	7.589188000	-0.659612000	3.290063000
H	7.544502000	-0.574347000	4.382682000
H	8.558550000	-0.259850000	2.959064000
C	7.384495000	-2.095322000	2.798702000
H	8.324935000	-2.644278000	2.697446000
H	6.742596000	-2.651076000	3.491795000
C	6.657629000	-1.872441000	1.470135000
H	6.082954000	-2.740832000	1.135666000
H	7.370297000	-1.608797000	0.680689000
C	5.779467000	-0.672857000	1.810918000
H	5.520750000	-0.056808000	0.944549000
H	4.845500000	-0.997550000	2.296957000
N	4.983849000	7.406632000	-2.051046000
N	2.076156000	4.877980000	-0.286798000
N	7.777071000	9.768382000	-1.193459000
O	6.544289000	0.125606000	2.713326000
Si	7.125412000	3.120292000	-1.316853000
Si	3.228840000	3.267255000	4.526394000
Y	4.389662000	4.946526000	0.678044000
C	4.095149000	8.057197000	1.790773000
C	5.533559000	6.941261000	3.247445000
H	3.536478000	8.001502000	0.858527000
C	4.080001000	9.205451000	2.557402000
C	5.596998000	8.099662000	4.068791000
H	3.495437000	10.065466000	2.252323000

H	6.204861000	8.102029000	4.964519000
C	4.864804000	9.213364000	3.720711000
H	4.902216000	10.097279000	4.351884000
N	4.800883000	6.950520000	2.100279000
N	6.196765000	5.801176000	3.545140000
C	7.129424000	5.772278000	4.656353000
H	7.550100000	4.769862000	4.727898000
H	7.957785000	6.481718000	4.518315000
H	6.632010000	5.997163000	5.607245000
C	6.109880000	4.688927000	2.614753000
H	6.548069000	3.801056000	3.073530000
H	4.779455000	4.277468000	2.658785000
H	6.727255000	4.889814000	1.714068000

C

C	-0.035521000	1.452529000	-1.909344000
C	-1.386851000	1.440497000	-2.348438000
C	-1.511098000	2.278953000	-3.522370000
C	-2.553246000	2.646282000	-4.382711000
H	-3.562987000	2.274113000	-4.228814000
C	-2.279506000	3.497634000	-5.447669000
H	-3.080647000	3.787377000	-6.121980000
C	-0.982747000	3.988094000	-5.668902000
H	-0.796418000	4.649368000	-6.510331000
C	0.069309000	3.639658000	-4.827302000
H	1.071110000	4.020092000	-5.003639000
C	-0.213673000	2.786630000	-3.760046000
C	-2.423145000	0.695391000	-1.727974000
H	-3.410324000	0.725994000	-2.203732000
C	-3.441450000	-0.746254000	-0.192144000
C	-3.708952000	-2.029158000	-0.719814000
C	-4.835855000	-2.715789000	-0.254976000
H	-5.062037000	-3.698091000	-0.660803000
C	-5.672682000	-2.166096000	0.708566000
H	-6.544493000	-2.715611000	1.053306000
C	-5.389483000	-0.907157000	1.227483000
H	-6.047275000	-0.478362000	1.978139000
C	-4.278057000	-0.177752000	0.795840000
C	-2.831614000	-2.660912000	-1.790389000
H	-1.906807000	-2.077965000	-1.850501000
C	-3.507991000	-2.592299000	-3.168150000
H	-4.449569000	-3.153260000	-3.171269000
H	-2.858017000	-3.019403000	-3.939554000
H	-3.736748000	-1.560730000	-3.453457000

C	-2.434671000	-4.103712000	-1.452250000
H	-1.957656000	-4.166223000	-0.469771000
H	-1.727326000	-4.483509000	-2.197018000
H	-3.298119000	-4.777842000	-1.450238000
C	-4.013105000	1.215015000	1.344024000
H	-2.959205000	1.442474000	1.153357000
C	-4.851376000	2.263259000	0.595764000
H	-4.651191000	2.246536000	-0.480089000
H	-4.631715000	3.270867000	0.965995000
H	-5.922132000	2.076776000	0.736076000
C	-4.234915000	1.328896000	2.856206000
H	-5.290826000	1.222659000	3.128904000
H	-3.909155000	2.313619000	3.207278000
H	-3.668473000	0.569765000	3.403438000
C	2.035641000	2.617834000	-2.667945000
H	2.480478000	2.654578000	-3.667602000
H	2.528247000	1.812255000	-2.120861000
C	2.236829000	3.970910000	-1.972897000
H	1.670638000	4.726082000	-2.529566000
H	1.792523000	3.925934000	-0.960380000
C	3.797562000	5.814450000	-1.834870000
H	3.414114000	6.184663000	-0.860495000
H	3.197452000	6.294753000	-2.616467000
C	5.263204000	6.215644000	-1.984314000
H	5.595103000	5.954726000	-2.997221000
H	5.356335000	7.303168000	-1.880129000
C	6.133987000	5.492885000	-0.956163000
H	5.880704000	5.853642000	0.051169000
H	7.194051000	5.722110000	-1.115339000
C	5.887344000	3.985913000	-1.028342000
H	6.428173000	3.462119000	-0.231525000
H	6.256935000	3.595462000	-1.984798000
C	4.397021000	3.675315000	-0.917994000
H	4.239405000	2.596866000	-1.017061000
H	4.034077000	3.960304000	0.092767000
C	1.173360000	-2.057988000	-0.685988000
H	1.568182000	-2.501670000	0.246188000
H	0.366532000	-2.733245000	-1.026427000
C	3.242718000	-3.914358000	-2.197343000
H	3.667208000	-4.296759000	-1.262183000
H	4.031647000	-3.939994000	-2.958271000
H	2.452528000	-4.606150000	-2.510727000
C	4.017264000	-1.064698000	-1.414956000
H	3.721643000	-0.014743000	-1.310167000

H	4.838461000	-1.110949000	-2.138922000
H	4.404413000	-1.393554000	-0.443855000
C	1.941141000	-1.563257000	-3.661216000
H	1.144702000	-2.217186000	-4.035091000
H	2.752171000	-1.575360000	-4.398144000
H	1.536279000	-0.547149000	-3.613219000
C	-1.197173000	-1.870419000	2.556545000
H	-2.108376000	-1.631573000	1.997606000
H	-0.478787000	-2.370695000	1.894994000
C	-0.058315000	-3.447310000	4.972495000
H	0.689569000	-3.923005000	4.328654000
H	-0.279358000	-4.127672000	5.802382000
H	0.384916000	-2.539204000	5.395798000
C	-2.392168000	-4.621100000	3.286472000
H	-3.274036000	-4.389245000	2.680214000
H	-2.699306000	-5.307605000	4.082625000
H	-1.673424000	-5.147479000	2.649770000
C	-2.890270000	-2.181967000	5.128411000
H	-2.488711000	-1.246055000	5.531709000
H	-3.156264000	-2.822338000	5.976308000
H	-3.810577000	-1.948332000	4.583074000
C	3.402657000	-5.805420000	3.488193000
H	3.140562000	-5.885126000	4.550248000
H	4.354403000	-5.260256000	3.414653000
C	3.487425000	-7.167933000	2.794498000
H	4.494705000	-7.592931000	2.822280000
H	2.806386000	-7.884100000	3.268427000
C	3.000876000	-6.833053000	1.382404000
H	2.620890000	-7.699437000	0.833816000
H	3.807820000	-6.383096000	0.793320000
C	1.921786000	-5.797267000	1.679932000
H	1.745218000	-5.096256000	0.858457000
H	0.967339000	-6.291149000	1.924793000
N	0.630795000	2.265078000	-2.775565000
N	-2.289319000	-0.022762000	-0.636103000
N	3.635128000	4.368305000	-1.953937000
O	2.391437000	-5.059748000	2.807528000
Si	2.543338000	-2.151560000	-1.952328000
Si	-1.628735000	-3.038869000	3.999234000
Y	0.117284000	-0.020687000	0.056057000
C	-0.816877000	3.170914000	0.973323000
C	0.670179000	2.249465000	2.518761000
H	-1.331924000	3.028012000	0.025923000
C	-0.970968000	4.342456000	1.689715000

C	0.574133000	3.435151000	3.303211000
H	-1.613275000	5.135604000	1.324796000
H	1.152409000	3.537344000	4.212568000
C	-0.245794000	4.460528000	2.885235000
H	-0.315648000	5.366295000	3.482420000
N	-0.033236000	2.145164000	1.355317000
N	1.447155000	1.201443000	2.871040000
C	2.268253000	1.288994000	4.064924000
H	2.694435000	0.303112000	4.252384000
H	3.098172000	2.004352000	3.953962000
H	1.679004000	1.575826000	4.944064000
C	1.702465000	0.139879000	1.897460000
H	1.809637000	-0.804530000	2.448172000
H	-0.744513000	-0.949745000	2.943269000
H	2.692627000	0.322215000	1.431146000

D

C	0.039938000	0.754092000	-1.497323000
C	-1.225087000	0.695312000	-2.135733000
C	-1.176106000	1.447434000	-3.369776000
C	-2.074639000	1.737500000	-4.403966000
H	-3.095634000	1.364935000	-4.377600000
C	-1.643216000	2.511986000	-5.475617000
H	-2.333428000	2.742327000	-6.282615000
C	-0.328112000	2.999606000	-5.534758000
H	-0.016192000	3.598919000	-6.385464000
C	0.584110000	2.726285000	-4.519521000
H	1.601559000	3.103053000	-4.570529000
C	0.142708000	1.952137000	-3.446008000
C	-2.321773000	-0.023050000	-1.601378000
H	-3.260291000	-0.015552000	-2.167838000
C	-3.462354000	-1.389827000	-0.074672000
C	-3.718732000	-2.686699000	-0.576651000
C	-4.865498000	-3.355899000	-0.136042000
H	-5.080925000	-4.348668000	-0.521645000
C	-5.736394000	-2.775789000	0.778621000
H	-6.623460000	-3.312015000	1.105258000
C	-5.470303000	-1.500608000	1.266436000
H	-6.159441000	-1.044793000	1.972066000
C	-4.339795000	-0.787498000	0.856527000
C	-2.805137000	-3.346017000	-1.599056000
H	-1.858822000	-2.795507000	-1.600060000
C	-3.401252000	-3.245929000	-3.012212000
H	-4.360976000	-3.772390000	-3.067900000

H	-2.726193000	-3.693186000	-3.749866000
H	-3.576729000	-2.206252000	-3.304065000
C	-2.483293000	-4.807419000	-1.261346000
H	-2.080284000	-4.908499000	-0.249096000
H	-1.736803000	-5.198814000	-1.960095000
H	-3.366080000	-5.451694000	-1.337013000
C	-4.101531000	0.627291000	1.359717000
H	-3.045038000	0.860126000	1.190182000
C	-4.930181000	1.637124000	0.550221000
H	-4.696085000	1.583219000	-0.517322000
H	-4.731952000	2.660695000	0.887385000
H	-6.002732000	1.443104000	0.665933000
C	-4.369753000	0.788872000	2.860056000
H	-5.430267000	0.666899000	3.107270000
H	-4.076553000	1.791969000	3.187587000
H	-3.800707000	0.060997000	3.446566000
C	2.201311000	1.888886000	-2.023024000
H	2.798979000	1.814377000	-2.938249000
H	2.587725000	1.159388000	-1.309009000
C	2.301300000	3.320017000	-1.477171000
H	1.722535000	3.973486000	-2.139288000
H	1.812179000	3.362833000	-0.484411000
C	3.726755000	5.264372000	-1.381076000
H	3.301506000	5.640204000	-0.426010000
H	3.105958000	5.672437000	-2.187172000
C	5.161961000	5.765782000	-1.524012000
H	5.529226000	5.491721000	-2.521068000
H	5.175289000	6.860310000	-1.460185000
C	6.063701000	5.145869000	-0.456292000
H	5.767182000	5.524247000	0.532713000
H	7.107499000	5.445072000	-0.607549000
C	5.926222000	3.623656000	-0.476022000
H	6.488802000	3.168991000	0.347804000
H	6.340630000	3.227421000	-1.411644000
C	4.460120000	3.208729000	-0.377014000
H	4.383083000	2.119102000	-0.437917000
H	4.060579000	3.500045000	0.617199000
C	1.116112000	-2.664392000	0.242533000
H	1.642136000	-2.999300000	1.154307000
H	0.209423000	-3.304940000	0.196190000
C	2.434964000	-5.106048000	-1.262056000
H	2.995975000	-5.416155000	-0.372861000
H	3.008123000	-5.414565000	-2.144453000
H	1.490841000	-5.662885000	-1.265329000

C	3.841165000	-2.407786000	-1.335444000
H	3.781000000	-1.315668000	-1.393268000
H	4.369261000	-2.756994000	-2.230059000
H	4.461884000	-2.669760000	-0.470447000
C	1.211938000	-2.800552000	-2.867084000
H	0.245036000	-3.313180000	-2.924613000
H	1.801160000	-3.111148000	-3.737385000
H	1.023011000	-1.725147000	-2.949238000
C	-0.409598000	-1.536990000	3.870700000
H	-0.409252000	-0.458508000	4.037133000
H	0.627768000	-1.896980000	3.856930000
C	-1.260681000	-2.339535000	4.839619000
H	-0.737656000	-2.556244000	5.775015000
H	-2.182478000	-1.797029000	5.076766000
C	-1.564352000	-3.591840000	4.012905000
H	-2.456904000	-4.126197000	4.348544000
H	-0.718203000	-4.285987000	4.056072000
C	-1.730251000	-3.033838000	2.599074000
H	-1.306279000	-3.688155000	1.832638000
H	-2.773098000	-2.817732000	2.351330000
N	0.828356000	1.514115000	-2.308844000
N	-2.282287000	-0.693286000	-0.472834000
N	3.670520000	3.807732000	-1.449975000
O	-1.009389000	-1.774393000	2.578126000
Si	2.112990000	-3.220214000	-1.242068000
Y	-0.038146000	-0.524537000	0.640455000
C	1.953042000	1.246450000	2.739738000
C	3.207093000	-0.416920000	1.685948000
C	3.131192000	1.700367000	3.400042000
C	4.383088000	-0.045273000	2.310028000
H	3.090407000	2.553383000	4.065047000
H	5.304981000	-0.580946000	2.115314000
C	4.326526000	1.049785000	3.183409000
H	5.223386000	1.396171000	3.691138000
N	2.021930000	0.197967000	1.867943000
N	0.744880000	1.814913000	2.949857000
H	3.180231000	-1.250581000	0.992687000
C	0.647642000	2.975023000	3.818735000
H	1.150358000	3.859610000	3.398646000
H	-0.409163000	3.212821000	3.940146000
H	1.069095000	2.780828000	4.813592000
C	-0.402424000	1.422895000	2.130809000
H	-0.630066000	2.259341000	1.440161000
H	-1.275371000	1.350809000	2.799096000

TS(D-E)

C	-0.301208000	1.696335000	-1.606233000
C	-1.658565000	1.796994000	-2.197301000
C	-1.670232000	2.906406000	-3.133725000
C	-2.644333000	3.503987000	-3.933963000
H	-3.673762000	3.154893000	-3.904956000
C	-2.283572000	4.548160000	-4.791464000
H	-3.039771000	5.013426000	-5.418211000
C	-0.961709000	4.990803000	-4.858101000
H	-0.695107000	5.796387000	-5.537076000
C	0.031733000	4.411638000	-4.058246000
H	1.060495000	4.754721000	-4.122536000
C	-0.339648000	3.385046000	-3.195224000
C	-2.667385000	0.932811000	-1.850919000
H	-3.655106000	1.042074000	-2.306613000
C	-3.612349000	-0.880671000	-0.633459000
C	-3.701449000	-2.199149000	-1.153694000
C	-4.769029000	-3.013607000	-0.764840000
H	-4.841932000	-4.022583000	-1.161460000
C	-5.753664000	-2.552922000	0.103315000
H	-6.579035000	-3.199794000	0.389249000
C	-5.683122000	-1.250538000	0.582864000
H	-6.466289000	-0.882337000	1.241834000
C	-4.629150000	-0.399744000	0.231645000
C	-2.704753000	-2.694486000	-2.189621000
H	-1.784716000	-2.114857000	-2.057681000
C	-3.219735000	-2.393200000	-3.606391000
H	-4.164080000	-2.916574000	-3.796558000
H	-2.493284000	-2.716782000	-4.360389000
H	-3.393545000	-1.322241000	-3.743836000
C	-2.347643000	-4.177898000	-2.051356000
H	-2.015475000	-4.424429000	-1.037269000
H	-1.537603000	-4.434726000	-2.741831000
H	-3.193634000	-4.830822000	-2.294336000
C	-4.621114000	1.024030000	0.767973000
H	-3.665184000	1.473942000	0.484759000
C	-5.734442000	1.865525000	0.126030000
H	-5.639175000	1.886003000	-0.963491000
H	-5.698940000	2.899223000	0.488616000
H	-6.724140000	1.459610000	0.364828000
C	-4.725555000	1.078583000	2.297894000
H	-5.686368000	0.693236000	2.656538000
H	-4.636169000	2.111956000	2.652005000

H	-3.935001000	0.486695000	2.769823000
C	1.898891000	2.644832000	-2.420126000
H	2.189277000	2.686241000	-3.479613000
H	2.261353000	1.696577000	-2.015690000
C	2.552957000	3.843569000	-1.712337000
H	1.902221000	4.713413000	-1.855971000
H	2.594698000	3.651037000	-0.622037000
C	4.312223000	5.481263000	-1.778313000
H	4.450526000	5.483342000	-0.674693000
H	3.529108000	6.215787000	-2.001131000
C	5.621042000	5.894708000	-2.446373000
H	5.443086000	6.008923000	-3.523009000
H	5.935693000	6.872279000	-2.061910000
C	6.703869000	4.841385000	-2.213119000
H	6.961719000	4.816721000	-1.144386000
H	7.622221000	5.100711000	-2.752762000
C	6.192415000	3.466203000	-2.640623000
H	6.919299000	2.683560000	-2.393654000
H	6.050280000	3.447388000	-3.728451000
C	4.858094000	3.147689000	-1.969464000
H	4.486349000	2.184977000	-2.333458000
H	5.013533000	3.038342000	-0.873896000
C	0.950823000	-2.115793000	-0.580397000
H	1.363862000	-2.534871000	0.356825000
H	0.188416000	-2.847034000	-0.907408000
C	2.960184000	-3.945002000	-2.194169000
H	3.351590000	-4.400545000	-1.277425000
H	3.762093000	-3.953149000	-2.941629000
H	2.152963000	-4.587746000	-2.563274000
C	3.821029000	-1.161638000	-1.263318000
H	3.547098000	-0.123799000	-1.044453000
H	4.615715000	-1.148143000	-2.017588000
H	4.242773000	-1.592611000	-0.347638000
C	1.719349000	-1.472885000	-3.521886000
H	0.895869000	-2.075427000	-3.922140000
H	2.521099000	-1.471231000	-4.268973000
H	1.351295000	-0.447267000	-3.412034000
C	-1.123447000	-0.474182000	3.412605000
H	-1.575402000	0.521402000	3.425904000
H	-0.063074000	-0.383485000	3.671485000
C	-1.845166000	-1.482422000	4.300383000
H	-1.431441000	-1.507017000	5.311933000
H	-2.910210000	-1.238563000	4.374251000
C	-1.654280000	-2.793051000	3.533129000

H	-2.389858000	-3.557153000	3.796728000
H	-0.653785000	-3.203082000	3.710391000
C	-1.797064000	-2.333771000	2.091098000
H	-1.245190000	-2.944826000	1.372239000
H	-2.843710000	-2.259948000	1.778141000
N	0.456086000	2.626569000	-2.327381000
N	-2.489369000	-0.075623000	-0.951818000
N	3.862707000	4.177597000	-2.251834000
O	-1.214428000	-1.001295000	2.066182000
Si	2.318663000	-2.177288000	-1.859219000
Y	-0.304131000	-0.102341000	-0.078867000
C	1.254516000	2.437493000	1.611611000
C	2.143856000	0.316450000	2.031497000
C	2.220548000	3.004965000	2.490850000
C	3.127666000	0.801604000	2.865674000
H	2.224962000	4.069819000	2.684113000
H	3.849967000	0.132679000	3.318462000
C	3.143175000	2.188257000	3.102665000
H	3.881080000	2.622135000	3.772032000
N	1.210943000	1.085826000	1.428032000
N	0.342848000	3.185340000	0.951436000
H	2.077179000	-0.747451000	1.812582000
C	0.354711000	4.631606000	1.101714000
H	1.361294000	5.037172000	0.959632000
H	-0.287487000	5.062798000	0.334626000
H	-0.021088000	4.945471000	2.085922000
C	-0.718217000	2.568962000	0.198708000
H	-1.296034000	3.347488000	-0.289819000
H	-1.413894000	2.034802000	0.875716000

E

C	-0.003536000	1.184439000	-0.583096000
C	-1.120359000	0.653493000	-1.423127000
C	-0.841484000	1.067634000	-2.800724000
C	-1.492255000	0.817536000	-4.006454000
H	-2.396971000	0.215467000	-4.031996000
C	-0.961284000	1.325643000	-5.194370000
H	-1.464532000	1.133419000	-6.137548000
C	0.228113000	2.057063000	-5.173617000
H	0.647090000	2.429754000	-6.104775000
C	0.895153000	2.319967000	-3.975388000
H	1.822210000	2.884673000	-3.978142000
C	0.334146000	1.848179000	-2.783913000
C	-2.178233000	-0.179358000	-1.073590000

H	-2.871779000	-0.444666000	-1.873039000
C	-3.591029000	-1.393429000	0.461905000
C	-4.026210000	-2.555460000	-0.232126000
C	-5.233608000	-3.157264000	0.143486000
H	-5.570104000	-4.041493000	-0.392771000
C	-6.005693000	-2.661449000	1.184742000
H	-6.936646000	-3.149635000	1.460521000
C	-5.577389000	-1.525872000	1.866076000
H	-6.188878000	-1.128785000	2.671302000
C	-4.391865000	-0.876059000	1.518204000
C	-3.238556000	-3.181945000	-1.375681000
H	-2.268242000	-2.677478000	-1.434666000
C	-3.952011000	-2.983111000	-2.722593000
H	-4.913321000	-3.509371000	-2.735064000
H	-3.344372000	-3.374689000	-3.545966000
H	-4.157403000	-1.927187000	-2.922862000
C	-2.955830000	-4.675549000	-1.155604000
H	-2.431682000	-4.854690000	-0.212456000
H	-2.329949000	-5.065598000	-1.965598000
H	-3.878265000	-5.266015000	-1.141496000
C	-3.994047000	0.423620000	2.200614000
H	-2.898449000	0.434888000	2.241887000
C	-4.422215000	1.625015000	1.342005000
H	-3.982500000	1.569859000	0.342548000
H	-4.107939000	2.568919000	1.803986000
H	-5.512609000	1.649516000	1.233706000
C	-4.520915000	0.577423000	3.630055000
H	-5.609317000	0.701952000	3.656696000
H	-4.088545000	1.470364000	4.094838000
H	-4.269931000	-0.285463000	4.256546000
C	2.220070000	2.232003000	-1.274033000
H	2.814843000	1.754743000	-2.068631000
H	2.495736000	1.753623000	-0.331681000
C	2.563105000	3.728187000	-1.258075000
H	2.066577000	4.196335000	-2.114732000
H	2.121815000	4.197730000	-0.356370000
C	4.250563000	5.387041000	-1.708994000
H	3.917308000	6.067367000	-0.895364000
H	3.659519000	5.643002000	-2.596139000
C	5.733396000	5.623250000	-1.984086000
H	6.022461000	5.040642000	-2.867795000
H	5.897325000	6.680929000	-2.222164000
C	6.581650000	5.195651000	-0.786713000
H	6.374068000	5.863762000	0.061790000

H	7.650241000	5.294154000	-1.010838000
C	6.239608000	3.758930000	-0.393857000
H	6.768839000	3.466436000	0.520937000
H	6.558682000	3.072744000	-1.188263000
C	4.735526000	3.593462000	-0.185675000
H	4.512279000	2.546800000	0.042152000
H	4.420763000	4.189823000	0.699971000
C	0.948415000	-3.027208000	-0.622059000
H	1.372436000	-3.571019000	0.244487000
H	0.149448000	-3.683223000	-1.012509000
C	2.990384000	-4.690971000	-2.357842000
H	3.413704000	-5.178937000	-1.472312000
H	3.778866000	-4.631804000	-3.117278000
H	2.199100000	-5.341816000	-2.746865000
C	3.765279000	-1.923096000	-1.293848000
H	3.466087000	-0.884888000	-1.110859000
H	4.584138000	-1.909346000	-2.021813000
H	4.161894000	-2.330325000	-0.356152000
C	1.647889000	-2.193182000	-3.534662000
H	0.813190000	-2.778659000	-3.937035000
H	2.429857000	-2.162296000	-4.301692000
H	1.289453000	-1.169677000	-3.381758000
C	-0.859880000	-1.760600000	3.708550000
H	-1.313601000	-0.771886000	3.602593000
H	0.100832000	-1.655648000	4.224619000
C	-1.773490000	-2.772464000	4.394400000
H	-1.615399000	-2.801763000	5.475698000
H	-2.823335000	-2.526837000	4.205707000
C	-1.409393000	-4.079849000	3.687142000
H	-2.188888000	-4.842054000	3.764267000
H	-0.477948000	-4.496045000	4.087591000
C	-1.213763000	-3.601456000	2.258546000
H	-0.543810000	-4.217447000	1.655112000
H	-2.172356000	-3.483365000	1.740376000
N	0.803224000	1.999592000	-1.490094000
N	-2.371418000	-0.742957000	0.176842000
N	3.988900000	3.991948000	-1.372982000
O	-0.597003000	-2.294966000	2.387206000
Si	2.294884000	-2.965281000	-1.922981000
Y	-0.128172000	-1.063492000	0.275729000
C	1.406418000	1.429901000	2.222679000
C	2.138930000	-0.763144000	2.525093000
C	2.403937000	1.869212000	3.136068000
C	3.150980000	-0.403869000	3.394114000

H	2.501323000	2.919393000	3.374580000
H	3.813922000	-1.152183000	3.812484000
C	3.265851000	0.955031000	3.706756000
H	4.031674000	1.300498000	4.395911000
N	1.278270000	0.102376000	1.951450000
N	0.576885000	2.317633000	1.612929000
H	1.987876000	-1.809264000	2.264047000
C	0.591795000	3.700679000	2.057158000
H	1.563823000	4.176594000	1.883121000
H	-0.151534000	4.257906000	1.488335000
H	0.346018000	3.791444000	3.124366000
C	-0.477898000	1.903840000	0.666847000
H	-1.020016000	2.821999000	0.404847000
H	-1.212781000	1.271901000	1.193953000

TS(E-F)

C	-0.067112000	1.086312000	-1.168264000
C	-1.107012000	0.430877000	-1.981080000
C	-0.659364000	0.555317000	-3.371057000
C	-1.226622000	0.159646000	-4.579868000
H	-2.182949000	-0.356815000	-4.596808000
C	-0.558594000	0.429487000	-5.776944000
H	-0.998314000	0.124366000	-6.721745000
C	0.676566000	1.083635000	-5.760037000
H	1.190458000	1.284309000	-6.696541000
C	1.266967000	1.490435000	-4.563424000
H	2.225393000	2.000813000	-4.566855000
C	0.587476000	1.227435000	-3.367778000
C	-2.239217000	-0.269962000	-1.562114000
H	-2.906882000	-0.636119000	-2.346343000
C	-3.820823000	-1.037151000	0.073869000
C	-4.306202000	-2.301960000	-0.349701000
C	-5.588626000	-2.704136000	0.043954000
H	-5.962005000	-3.671922000	-0.283506000
C	-6.390857000	-1.906341000	0.847681000
H	-7.381138000	-2.242887000	1.142947000
C	-5.912305000	-0.669723000	1.269635000
H	-6.542259000	-0.042102000	1.893918000
C	-4.647107000	-0.217358000	0.891737000
C	-3.488308000	-3.259552000	-1.202908000
H	-2.502488000	-2.812997000	-1.375706000
C	-4.132541000	-3.482514000	-2.579103000
H	-5.112110000	-3.964715000	-2.484778000
H	-3.501849000	-4.124068000	-3.203302000

H	-4.283198000	-2.536362000	-3.108217000
C	-3.254838000	-4.601015000	-0.493294000
H	-2.765201000	-4.455186000	0.474825000
H	-2.616194000	-5.251130000	-1.100952000
H	-4.196636000	-5.132078000	-0.316199000
C	-4.166683000	1.165200000	1.297631000
H	-3.075626000	1.093340000	1.370095000
C	-4.480891000	2.189202000	0.195246000
H	-4.030463000	1.893837000	-0.756514000
H	-4.098406000	3.182313000	0.460856000
H	-5.563333000	2.274429000	0.045896000
C	-4.703745000	1.647125000	2.648301000
H	-5.778260000	1.858791000	2.612744000
H	-4.208401000	2.580101000	2.939673000
H	-4.535281000	0.910096000	3.440977000
C	2.132314000	2.275241000	-1.725667000
H	2.981907000	1.935421000	-2.330811000
H	2.387154000	2.044206000	-0.686967000
C	1.969282000	3.790956000	-1.934358000
H	1.693424000	3.953879000	-2.981887000
H	1.117696000	4.163663000	-1.331304000
C	3.275776000	5.783502000	-2.384890000
H	2.493613000	6.493155000	-2.041396000
H	3.083219000	5.587326000	-3.445820000
C	4.649332000	6.428258000	-2.215249000
H	5.401689000	5.772104000	-2.670783000
H	4.675629000	7.381078000	-2.756973000
C	4.974775000	6.634574000	-0.735862000
H	4.291523000	7.386845000	-0.316163000
H	5.990603000	7.027589000	-0.611876000
C	4.804684000	5.320155000	0.025864000
H	4.938359000	5.473286000	1.103517000
H	5.568073000	4.602347000	-0.299776000
C	3.426594000	4.716987000	-0.236331000
H	3.343603000	3.753655000	0.277700000
H	2.647107000	5.380797000	0.197471000
C	0.557261000	-3.327411000	-0.995423000
H	1.364095000	-3.553198000	-0.270111000
H	-0.222587000	-4.085608000	-0.796924000
C	2.030171000	-5.472620000	-2.758398000
H	2.841611000	-5.571799000	-2.027866000
H	2.443304000	-5.695945000	-3.749067000
H	1.283237000	-6.240606000	-2.526709000
C	2.629654000	-2.502115000	-3.185297000

H	2.251248000	-1.475406000	-3.229580000
H	3.031107000	-2.750451000	-4.174247000
H	3.467479000	-2.529529000	-2.478330000
C	-0.102915000	-3.662912000	-4.016947000
H	-0.925667000	-4.341487000	-3.765143000
H	0.287563000	-3.962037000	-4.996004000
H	-0.510369000	-2.651552000	-4.114420000
C	0.102440000	-3.489721000	2.480331000
H	1.139263000	-3.148998000	2.416768000
H	-0.016413000	-4.378536000	1.852723000
C	-0.380731000	-3.716678000	3.908805000
H	-0.218183000	-4.746489000	4.237222000
H	0.144283000	-3.051731000	4.603654000
C	-1.859731000	-3.332249000	3.819955000
H	-2.299800000	-3.077041000	4.787511000
H	-2.445794000	-4.147503000	3.382200000
C	-1.817108000	-2.142716000	2.874209000
H	-2.732320000	-1.986257000	2.299828000
H	-1.560960000	-1.216412000	3.402414000
N	0.958384000	1.522554000	-2.080283000
N	-2.527118000	-0.564995000	-0.246604000
N	3.200127000	4.516408000	-1.663522000
O	-0.752425000	-2.449328000	1.941366000
Si	1.254807000	-3.725331000	-2.687204000
Y	-0.300459000	-1.237721000	-0.134291000
C	1.578310000	0.442513000	1.565846000
C	3.158479000	-0.941381000	0.540363000
C	2.591185000	1.079143000	2.311310000
C	4.200883000	-0.366754000	1.243081000
H	2.343242000	1.877946000	3.001833000
H	5.217648000	-0.713385000	1.094363000
C	3.902258000	0.660820000	2.154711000
H	4.694836000	1.128481000	2.732410000
N	1.874454000	-0.567948000	0.699396000
N	0.238204000	0.750480000	1.554139000
H	3.329493000	-1.744432000	-0.171053000
C	-0.254613000	1.514601000	2.686116000
H	0.141437000	2.542895000	2.724398000
H	-1.343396000	1.586954000	2.623049000
H	0.000690000	1.017559000	3.627960000
C	-0.253678000	1.683212000	0.115922000
H	0.315403000	2.596952000	0.297993000
H	-1.296481000	1.785668000	0.406047000

F

C	0.112764000	1.361513000	-1.361680000
C	-1.150105000	0.923788000	-1.884687000
C	-1.162990000	1.252571000	-3.298491000
C	-2.095014000	1.108805000	-4.328280000
H	-3.076091000	0.682012000	-4.136609000
C	-1.755783000	1.525213000	-5.615476000
H	-2.479840000	1.422214000	-6.418851000
C	-0.496941000	2.070462000	-5.887289000
H	-0.252615000	2.387327000	-6.897050000
C	0.455110000	2.213284000	-4.875744000
H	1.432696000	2.634291000	-5.090937000
C	0.103307000	1.801844000	-3.595361000
C	-2.153050000	0.232719000	-1.198332000
H	-3.099989000	0.122883000	-1.738768000
C	-3.319833000	-0.867951000	0.492705000
C	-3.713942000	-2.181941000	0.148403000
C	-4.910392000	-2.680457000	0.677898000
H	-5.228146000	-3.685840000	0.414052000
C	-5.704982000	-1.915428000	1.521828000
H	-6.631685000	-2.321467000	1.918666000
C	-5.313926000	-0.619924000	1.844563000
H	-5.947592000	-0.020711000	2.491957000
C	-4.129447000	-0.073031000	1.342170000
C	-2.909959000	-3.049035000	-0.808390000
H	-1.938058000	-2.569573000	-0.962314000
C	-3.600145000	-3.138668000	-2.178299000
H	-4.586997000	-3.607732000	-2.091047000
H	-3.001583000	-3.737783000	-2.872853000
H	-3.741903000	-2.149410000	-2.623613000
C	-2.643569000	-4.452325000	-0.248873000
H	-2.170792000	-4.399037000	0.735777000
H	-1.976240000	-5.005579000	-0.917865000
H	-3.565195000	-5.036985000	-0.151242000
C	-3.758572000	1.368156000	1.658021000
H	-2.670975000	1.451698000	1.548855000
C	-4.392906000	2.329326000	0.639302000
H	-4.076644000	2.101224000	-0.382357000
H	-4.108066000	3.365068000	0.855738000
H	-5.486296000	2.263459000	0.675022000
C	-4.122324000	1.796847000	3.083992000
H	-5.205589000	1.879717000	3.224320000
H	-3.698727000	2.783900000	3.297677000
H	-3.741028000	1.094037000	3.831694000

C	2.151628000	2.474250000	-2.305808000
H	2.713507000	2.285852000	-3.224747000
H	2.706141000	1.988497000	-1.500129000
C	2.040880000	3.987047000	-2.073296000
H	1.529067000	4.425467000	-2.937203000
H	1.393615000	4.174617000	-1.195837000
C	3.351594000	6.007653000	-2.349301000
H	2.712852000	6.623345000	-1.681591000
H	2.919036000	6.074952000	-3.354323000
C	4.769000000	6.575194000	-2.351347000
H	5.359270000	6.039148000	-3.105256000
H	4.738924000	7.629998000	-2.649015000
C	5.421390000	6.414519000	-0.978685000
H	4.894362000	7.047286000	-0.250281000
H	6.461830000	6.758885000	-1.000609000
C	5.341874000	4.956042000	-0.529886000
H	5.719137000	4.839233000	0.492749000
H	5.966921000	4.332997000	-1.181790000
C	3.903887000	4.448655000	-0.600001000
H	3.873737000	3.390082000	-0.321048000
H	3.285347000	4.992557000	0.145241000
C	1.057309000	-2.757008000	-0.062987000
H	1.726769000	-3.207905000	0.691464000
H	0.236601000	-3.487543000	-0.189651000
C	2.840703000	-4.431598000	-2.047425000
H	3.538898000	-4.711396000	-1.249965000
H	3.401268000	-4.408898000	-2.989405000
H	2.091341000	-5.227815000	-2.123248000
C	3.407858000	-1.452812000	-1.633794000
H	2.994265000	-0.452245000	-1.471034000
H	3.971817000	-1.441274000	-2.573124000
H	4.115056000	-1.656950000	-0.821778000
C	0.864437000	-2.361650000	-3.140720000
H	0.076683000	-3.119480000	-3.223097000
H	1.415820000	-2.355177000	-4.087513000
H	0.378830000	-1.386812000	-3.028827000
C	-0.169956000	-3.680865000	3.062897000
H	0.886612000	-3.413285000	2.999195000
H	-0.366715000	-4.520940000	2.388505000
C	-0.645241000	-3.954916000	4.484772000
H	-0.546234000	-5.010087000	4.753066000
H	-0.064883000	-3.364280000	5.201725000
C	-2.095515000	-3.469678000	4.446780000
H	-2.501482000	-3.240391000	5.435629000

H	-2.742279000	-4.217746000	3.975415000
C	-1.987102000	-2.232945000	3.569314000
H	-2.900135000	-1.994869000	3.019910000
H	-1.657116000	-1.355657000	4.137991000
N	0.853994000	1.837918000	-2.415104000
N	-2.086680000	-0.323901000	0.006831000
N	3.350984000	4.604286000	-1.943613000
O	-0.955967000	-2.548193000	2.599540000
Si	2.010978000	-2.749897000	-1.671837000
Y	0.079065000	-0.872968000	1.097171000
C	1.607713000	-0.036177000	3.429678000
C	3.346416000	-1.402087000	2.631053000
C	2.451668000	0.419496000	4.484970000
C	4.214951000	-1.011373000	3.639105000
H	2.084222000	1.142230000	5.204805000
H	5.221548000	-1.410019000	3.691502000
C	3.737088000	-0.077901000	4.573564000
H	4.386238000	0.261184000	5.378224000
N	2.096939000	-0.943366000	2.522097000
N	0.340099000	0.314543000	3.169205000
H	3.654156000	-2.112572000	1.866293000
C	-0.256382000	1.331606000	3.999604000
H	0.308204000	2.279278000	3.988764000
H	-1.265585000	1.554429000	3.643424000
H	-0.345619000	1.027346000	5.056998000
C	0.538931000	1.332291000	-0.011517000
H	1.458478000	1.858343000	0.235640000
H	-0.270991000	1.607073000	0.676660000

G

C	-0.093123000	1.327695000	-1.342673000
C	-1.463298000	0.953220000	-1.547397000
C	-1.776207000	1.225052000	-2.937320000
C	-2.921936000	1.099245000	-3.726252000
H	-3.858112000	0.751007000	-3.297536000
C	-2.857894000	1.435450000	-5.078699000
H	-3.749305000	1.348652000	-5.693761000
C	-1.664013000	1.882514000	-5.653493000
H	-1.635561000	2.139895000	-6.708348000
C	-0.502658000	2.005118000	-4.887187000
H	0.422900000	2.352227000	-5.336832000
C	-0.579614000	1.673891000	-3.539381000
C	-2.317440000	0.346838000	-0.618227000
H	-3.375389000	0.308873000	-0.902097000

C	-3.057803000	-0.706555000	1.336846000
C	-3.785481000	-1.858043000	0.948941000
C	-4.798804000	-2.325366000	1.795503000
H	-5.366502000	-3.205774000	1.504418000
C	-5.094064000	-1.690775000	2.994421000
H	-5.884252000	-2.071198000	3.636181000
C	-4.377363000	-0.556149000	3.362872000
H	-4.622643000	-0.054857000	4.294050000
C	-3.361970000	-0.042587000	2.552763000
C	-3.519076000	-2.607605000	-0.348950000
H	-2.634204000	-2.164751000	-0.814276000
C	-4.690151000	-2.461030000	-1.332344000
H	-5.605238000	-2.906140000	-0.926040000
H	-4.466010000	-2.964965000	-2.279020000
H	-4.907151000	-1.410849000	-1.550911000
C	-3.204239000	-4.089906000	-0.106769000
H	-2.365129000	-4.199651000	0.584793000
H	-2.936399000	-4.582030000	-1.048113000
H	-4.063156000	-4.626124000	0.311530000
C	-2.654654000	1.250098000	2.931267000
H	-1.628218000	1.185936000	2.551906000
C	-3.324416000	2.448553000	2.238603000
H	-3.325614000	2.336052000	1.150816000
H	-2.797365000	3.378023000	2.480739000
H	-4.364336000	2.551860000	2.568871000
C	-2.567443000	1.491374000	4.440871000
H	-3.547052000	1.711813000	4.879728000
H	-1.927344000	2.355899000	4.642174000
H	-2.144813000	0.630322000	4.968297000
C	1.751751000	2.227512000	-2.782792000
H	2.062988000	1.968381000	-3.798802000
H	2.434991000	1.710311000	-2.105232000
C	1.818000000	3.749918000	-2.604983000
H	1.091853000	4.196109000	-3.293853000
H	1.485245000	4.013231000	-1.582829000
C	3.084654000	5.692184000	-3.286668000
H	2.750926000	6.319331000	-2.433465000
H	2.340117000	5.814614000	-4.081947000
C	4.447472000	6.182604000	-3.769240000
H	4.710242000	5.638425000	-4.685217000
H	4.381873000	7.245980000	-4.028145000
C	5.519412000	5.945529000	-2.705445000
H	5.316964000	6.587913000	-1.836508000
H	6.509590000	6.227762000	-3.081664000

C	5.503495000	4.481935000	-2.265075000
H	6.198060000	4.315892000	-1.433372000
H	5.828704000	3.842256000	-3.095264000
C	4.098294000	4.058480000	-1.843504000
H	4.101078000	2.996658000	-1.576447000
H	3.803962000	4.617196000	-0.930089000
C	1.087368000	-0.223971000	3.204866000
H	1.595610000	-1.139987000	3.564745000
H	0.185071000	-0.126795000	3.837263000
C	1.373490000	2.889944000	3.322488000
H	1.184406000	3.039819000	2.254853000
H	2.008800000	3.712974000	3.668798000
H	0.415264000	2.969723000	3.847826000
C	3.840640000	1.159097000	2.690246000
H	4.419847000	0.262501000	2.938046000
H	4.464927000	2.029024000	2.924089000
H	3.658891000	1.151982000	1.610037000
C	2.674751000	1.208113000	5.518357000
H	1.780614000	1.275754000	6.148569000
H	3.329264000	2.049508000	5.774622000
H	3.198092000	0.283378000	5.787518000
C	0.351786000	-4.236369000	1.881380000
H	1.321745000	-3.975435000	1.453394000
H	-0.202781000	-4.858702000	1.168172000
C	0.410391000	-4.879255000	3.257307000
H	0.556369000	-5.961480000	3.203149000
H	1.228906000	-4.449789000	3.845332000
C	-0.943667000	-4.478658000	3.846362000
H	-0.972016000	-4.522901000	4.938277000
H	-1.735089000	-5.130051000	3.459551000
C	-1.119287000	-3.054818000	3.329649000
H	-2.157572000	-2.785285000	3.123893000
H	-0.677062000	-2.315729000	4.005403000
N	0.417152000	1.708889000	-2.559703000
N	-1.983454000	-0.203154000	0.541389000
N	3.135106000	4.279116000	-2.920070000
O	-0.379280000	-2.998415000	2.077747000
Si	2.202788000	1.208199000	3.665667000
Y	0.377185000	-0.887724000	0.983769000
C	1.899545000	-2.439086000	-0.947757000
C	0.025764000	-2.571888000	-2.347446000
C	2.693811000	-3.068191000	-1.945935000
C	0.738336000	-3.190872000	-3.364595000
H	3.748788000	-3.245471000	-1.770417000

H	0.254169000	-3.460135000	-4.296244000
C	2.099766000	-3.438329000	-3.138020000
H	2.698884000	-3.919984000	-3.907798000
N	0.564802000	-2.219291000	-1.177730000
N	2.296780000	-1.998482000	0.262311000
H	-1.029332000	-2.338300000	-2.472275000
C	3.683600000	-2.162997000	0.627074000
H	4.370251000	-1.629211000	-0.050032000
H	3.843767000	-1.765150000	1.631672000
H	3.997731000	-3.220591000	0.634285000
C	0.628705000	1.332265000	-0.124679000
H	0.004665000	1.646996000	0.721309000
H	1.595569000	1.829277000	-0.115792000

TS(G-H)

C	-0.905645000	1.095140000	-2.412065000
C	-2.360830000	0.985212000	-2.392933000
C	-2.878222000	1.877125000	-3.420239000
C	-4.158677000	2.211758000	-3.858707000
H	-5.038377000	1.776209000	-3.390993000
C	-4.308690000	3.116166000	-4.913204000
H	-5.305511000	3.381516000	-5.254450000
C	-3.191538000	3.680152000	-5.532654000
H	-3.324333000	4.382173000	-6.351251000
C	-1.897788000	3.355823000	-5.112743000
H	-1.032771000	3.801130000	-5.595392000
C	-1.761535000	2.456052000	-4.059987000
C	-3.148756000	0.165712000	-1.610773000
H	-4.228680000	0.301883000	-1.724955000
C	-3.812591000	-1.337270000	0.054354000
C	-4.305579000	-2.639453000	-0.212820000
C	-5.300362000	-3.171988000	0.613704000
H	-5.690435000	-4.164824000	0.403935000
C	-5.820714000	-2.446437000	1.679470000
H	-6.600235000	-2.873239000	2.305001000
C	-5.347204000	-1.162814000	1.926254000
H	-5.765013000	-0.590310000	2.750521000
C	-4.346044000	-0.587339000	1.135836000
C	-3.840091000	-3.428715000	-1.425533000
H	-2.936670000	-2.936719000	-1.801824000
C	-4.889431000	-3.357520000	-2.545932000
H	-5.833842000	-3.812779000	-2.226771000
H	-4.544015000	-3.891655000	-3.438618000
H	-5.096685000	-2.321259000	-2.829062000

C	-3.480716000	-4.883884000	-1.104376000
H	-2.739067000	-4.942796000	-0.301956000
H	-3.059774000	-5.374993000	-1.988068000
H	-4.357715000	-5.464398000	-0.797351000
C	-3.872520000	0.824098000	1.454730000
H	-2.983897000	1.020510000	0.847617000
C	-4.936172000	1.864946000	1.072153000
H	-5.191456000	1.805941000	0.010400000
H	-4.573778000	2.878714000	1.274480000
H	-5.858186000	1.716012000	1.646072000
C	-3.471463000	0.989833000	2.927246000
H	-4.326162000	0.871833000	3.602358000
H	-3.061081000	1.990939000	3.096691000
H	-2.710563000	0.260592000	3.223414000
C	0.723643000	2.323530000	-3.906033000
H	0.706772000	2.460467000	-4.992738000
H	1.385064000	1.476381000	-3.703694000
C	1.239108000	3.613862000	-3.255506000
H	0.476761000	4.386513000	-3.407018000
H	1.324153000	3.466231000	-2.161870000
C	2.710128000	5.498085000	-3.593047000
H	2.850922000	5.691419000	-2.508500000
H	1.816084000	6.052860000	-3.900656000
C	3.929079000	6.009178000	-4.357005000
H	3.728162000	5.925766000	-5.432583000
H	4.080792000	7.072043000	-4.134317000
C	5.173129000	5.194548000	-4.002850000
H	5.439828000	5.377650000	-2.952051000
H	6.031723000	5.512591000	-4.605850000
C	4.893118000	3.704907000	-4.199671000
H	5.741526000	3.098859000	-3.860430000
H	4.746832000	3.494571000	-5.266691000
C	3.634583000	3.285124000	-3.443069000
H	3.427683000	2.227539000	-3.636153000
H	3.813091000	3.382479000	-2.351080000
C	0.357698000	0.103895000	1.241926000
H	1.054708000	-0.701266000	1.536866000
H	-0.556574000	-0.007292000	1.849585000
C	0.082835000	3.190485000	1.281626000
H	-0.125961000	3.175188000	0.207434000
H	0.560936000	4.145008000	1.526652000
H	-0.876909000	3.153492000	1.808089000
C	2.870902000	1.873917000	0.914428000
H	3.522592000	1.034848000	1.182362000

H	3.378907000	2.798318000	1.209670000
H	2.762751000	1.880576000	-0.174537000
C	1.460883000	1.762760000	3.648263000
H	0.513318000	1.665759000	4.189509000
H	1.928760000	2.703221000	3.960951000
H	2.113786000	0.942957000	3.968027000
C	-0.000886000	-4.086512000	1.801487000
H	0.773213000	-3.626568000	2.430608000
H	0.463148000	-4.449133000	0.884679000
C	-0.813604000	-5.126854000	2.581246000
H	-1.082352000	-5.972511000	1.942898000
H	-0.237261000	-5.519747000	3.423116000
C	-2.076206000	-4.357206000	3.037073000
H	-2.232316000	-4.401596000	4.118047000
H	-2.970337000	-4.756346000	2.552485000
C	-1.824186000	-2.925147000	2.567102000
H	-2.719663000	-2.397480000	2.238413000
H	-1.306215000	-2.331466000	3.333416000
N	-0.603368000	1.969109000	-3.461914000
N	-2.763563000	-0.794986000	-0.744721000
N	2.480794000	4.080076000	-3.854570000
O	-0.950877000	-3.065466000	1.429002000
Si	1.179993000	1.721161000	1.765254000
Y	-0.516253000	-1.532462000	-0.519878000
C	1.195104000	-3.350904000	-1.938188000
C	-0.579449000	-3.710396000	-3.438751000
C	2.055308000	-4.115363000	-2.778020000
C	0.202829000	-4.465921000	-4.296022000
H	3.094716000	-4.255930000	-2.504350000
H	-0.213427000	-4.879058000	-5.207421000
C	1.546546000	-4.663271000	-3.938241000
H	2.197426000	-5.249568000	-4.583159000
N	-0.123244000	-3.181680000	-2.297654000
N	1.505717000	-2.726830000	-0.790079000
H	-1.624433000	-3.511821000	-3.667560000
C	2.872768000	-2.784614000	-0.333229000
H	3.585451000	-2.367904000	-1.063366000
H	2.975160000	-2.200818000	0.586167000
H	3.206990000	-3.811889000	-0.108608000
C	0.032145000	0.495545000	-1.583364000
H	0.090497000	0.459494000	-0.166896000
H	1.067055000	0.788574000	-1.787842000

H

C	-0.491243000	0.978774000	-2.410427000
C	-1.882820000	0.484241000	-2.557646000
C	-2.409210000	1.070150000	-3.786907000
C	-3.615513000	0.930961000	-4.469850000
H	-4.373742000	0.234463000	-4.119528000
C	-3.844183000	1.687603000	-5.622841000
H	-4.782940000	1.581948000	-6.159133000
C	-2.870660000	2.571541000	-6.092339000
H	-3.058459000	3.151983000	-6.991667000
C	-1.650795000	2.722196000	-5.426943000
H	-0.902587000	3.416560000	-5.797418000
C	-1.430874000	1.960760000	-4.280657000
C	-2.698759000	-0.192014000	-1.659131000
H	-3.762519000	-0.223950000	-1.918679000
C	-3.326449000	-1.113686000	0.434517000
C	-3.808761000	-2.433044000	0.614450000
C	-4.767486000	-2.671006000	1.604582000
H	-5.153779000	-3.678370000	1.738985000
C	-5.251954000	-1.644077000	2.406115000
H	-6.000766000	-1.849511000	3.166468000
C	-4.778080000	-0.350247000	2.219235000
H	-5.164792000	0.453259000	2.840840000
C	-3.816903000	-0.058803000	1.246577000
C	-3.378258000	-3.576792000	-0.290468000
H	-2.500286000	-3.241326000	-0.855585000
C	-4.470902000	-3.894049000	-1.322864000
H	-5.389581000	-4.228012000	-0.827323000
H	-4.144971000	-4.687101000	-2.005105000
H	-4.717804000	-3.010988000	-1.919749000
C	-2.973283000	-4.841053000	0.476752000
H	-2.205198000	-4.626992000	1.227044000
H	-2.575147000	-5.593240000	-0.212678000
H	-3.824848000	-5.293524000	0.996266000
C	-3.334297000	1.374014000	1.066012000
H	-2.432526000	1.339036000	0.445610000
C	-4.380495000	2.219951000	0.323235000
H	-4.611744000	1.799641000	-0.659495000
H	-4.014715000	3.241775000	0.173134000
H	-5.315871000	2.276204000	0.892508000
C	-2.955222000	2.048121000	2.391565000
H	-3.823831000	2.196744000	3.042362000
H	-2.522244000	3.035833000	2.199633000
H	-2.219410000	1.460510000	2.949733000
C	0.922675000	2.591816000	-3.726905000

H	1.018973000	2.753663000	-4.805468000
H	1.740864000	1.927431000	-3.428310000
C	1.014800000	3.943844000	-3.007466000
H	0.157875000	4.548358000	-3.326076000
H	0.899629000	3.785232000	-1.918019000
C	2.095729000	6.104074000	-3.123708000
H	1.942078000	6.339236000	-2.048925000
H	1.200242000	6.447491000	-3.654655000
C	3.323018000	6.857137000	-3.631302000
H	3.393904000	6.718119000	-4.717489000
H	3.195749000	7.930539000	-3.446928000
C	4.595290000	6.336720000	-2.962383000
H	4.572126000	6.590766000	-1.892817000
H	5.483220000	6.823659000	-3.382406000
C	4.683646000	4.818738000	-3.117690000
H	5.538517000	4.417778000	-2.560259000
H	4.833874000	4.563461000	-4.174246000
C	3.400326000	4.148207000	-2.632285000
H	3.465948000	3.067666000	-2.795393000
H	3.297504000	4.299980000	-1.536111000
C	0.598974000	-2.912193000	2.009541000
H	1.672122000	-2.988155000	2.229830000
H	0.294062000	-3.786695000	1.432579000
C	-0.220826000	-2.660624000	3.280855000
H	-1.180642000	-3.180667000	3.236968000
H	0.312123000	-3.018863000	4.165624000
C	-0.436910000	-1.127366000	3.297363000
H	-0.084092000	-0.663240000	4.222062000
H	-1.497679000	-0.893330000	3.183731000
C	0.349894000	-0.625390000	2.086710000
H	-0.104224000	0.204404000	1.543023000
H	1.384377000	-0.362752000	2.346308000
N	-0.318169000	1.909290000	-3.458640000
N	-2.323698000	-0.836318000	-0.527653000
N	2.233405000	4.667136000	-3.339888000
O	0.385999000	-1.753096000	1.186135000
Y	-0.239344000	-1.516129000	-1.126523000
C	0.574799000	-3.737894000	-2.722233000
C	-0.972718000	-2.968020000	-4.326647000
C	0.950263000	-4.795881000	-3.598813000
C	-0.650340000	-3.974224000	-5.222075000
H	1.709806000	-5.507970000	-3.297262000
H	-1.138954000	-4.034192000	-6.187544000
C	0.332953000	-4.897292000	-4.829859000

H	0.615812000	-5.703407000	-5.503359000
N	-0.396013000	-2.849515000	-3.125551000
N	1.063886000	-3.464803000	-1.498500000
H	-1.715951000	-2.211067000	-4.567657000
C	2.139565000	-4.293230000	-1.011154000
H	3.010416000	-4.299219000	-1.686910000
H	2.487878000	-3.912999000	-0.046579000
H	1.841532000	-5.345027000	-0.861683000
C	0.453463000	0.604852000	-1.477767000
H	1.375419000	1.191269000	-1.478270000

I

Y	9.590889000	6.123440000	12.039059000
O	9.084487000	8.579723000	12.086067000
N	7.260374000	5.483965000	11.919244000
N	9.785494000	6.062031000	9.522981000
N	7.510237000	6.769837000	16.213646000
N	11.414004000	6.964891000	10.822455000
C	6.415993000	5.594577000	12.954029000
H	5.365131000	5.389393000	12.723563000
C	5.557716000	6.134704000	15.229705000
C	6.640189000	5.953867000	14.275646000
C	6.136274000	6.646798000	16.409714000
C	11.050301000	6.602931000	9.583134000
C	9.188436000	6.209340000	14.445229000
H	9.922590000	6.690489000	15.119668000
C	7.885343000	6.310804000	14.943290000
C	8.400929000	7.207223000	17.263618000
H	9.409262000	6.848460000	17.049498000
H	8.089026000	6.721475000	18.194055000
C	4.179005000	5.920858000	15.191444000
H	3.700899000	5.524907000	14.298681000
C	6.620398000	5.091926000	10.697048000
C	5.377795000	6.942056000	17.538230000
H	5.833412000	7.337712000	18.441013000
C	3.998859000	6.715753000	17.479306000
H	3.385300000	6.936523000	18.348368000
C	6.473930000	3.718206000	10.384334000
C	9.295236000	5.640937000	8.351148000
H	8.294635000	5.217281000	8.384532000
N	9.330752000	9.207380000	18.433456000
C	3.406682000	6.213132000	16.318736000
H	2.333448000	6.045553000	16.290555000
C	6.122612000	6.075134000	9.807433000

C	6.867209000	2.627423000	11.368738000
H	7.572343000	3.069035000	12.081574000
C	8.415678000	8.734019000	17.403813000
H	8.746787000	9.150100000	16.445090000
H	7.382981000	9.100220000	17.566181000
C	11.821425000	6.719306000	8.388336000
H	12.822668000	7.132246000	8.427974000
C	5.516240000	5.665784000	8.615112000
H	5.124736000	6.416093000	7.933658000
C	5.872962000	3.360341000	9.172656000
H	5.760127000	2.308081000	8.927154000
C	6.177035000	7.557529000	10.140425000
H	6.902934000	7.678941000	10.949931000
C	5.399550000	4.320626000	8.286789000
H	4.929517000	4.022115000	7.353444000
C	12.740415000	7.500841000	11.011708000
H	12.905410000	8.437183000	10.449883000
H	13.530755000	6.796317000	10.712845000
H	12.896464000	7.723897000	12.070348000
C	9.991083000	5.729980000	7.153988000
H	9.545745000	5.381382000	6.229085000
C	5.633083000	2.159042000	12.158113000
H	5.183158000	2.974603000	12.730990000
H	5.899879000	1.359616000	12.859175000
H	4.868385000	1.765740000	11.478456000
C	8.197302000	9.247087000	13.016396000
H	8.304982000	8.748204000	13.979661000
H	7.164179000	9.124756000	12.668771000
C	9.708970000	9.556845000	11.212294000
H	9.583476000	9.225050000	10.179646000
H	10.777613000	9.578624000	11.443737000
C	6.647531000	8.422879000	8.964687000
H	7.609531000	8.078158000	8.575055000
H	6.758023000	9.465539000	9.284201000
H	5.928760000	8.420703000	8.137863000
C	9.026334000	10.883735000	11.525416000
H	9.689965000	11.735992000	11.355280000
H	8.135715000	11.018117000	10.901728000
C	7.549405000	1.422786000	10.709778000
H	6.843221000	0.836287000	10.110730000
H	7.940519000	0.750833000	11.482231000
H	8.375556000	1.711390000	10.053257000
C	11.280083000	6.286478000	7.194599000
H	11.863435000	6.373859000	6.280205000

C	4.815120000	8.047221000	10.658309000
H	4.039287000	7.919973000	9.894523000
H	4.856020000	9.111660000	10.918665000
H	4.500420000	7.494222000	11.548168000
C	10.621113000	11.135316000	19.285371000
H	11.577682000	10.650055000	19.054954000
H	10.763667000	12.214863000	19.156475000
C	8.867602000	8.892426000	19.784079000
H	8.699118000	7.814522000	19.861333000
H	7.896528000	9.390486000	19.992999000
C	10.210880000	10.805748000	20.719903000
H	9.319804000	11.391715000	20.987155000
H	10.999246000	11.091198000	21.426155000
C	8.623798000	10.705833000	12.990696000
H	7.821918000	11.378535000	13.306564000
H	9.485341000	10.866252000	13.648806000
C	9.571248000	10.641779000	18.293724000
H	8.633531000	11.219753000	18.437593000
H	9.907801000	10.832904000	17.268034000
C	9.890191000	9.316569000	20.835925000
H	9.503798000	9.075734000	21.833320000
H	10.805516000	8.729164000	20.690346000
Y	10.248671000	4.001035000	14.864964000
O	10.755105000	1.544757000	14.817952000
N	12.579193000	4.640492000	14.984783000
N	10.054069000	4.062435000	17.381047000
N	12.329306000	3.354651000	10.690366000
N	8.425567000	3.159566000	16.081574000
C	13.423568000	4.529865000	13.949996000
H	14.474433000	4.735038000	14.180459000
C	14.281842000	3.989697000	11.674330000
C	13.199368000	4.170569000	12.628381000
C	13.703275000	3.477637000	10.494311000
C	8.789266000	3.521527000	17.320896000
C	10.651119000	3.915138000	12.458793000
H	9.916965000	3.433988000	11.784352000
C	11.954209000	3.813663000	11.960732000
C	11.438599000	2.917348000	9.640370000
H	10.430285000	3.276163000	9.854496000
H	11.750535000	3.403106000	8.709949000
C	15.660561000	4.203494000	11.712604000
H	16.138675000	4.599415000	12.605376000
C	13.219172000	5.032531000	16.206975000
C	14.461750000	3.182383000	9.365791000

H	14.006126000	2.786769000	8.462993000
C	15.840693000	3.408636000	9.424729000
H	16.454250000	3.187866000	8.555664000
C	13.365656000	6.406251000	16.519677000
C	10.544331000	4.483527000	18.552879000
H	11.544932000	4.907185000	18.519492000
N	10.508680000	0.917288000	8.470445000
C	16.432881000	3.911212000	10.585313000
H	17.506121000	4.078752000	10.613504000
C	13.716937000	4.049321000	17.096600000
C	12.972371000	7.497026000	15.535265000
H	12.267211000	7.055413000	14.822455000
C	11.423744000	1.390558000	9.500138000
H	11.092557000	0.974484000	10.458837000
H	12.456419000	1.024275000	9.337815000
C	8.018146000	3.405148000	18.515695000
H	7.016903000	2.992206000	18.476058000
C	14.323309000	4.458674000	18.288920000
H	14.714798000	3.708368000	18.970386000
C	13.966622000	6.764119000	17.731355000
H	14.079464000	7.816379000	17.976851000
C	13.662490000	2.566925000	16.763615000
H	12.936605000	2.445523000	15.954095000
C	14.440016000	5.803835000	18.617231000
H	14.910045000	6.102346000	19.550579000
C	7.099166000	2.623591000	15.892323000
H	6.934182000	1.687257000	16.454165000
H	6.308811000	3.328105000	16.191169000
H	6.943128000	2.400512000	14.833687000
C	9.848489000	4.394477000	19.750041000
H	10.293828000	4.743072000	20.674944000
C	14.206479000	7.965382000	14.745847000
H	14.656386000	7.149807000	14.172974000
H	13.939666000	8.764793000	14.044775000
H	14.971198000	8.358695000	15.425475000
C	11.642294000	0.877397000	13.887623000
H	11.534619000	1.376285000	12.924359000
H	12.675414000	0.999727000	14.235256000
C	10.130602000	0.567626000	15.691704000
H	10.256072000	0.899417000	16.724357000
H	9.061965000	0.545845000	15.460236000
C	13.191956000	1.701584000	17.939344000
H	12.229968000	2.046338000	18.328979000
H	13.081423000	0.658930000	17.619822000

H	13.910727000	1.703723000	18.766168000
C	10.813248000	-0.759259000	15.378587000
H	10.149619000	-1.611520000	15.548715000
H	11.703861000	-0.893637000	16.002284000
C	12.290210000	8.701683000	16.194221000
H	12.996424000	9.288196000	16.793219000
H	11.899065000	9.373615000	15.421765000
H	11.464088000	8.413098000	16.850788000
C	8.559490000	3.837975000	19.709431000
H	7.976140000	3.750592000	20.623826000
C	15.024403000	2.077197000	16.245756000
H	15.800228000	2.204443000	17.009551000
H	14.983485000	1.012754000	15.985418000
H	15.339128000	2.630174000	15.355893000
C	9.218200000	-1.010532000	7.618449000
H	8.261662000	-0.525195000	7.848834000
H	9.075552000	-2.090070000	7.747324000
C	10.971910000	1.232228000	7.119848000
H	11.140478000	2.310121000	7.042616000
H	11.942955000	0.734097000	6.910960000
C	9.628518000	-0.680976000	6.183939000
H	10.519557000	-1.267011000	5.916714000
H	8.840158000	-0.966350000	5.477649000
C	11.215796000	-0.581350000	13.913312000
H	12.017678000	-1.254051000	13.597446000
H	10.354258000	-0.741765000	13.255195000
C	10.268067000	-0.517094000	8.610142000
H	11.205745000	-1.095138000	8.466298000
H	9.931466000	-0.708213000	9.635818000
C	9.949333000	0.808179000	6.067953000
H	10.335788000	1.048997000	5.070577000
H	9.034049000	1.395657000	6.213500000

TS(D-E)'

C	0.098825000	0.592345000	-1.458984000
C	-1.179105000	0.467183000	-2.191726000
C	-0.991620000	1.005165000	-3.529299000
C	-1.795862000	1.118960000	-4.662790000
H	-2.814181000	0.737852000	-4.657827000
C	-1.286775000	1.740229000	-5.809136000
H	-1.914551000	1.836379000	-6.690936000
C	0.015533000	2.239719000	-5.828941000
H	0.396580000	2.720837000	-6.725791000
C	0.845328000	2.129962000	-4.705038000

H	1.857380000	2.524790000	-4.726107000
C	0.331849000	1.509035000	-3.570616000
C	-2.322246000	-0.006001000	-1.593957000
H	-3.249452000	-0.045080000	-2.170335000
C	-3.545195000	-1.031889000	0.172657000
C	-4.099959000	-2.186668000	-0.449660000
C	-5.247273000	-2.770212000	0.102609000
H	-5.674157000	-3.647210000	-0.378675000
C	-5.847950000	-2.268828000	1.248768000
H	-6.734863000	-2.743407000	1.659940000
C	-5.306074000	-1.139412000	1.855995000
H	-5.789568000	-0.731769000	2.739075000
C	-4.176766000	-0.505824000	1.336759000
C	-3.500291000	-2.832162000	-1.694646000
H	-2.554420000	-2.329507000	-1.916509000
C	-4.417112000	-2.655049000	-2.915294000
H	-5.376628000	-3.162971000	-2.764332000
H	-3.952450000	-3.075805000	-3.813853000
H	-4.633290000	-1.600153000	-3.108912000
C	-3.184999000	-4.322187000	-1.494306000
H	-2.511976000	-4.483401000	-0.646952000
H	-2.700893000	-4.730805000	-2.388250000
H	-4.090129000	-4.912815000	-1.315162000
C	-3.691984000	0.800116000	1.946960000
H	-2.598521000	0.831315000	1.860292000
C	-4.223931000	1.994587000	1.139193000
H	-3.917821000	1.925145000	0.092198000
H	-3.846258000	2.940517000	1.544439000
H	-5.318917000	2.020751000	1.174667000
C	-4.019055000	0.968557000	3.433059000
H	-5.091692000	1.112541000	3.603675000
H	-3.512294000	1.855271000	3.828629000
H	-3.700537000	0.102463000	4.023700000
C	2.176142000	1.910345000	-1.933555000
H	2.912080000	1.830650000	-2.742346000
H	2.572477000	1.342639000	-1.086901000
C	1.998581000	3.393465000	-1.578376000
H	1.498050000	3.876316000	-2.424855000
H	1.312438000	3.480667000	-0.713585000
C	3.158001000	5.516487000	-1.539213000
H	2.485660000	5.972831000	-0.780991000
H	2.704064000	5.704042000	-2.518909000
C	4.528164000	6.186258000	-1.461916000
H	5.143747000	5.819905000	-2.293149000

H	4.414314000	7.269038000	-1.592229000
C	5.215596000	5.867087000	-0.134632000
H	4.656995000	6.341507000	0.685277000
H	6.228352000	6.286292000	-0.109612000
C	5.246535000	4.355188000	0.086942000
H	5.649172000	4.112749000	1.077865000
H	5.903458000	3.885730000	-0.656024000
C	3.847566000	3.759544000	-0.053597000
H	3.896019000	2.672551000	0.064380000
H	3.202615000	4.140629000	0.768355000
C	0.783357000	-1.381438000	-1.216245000
H	1.575501000	-1.464913000	-0.442423000
H	-0.039168000	-2.067100000	-0.938388000
C	2.239112000	-3.871321000	-2.296143000
H	3.035646000	-3.776132000	-1.549015000
H	2.665424000	-4.374611000	-3.172195000
H	1.465745000	-4.527093000	-1.880577000
C	2.957800000	-1.164003000	-3.507108000
H	2.597513000	-0.255165000	-3.995942000
H	3.480204000	-1.766830000	-4.258417000
H	3.689245000	-0.879146000	-2.742923000
C	0.197186000	-2.448633000	-4.091574000
H	-0.600712000	-3.097530000	-3.714760000
H	0.636476000	-2.935958000	-4.969256000
H	-0.253395000	-1.505666000	-4.411879000
C	-0.556493000	-1.987624000	3.589053000
H	-0.915253000	-1.000946000	3.895162000
H	0.495343000	-2.088388000	3.880201000
C	-1.406216000	-3.139279000	4.105396000
H	-1.094669000	-3.467540000	5.100448000
H	-2.460285000	-2.846396000	4.151130000
C	-1.195284000	-4.199165000	3.021430000
H	-1.979025000	-4.960492000	3.005827000
H	-0.231305000	-4.702003000	3.157751000
C	-1.193710000	-3.358743000	1.752169000
H	-0.564563000	-3.761858000	0.953902000
H	-2.204192000	-3.187251000	1.369389000
N	0.933275000	1.290169000	-2.328293000
N	-2.365844000	-0.414773000	-0.292258000
N	3.266370000	4.073299000	-1.353622000
O	-0.640802000	-2.072131000	2.143693000
Si	1.521960000	-2.162420000	-2.768421000
Y	-0.234709000	-0.086757000	0.734697000
C	2.090866000	1.134220000	2.825181000

C	2.779710000	-0.981959000	2.109924000
C	3.298693000	1.251047000	3.577492000
C	3.963377000	-0.938354000	2.817464000
H	3.491424000	2.140961000	4.162218000
H	4.662004000	-1.766210000	2.785309000
C	4.214213000	0.223644000	3.565053000
H	5.130802000	0.317763000	4.141731000
N	1.860929000	0.003923000	2.092655000
N	1.156652000	2.106495000	2.816689000
H	2.533703000	-1.856107000	1.509455000
C	1.386044000	3.313189000	3.595320000
H	2.315614000	3.819932000	3.305452000
H	0.557644000	3.994442000	3.404395000
H	1.423273000	3.111942000	4.676013000
C	-0.122265000	1.938634000	2.118237000
H	-0.250924000	2.802387000	1.444322000
H	-0.921541000	2.039717000	2.873348000

E'

C	0.438894000	-0.068229000	-1.427023000
C	-0.996028000	0.238392000	-1.709545000
C	-1.007485000	1.323021000	-2.699580000
C	-2.040794000	2.034303000	-3.305087000
H	-3.077386000	1.820088000	-3.056543000
C	-1.740718000	3.039470000	-4.228514000
H	-2.544048000	3.597360000	-4.701102000
C	-0.409833000	3.337629000	-4.532992000
H	-0.184949000	4.127513000	-5.245323000
C	0.642471000	2.640208000	-3.937805000
H	1.672363000	2.881018000	-4.185048000
C	0.334830000	1.615504000	-3.034822000
C	-2.142407000	-0.194416000	-1.044597000
H	-3.093547000	0.220237000	-1.389284000
C	-3.367500000	-1.657566000	0.426471000
C	-3.799284000	-2.768946000	-0.348763000
C	-4.962857000	-3.454067000	0.011238000
H	-5.284247000	-4.302027000	-0.589516000
C	-5.714601000	-3.083347000	1.118388000
H	-6.614434000	-3.631030000	1.385514000
C	-5.303285000	-1.990808000	1.871119000
H	-5.904794000	-1.678351000	2.721603000
C	-4.152268000	-1.265117000	1.548644000
C	-3.031555000	-3.250477000	-1.570264000
H	-2.117079000	-2.655308000	-1.640886000

C	-3.837431000	-3.018481000	-2.856752000
H	-4.782724000	-3.572967000	-2.838839000
H	-3.275156000	-3.350472000	-3.736812000
H	-4.075053000	-1.958525000	-2.986368000
C	-2.622246000	-4.725025000	-1.446686000
H	-2.013902000	-4.897829000	-0.552337000
H	-2.039358000	-5.037366000	-2.320210000
H	-3.493239000	-5.386451000	-1.383827000
C	-3.848601000	-0.013146000	2.355496000
H	-2.828217000	0.300339000	2.106772000
C	-4.780648000	1.134572000	1.937360000
H	-4.687542000	1.346226000	0.868141000
H	-4.545500000	2.052576000	2.488938000
H	-5.827586000	0.878606000	2.137637000
C	-3.907698000	-0.224708000	3.872766000
H	-4.926346000	-0.429223000	4.219998000
H	-3.564572000	0.674998000	4.396596000
H	-3.281237000	-1.065112000	4.189197000
C	2.569068000	1.127718000	-2.112096000
H	3.062875000	1.364296000	-3.062366000
H	3.070759000	0.239712000	-1.716968000
C	2.744379000	2.330136000	-1.172558000
H	2.127618000	3.146844000	-1.564306000
H	2.342860000	2.081628000	-0.170742000
C	4.205036000	4.163013000	-0.597177000
H	3.865913000	4.216402000	0.460026000
H	3.523942000	4.792686000	-1.181220000
C	5.629031000	4.705408000	-0.694767000
H	5.909440000	4.762740000	-1.754100000
H	5.661421000	5.725010000	-0.292495000
C	6.607793000	3.795127000	0.046947000
H	6.396639000	3.838446000	1.125293000
H	7.639706000	4.140751000	-0.086342000
C	6.450529000	2.354800000	-0.439090000
H	7.076755000	1.673073000	0.149030000
H	6.778404000	2.279853000	-1.483600000
C	4.992006000	1.907838000	-0.354267000
H	4.898659000	0.893521000	-0.755534000
H	4.681684000	1.862098000	0.712077000
C	0.871790000	-1.542932000	-1.432274000
H	1.775046000	-1.708111000	-0.818805000
H	0.078460000	-2.148768000	-0.970855000
C	1.296454000	-4.250703000	-2.810408000
H	2.099271000	-4.496272000	-2.105365000

H	1.493925000	-4.802370000	-3.736206000
H	0.357318000	-4.626466000	-2.392156000
C	2.913809000	-1.889065000	-3.856336000
H	2.927140000	-0.847383000	-4.186816000
H	3.137130000	-2.519832000	-4.724427000
H	3.723469000	-2.030447000	-3.131979000
C	-0.130134000	-1.978651000	-4.391955000
H	-1.118211000	-2.254972000	-4.014110000
H	0.042216000	-2.520112000	-5.328790000
H	-0.147262000	-0.907541000	-4.612781000
C	-0.089601000	-1.580698000	3.786207000
H	-0.738649000	-0.734087000	4.024988000
H	0.897705000	-1.400019000	4.226626000
C	-0.661020000	-2.928744000	4.202114000
H	-0.397015000	-3.187473000	5.230852000
H	-1.752511000	-2.926010000	4.116578000
C	-0.052917000	-3.869960000	3.160852000
H	-0.603717000	-4.807788000	3.054447000
H	0.985537000	-4.109161000	3.416508000
C	-0.117663000	-3.025268000	1.897395000
H	0.674293000	-3.245167000	1.177636000
H	-1.089000000	-3.090008000	1.397796000
N	1.190187000	0.770206000	-2.361662000
N	-2.171996000	-0.981898000	0.105182000
N	4.121977000	2.800543000	-1.112169000
O	0.061850000	-1.651368000	2.345473000
Si	1.223901000	-2.374194000	-3.134130000
Y	-0.398202000	0.226563000	0.808766000
C	0.908454000	2.538355000	2.847179000
C	2.298371000	0.658540000	2.855557000
C	1.831345000	3.200761000	3.711688000
C	3.226584000	1.232929000	3.700227000
H	1.646845000	4.219403000	4.027036000
H	4.116646000	0.693080000	4.001743000
C	2.967538000	2.545596000	4.128503000
H	3.668295000	3.056518000	4.783848000
N	1.173385000	1.264171000	2.432158000
N	-0.227136000	3.123545000	2.415707000
H	2.445412000	-0.353315000	2.481163000
C	-0.519153000	4.489714000	2.817449000
H	0.164844000	5.217381000	2.355724000
H	-1.532222000	4.723874000	2.490744000
H	-0.476055000	4.614260000	3.906504000
C	-1.046367000	2.499600000	1.370327000

H	-0.906439000	3.080050000	0.438098000
H	-2.100604000	2.639684000	1.647727000

Computational details

The optimization of yttrium complexes was carried out by employing DFT hybrid functional (B3PW91)[5] along with small core pseudopotential Stuttgart basis set for yttrium, and silicon atoms with additional polarization functions for silicon atoms.[6] Pople basis sets (6-31G**) were employed for the rest of the atoms.[7] Frequency calculations were performed to locate minima for the optimized structures (maxima for TS structures). All the calculations were performed using Gaussian 09 suite of programs.[8]

Table S16. Computed natural charges for **2d**

Atom Label	Natural Charges
Y1	2.06384
O2	-0.66034
N16	-0.62955
N34	-0.67278
C35	-0.25802
C84	-0.23958
C133	-1.69700

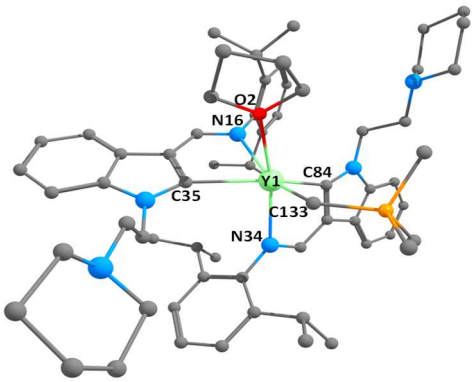


Table S17. Computed Wiberg bond index between selected atoms in **2d**

Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000
O2	0.0967	N16	0.1307	N34	0.1527
Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000
C35	0.2640	C84	0.2748	C133	0.3361

SD1. Bonding analysis from NBO computation for **2d**

(1.92570) BD(1) Y1-C35
(6.20%) 0.2489* Y1 s (17.47%) p 0.15 (2.63%) d 4.57 (79.89%)
(93.80%) 0.9685* C35 s (35.47%) p 1.82 (64.51%) d 0.00 (0.02%)
(1.92706) BD(1)Y1-C84
(6.61%) 0.2571* Y1 s (26.81%) p 0.09 (2.43%) d 2.64 (70.76%)
(93.39%) 0.9664* C84 s (35.60%) p 1.81 (64.38%) d 0.00 (0.02%)
(1.93417) BD(1) Y1-C133
(7.43%) 0.2726* Y1 s (28.55%) p 0.02 (0.68%) d 2.48 (70.77%)
(92.57%) 0.9621* C133 s (23.09%) p 3.33 (76.91%) d 0.00 (0.01%)

Table S18. DFT computed NBO second order perturbation analysis for **2d**

Donor NBO	Acceptor NBO	E(2) kcal/mol
(1.97498) BD(1) N16-C55 (60.16%) 0.7756* N16 s(37.57%)p 1.66(62.32%)d 0.00(0.12%) (39.84%) 0.6312* C 55 s(26.58%)p 2.76(73.30%)d 0.00(0.12%)	(0.08910) LV (2) Y1 s(1.72%)p 0.26(0.45%)d56.80(97.83%)	6.01
(1.90075) BD (2) N16-C55 (93.69%) 0.9679* N16 s(19.93%)p 4.01(80.02%)d 0.00(0.05%) (6.31%) 0.2513* C55 s(1.77%)p55.43(97.92%)d 0.18(0.32%)	(0.08910) LV (2) Y1 s(1.72%)p 0.26(0.45%)d56.80(97.83%)	11.00
(1.97950) BD (1) N34-C102 (60.35%) 0.7768* N34 s(41.47%)p 1.41(58.40%)d 0.00(0.12%) (39.65%) 0.6297* C102 s(32.39%)p 2.08(67.48%)d 0.00(0.13%)	(0.13861) LV (1) Y1 s(23.65%)p 0.01(0.15%)d 3.22(76.19%)	8.43
(1.97647) BD (1) N34-C104 (60.29%) 0.7765* N34 s(36.67%)p 1.72(63.22%)d 0.00(0.11%) (39.71%) 0.6301* C104 s(26.87%)p 2.72(73.02%)d 0.00(0.12%)	(0.13861) LV (1) Y1 s(23.65%)p 0.01(0.15%)d 3.22(76.19%)	7.60
(1.96148) BD (1) C35-C36 (46.92%) 0.6850* C35 s(35.46%)p 1.82(64.43%)d 0.00(0.12%) (53.08%) 0.7286* C36 s(32.66%)p 2.06(67.28%)d 0.00(0.06%)	(0.13861) LV (1) Y1 s(23.65%)p 0.01(0.15%)d 3.22(76.19%)	25.30
(1.93816) LP (1) O2 s(36.19%)p 1.76(63.79%)d 0.00(0.02%)	(0.13861) LV (1) Y1 s(23.65%)p 0.01(0.15%)d 3.22(76.19%)	20.82
(1.93585) LP(2) O2 s(4.44%)p21.49(95.50%)d 0.01(0.05%)	(0.13861) LV (1) Y1 s(23.65%)p 0.01(0.15%)d 3.22(76.19%)	4.54

Fig. S52. Computed MOs for **2d**. Left-HOMO, Right-LUMO

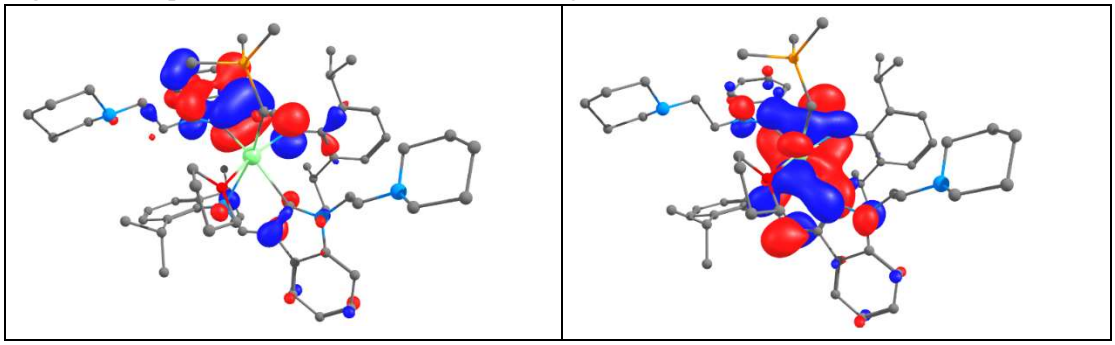


Table S19. Computed natural charges for **A3**

Atom Label	Natural Charges
Y1	2.05247
N3	-0.66626
N21	-0.67304
C22	-0.21544
C71	-0.20662
N139	-0.65335
C151	-0.90134

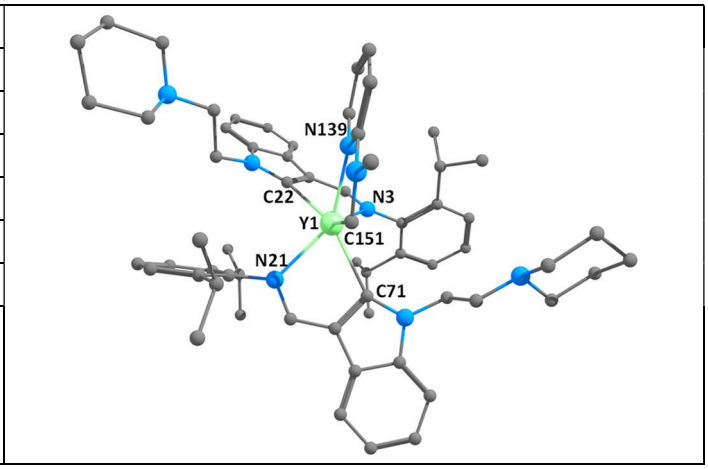


Table S20. Computed Wiberg bond index between selected atoms in **A3**

Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000
N3	0.1645	N21	0.1702	C22	0.2730
Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000
C71	0.2830	N139	0.1475	C151	0.3151

SD2. Bonding analysis from NBO computation for **A3**

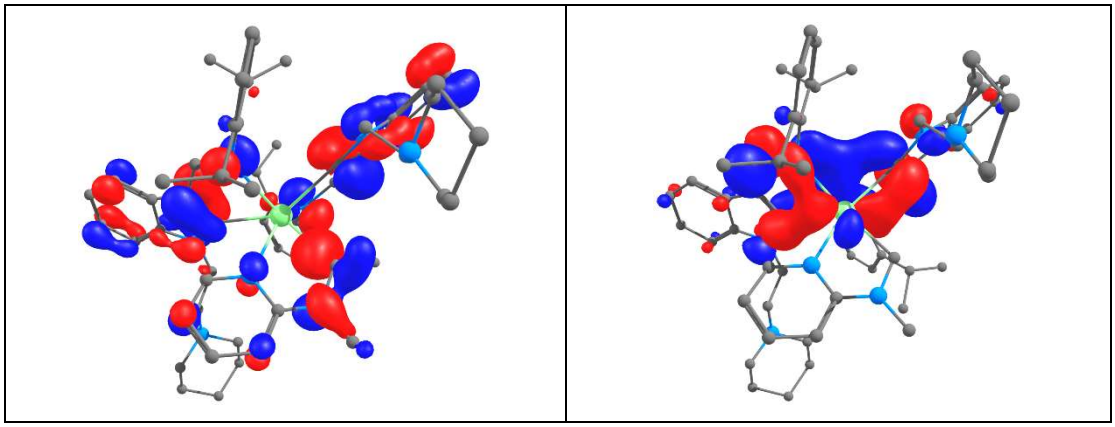
(1.92335) BD (1) Y1-C22
(6.52%) 0.2553* Y1 s(15.05%)p 0.18(2.75%)d 5.46(82.20%)
(93.48%) 0.9669* C22 s(36.43%)p 1.74(63.55%)d 0.00(0.02%)
(1.92694) BD (1) Y1-C71
(7.08%) 0.2661* Y1 s(28.76%)p 0.08(2.42%)d 2.39(68.82%)
(92.92%) 0.9639* C71 s(36.47%)p 1.74(63.51%)d 0.00(0.02%)
(1.94910) BD (1) Y1-C151
(7.92%) 0.2814* Y1 s(26.29%)p 0.03(0.70%)d 2.78(73.01%)
(92.08%) 0.9596* C151 s(26.65%)p 2.75(73.35%)d 0.00(0.00%)

Table S21. DFT computed NBO second order perturbation analysis for **A3**

Donor NBO	Acceptor NBO	E(2) kcal/mol
(1.87237) LP(1) N139 s(26.18%)p 2.82(73.78%)d 0.00(0.04%)	(0.15254) LV(1) Y1 s(28.05%)p 0.01(0.23%)d 2.56(71.73%)	12.85
(1.87237) LP(1) N139 s(26.18%)p 2.82(73.78%)d 0.00(0.04%)	(0.09759) LV(2) Y1 s(0.68%)p 0.25(0.17%)d99.99(99.15%)	7.98
(1.87237) LP(1) N139 s(26.18%)p 2.82(73.78%)d 0.00(0.04%)	(0.06919) BD*(1) Y1-C71 (92.92%) 0.9639* Y1 s(28.76%)p 0.08(2.42%)d 2.39(68.82%) (7.08%)-0.2661* C71 s(36.47%)p	11.74

	1.74(63.51%)d 0.00(0.02%)	
(1.97866) BD(1) N3-C40 (60.30%) 0.7765* N3 s(40.59%)p 1.46(59.29%)d 0.00(0.13%) (39.70%) 0.6301* C40 s(32.31%)p 2.09(67.56%)d 0.00(0.13%)	(0.09759) LV(2) Y1 s(0.68%)p 0.25(0.17%)d99.99(99.15%)	6.85
(1.97652) BD(1) N3-C42 (60.27%) 0.7764* N3 s(35.61%)p 1.80(64.28%)d 0.00(0.11%) (39.73%) 0.6303* C42 s(27.08%)p 2.69(72.81%)d 0.00(0.11%)	(0.09759) LV (2) Y1 s(0.68%)p 0.25(0.17%)d99.99(99.15%)	6.04
(1.89204) BD(2) N3-C42 (94.21%) 0.9706* N3 s(22.73%)p 3.40(77.24%)d 0.00(0.03%) (5.79%) 0.2407* C42 s(1.10%)p89.26(98.59%)d 0.28(0.31%)	(0.15254) LV (1) Y1 s(28.05%)p 0.01(0.23%)d 2.56(71.73%)	6.74
(1.89204) BD(2) N3-C42 (94.21%) 0.9706* N3 s(22.73%)p 3.40(77.24%)d 0.00(0.03%) (5.79%) 0.2407*C42 s(1.10%)p89.26(98.59%)d 0.28(0.31%)	(0.09759) LV (2) Y1 s(0.68%)p 0.25(0.17%)d99.99(99.15%)	13.17
(1.97818) BD(1) N21-C89 (60.34%) 0.7768* N21 s(41.37%)p 1.41(58.50%)d 0.00(0.13%) (39.66%) 0.6297* C89 s(32.44%)p 2.08(67.43%)d 0.00(0.13%)	(0.15254) LV (1) Y1 s(28.05%)p 0.01(0.23%)d 2.56(71.73%)	8.94
(1.97681) BD(1) N21-C91 (60.13%) 0.7754* N 21 s(35.46%)p 1.82(64.43%)d 0.00(0.11%) (39.87%) 0.6314* C 91 s(27.15%)p 2.68(72.74%)d 0.00(0.11%)	(0.15254) LV (1) Y1 s(28.05%)p 0.01(0.23%)d 2.56(71.73%)	8.04
(1.89161) BD(2) N21-C91 (94.23%) 0.9707* N 21 s(23.13%)p 3.32(76.84%)d 0.00(0.03%) (5.77%) 0.2401* C91 s(1.01%)p97.69(98.70%)d 0.28(0.29%)	(0.15254) LV (1) Y1 s(28.05%)p 0.01(0.23%)d 2.56(71.73%)	31.12

Fig. S53. Computed MOs for **A3**. Left-HOMO, Right-LUMO



Optimized geometries

2d

Y	11.199573000	8.364359000	13.878395000
O	9.531988000	10.238444000	14.045355000
C	8.948907000	10.961106000	12.928841000
H	8.633642000	10.226280000	12.181534000
H	9.721490000	11.594424000	12.489408000
C	7.768710000	11.730707000	13.507925000
H	6.979395000	11.885114000	12.767284000
H	8.088777000	12.713484000	13.871177000
C	7.340412000	10.843095000	14.678307000
H	6.757463000	11.373280000	15.436029000
H	6.749171000	9.992953000	14.321039000
C	8.682661000	10.367097000	15.210663000
H	9.130934000	11.102476000	15.888379000
H	8.646956000	9.393164000	15.698191000
N	10.727899000	8.814425000	10.263808000
N	12.698207000	10.537692000	13.626560000
N	13.196310000	8.174943000	16.986839000
N	11.332982000	10.371557000	19.419294000
C	10.137069000	10.117979000	20.222237000
H	10.363784000	9.436309000	21.068979000
H	9.401454000	9.605672000	19.592448000
C	9.545596000	11.414032000	20.767993000
H	9.217256000	12.034502000	19.924253000
H	8.657131000	11.183424000	21.367534000
C	10.579886000	12.176616000	21.595387000
H	10.810540000	11.603356000	22.504688000
H	10.180875000	13.142960000	21.924989000
C	11.858202000	12.366476000	20.780204000
H	11.663522000	13.045252000	19.940332000
H	12.647200000	12.822514000	21.389766000
C	12.358072000	11.034648000	20.224978000

H	13.240605000	11.212472000	19.603442000
H	12.678332000	10.382477000	21.065529000
N	12.483764000	6.304290000	13.247572000
C	11.247472000	9.103688000	11.495591000
C	11.960720000	10.316496000	11.336866000
C	11.852746000	10.761034000	9.965976000
C	12.328960000	11.850457000	9.223620000
H	12.940320000	12.619210000	9.689783000
C	12.010996000	11.937618000	7.872828000
H	12.375880000	12.778765000	7.289682000
C	11.226136000	10.955143000	7.246723000
H	10.994041000	11.048172000	6.189542000
C	10.739987000	9.863779000	7.960019000
H	10.133017000	9.105736000	7.473369000
C	11.061464000	9.784039000	9.316482000
C	9.914499000	7.654557000	9.941165000
H	10.128347000	6.892354000	10.692432000
H	10.228704000	7.257207000	8.969821000
C	8.420428000	8.001540000	9.875090000
H	8.032740000	8.133924000	10.906299000
H	8.321223000	8.970261000	9.371803000
C	12.680180000	10.952352000	12.388097000
H	13.261836000	11.844687000	12.124894000
C	13.520998000	11.266330000	14.543729000
C	12.993564000	12.371843000	15.251078000
C	13.817343000	13.043098000	16.161212000
H	13.423870000	13.899394000	16.701398000
C	15.127474000	12.640813000	16.385347000
H	15.751757000	13.175121000	17.096662000
C	15.637173000	11.556482000	15.681083000
H	16.666177000	11.250833000	15.845804000
C	14.858821000	10.856790000	14.754244000
C	11.578999000	12.874914000	15.011600000
H	11.017418000	12.049396000	14.563033000
C	11.575604000	14.044815000	14.014064000
H	12.157236000	14.887906000	14.403744000
H	10.554562000	14.399644000	13.829761000
H	12.012684000	13.759767000	13.052462000
C	10.860227000	13.283438000	16.304863000
H	10.897236000	12.492770000	17.061587000
H	9.809134000	13.514500000	16.096592000
H	11.294785000	14.187029000	16.746805000
C	15.485241000	9.737151000	13.939742000
H	14.671096000	9.096182000	13.584099000

C	16.445227000	8.856038000	14.745707000
H	17.358633000	9.392853000	15.025659000
H	16.753503000	7.995053000	14.144528000
H	15.977437000	8.477973000	15.658068000
C	16.202867000	10.321963000	12.711867000
H	15.514981000	10.870742000	12.061654000
H	16.669433000	9.529427000	12.117070000
H	16.991481000	11.016903000	13.022449000
C	12.745516000	7.800995000	15.754402000
C	13.392120000	6.572790000	15.465247000
C	14.249321000	6.209167000	16.570518000
C	15.120779000	5.150234000	16.856582000
H	15.253080000	4.330897000	16.154443000
C	15.822010000	5.158568000	18.057085000
H	16.498536000	4.340414000	18.288497000
C	15.672215000	6.209021000	18.976931000
H	16.235104000	6.192663000	19.905906000
C	14.811059000	7.270894000	18.717798000
H	14.697999000	8.080625000	19.432472000
C	14.104717000	7.252947000	17.514136000
C	12.813145000	9.395294000	17.674932000
H	12.362941000	10.063333000	16.939265000
H	13.723977000	9.884726000	18.035006000
C	11.819131000	9.138517000	18.812279000
H	10.962335000	8.605747000	18.385883000
H	12.267136000	8.458350000	19.562210000
C	13.239363000	5.885837000	14.233745000
H	13.804009000	4.956469000	14.098970000
C	12.431388000	5.514054000	12.054650000
C	13.188822000	5.920434000	10.929299000
C	13.065152000	5.198374000	9.739766000
H	13.639325000	5.504827000	8.870786000
C	12.236275000	4.085521000	9.651414000
H	12.154379000	3.536019000	8.717376000
C	11.536061000	3.666653000	10.774251000
H	10.918026000	2.774987000	10.714077000
C	11.616630000	4.359075000	11.989073000
C	14.209423000	7.041140000	11.032544000
H	13.861732000	7.733733000	11.807084000
C	15.559101000	6.458437000	11.485102000
H	15.481705000	5.959496000	12.455649000
H	16.315878000	7.245630000	11.568400000
H	15.919879000	5.720305000	10.759608000
C	14.388287000	7.846292000	9.742737000

H	14.869181000	7.256604000	8.953945000
H	15.032369000	8.710792000	9.931158000
H	13.434310000	8.217657000	9.360306000
C	10.887254000	3.803270000	13.202146000
H	10.863939000	4.585891000	13.965699000
C	9.435857000	3.407367000	12.904671000
H	8.868877000	4.241211000	12.480759000
H	8.936095000	3.095424000	13.827397000
H	9.374708000	2.565972000	12.205991000
C	11.648367000	2.601564000	13.787215000
H	11.704272000	1.783595000	13.059918000
H	11.143655000	2.222436000	14.682757000
H	12.673506000	2.864701000	14.064754000
C	9.186335000	7.121699000	14.418371000
H	8.360202000	7.716994000	13.986036000
H	9.330966000	6.292719000	13.697607000
Si	8.510627000	6.288791000	15.958698000
C	7.971006000	7.527686000	17.313469000
H	8.792308000	8.172607000	17.643920000
H	7.617519000	6.972942000	18.190226000
H	7.145043000	8.166917000	16.980887000
C	6.940038000	5.255734000	15.610891000
H	6.132808000	5.894439000	15.233728000
H	6.575004000	4.755884000	16.515874000
H	7.129750000	4.486759000	14.855012000
C	9.787303000	5.133939000	16.768777000
H	10.019004000	4.276695000	16.128448000
H	9.405575000	4.740988000	17.718028000
H	10.725445000	5.661504000	16.967830000
N	7.647883000	7.031602000	9.118256000
C	6.312635000	7.540324000	8.819517000
H	6.418411000	8.519941000	8.338212000
H	5.726785000	7.700679000	9.750204000
C	5.547739000	6.588106000	7.904156000
H	6.070698000	6.532233000	6.941034000
H	4.548052000	6.994127000	7.709475000
C	5.460112000	5.194033000	8.524565000
H	4.832329000	5.236811000	9.426109000
H	4.975870000	4.491522000	7.836368000
C	6.857139000	4.705657000	8.905257000
H	7.451195000	4.542125000	7.997146000
H	6.805759000	3.748744000	9.437446000
C	7.575823000	5.730879000	9.779792000
H	7.052969000	5.813624000	10.756668000

H	8.591327000	5.381170000	9.989934000

A1

Y	-0.165542000	-0.124800000	0.077244000
N	-0.810952000	0.146105000	-3.541015000
N	1.358086000	1.999073000	-0.367138000
N	2.199947000	-0.665680000	2.971038000
N	0.821250000	1.572293000	5.665833000
C	-0.075821000	1.276818000	6.784947000
H	0.439445000	0.658383000	7.548924000
H	-0.909227000	0.674470000	6.404141000
C	-0.599791000	2.548602000	7.446087000
H	-1.214855000	3.102141000	6.724801000
H	-1.251865000	2.277248000	8.284338000
C	0.555098000	3.433589000	7.912180000
H	1.094654000	2.928131000	8.725575000
H	0.180805000	4.378770000	8.321889000
C	1.512160000	3.685573000	6.749548000
H	1.013888000	4.293842000	5.984019000
H	2.394316000	4.244858000	7.081965000
C	1.963246000	2.373504000	6.113343000
H	2.600891000	2.595061000	5.252824000
H	2.579141000	1.804487000	6.841133000
N	0.911297000	-2.277982000	-0.754105000
C	-0.220609000	0.477097000	-2.350927000
C	0.530941000	1.648795000	-2.611691000
C	0.381289000	2.020417000	-4.000213000
C	0.870405000	3.042249000	-4.825333000
H	1.533397000	3.809097000	-4.432459000
C	0.497797000	3.064044000	-6.164728000
H	0.872275000	3.852550000	-6.811886000
C	-0.354437000	2.083023000	-6.698156000
H	-0.627966000	2.124572000	-7.748702000
C	-0.855575000	1.058446000	-5.900987000
H	-1.516414000	0.301015000	-6.312666000
C	-0.477902000	1.045017000	-4.556618000
C	-1.705741000	-0.975930000	-3.772926000
H	-1.549881000	-1.687517000	-2.961109000
H	-1.414259000	-1.472016000	-4.705405000
C	-3.172842000	-0.530078000	-3.885141000
H	-3.594730000	-0.388890000	-2.870046000
H	-3.193056000	0.450259000	-4.375121000
C	1.303029000	2.327145000	-1.631212000
H	1.898195000	3.181780000	-1.974230000

C	2.221733000	2.777758000	0.465862000
C	1.760698000	3.987451000	1.039298000
C	2.614401000	4.685404000	1.901710000
H	2.273971000	5.616760000	2.345276000
C	3.890503000	4.220536000	2.192546000
H	4.536920000	4.778795000	2.864760000
C	4.344636000	3.049899000	1.594857000
H	5.354644000	2.705629000	1.797185000
C	3.535549000	2.316642000	0.722440000
C	0.403152000	4.580231000	0.688722000
H	-0.227810000	3.767329000	0.314250000
C	0.534270000	5.621056000	-0.436392000
H	1.176791000	6.451350000	-0.121625000
H	-0.447184000	6.032019000	-0.698086000
H	0.969578000	5.191331000	-1.342541000
C	-0.311212000	5.214377000	1.889587000
H	-0.342963000	4.537034000	2.747524000
H	-1.340705000	5.471114000	1.618275000
H	0.176552000	6.141226000	2.211184000
C	4.106061000	1.116534000	-0.015598000
H	3.264824000	0.471711000	-0.292804000
C	5.076627000	0.273016000	0.816052000
H	6.011085000	0.806249000	1.024691000
H	5.343463000	-0.634602000	0.265888000
H	4.636638000	-0.033951000	1.767965000
C	4.793334000	1.585179000	-1.309496000
H	4.100039000	2.109612000	-1.973651000
H	5.208707000	0.733722000	-1.859205000
H	5.616606000	2.271345000	-1.079769000
C	1.566491000	-0.917083000	1.779674000
C	2.028981000	-2.195792000	1.382220000
C	2.950458000	-2.715663000	2.364516000
C	3.710835000	-3.884081000	2.504593000
H	3.658516000	-4.677096000	1.763061000
C	4.541385000	-4.019245000	3.610950000
H	5.133491000	-4.922437000	3.730302000
C	4.630672000	-3.004688000	4.577848000
H	5.292005000	-3.132691000	5.430131000
C	3.882473000	-1.837298000	4.462553000
H	3.957854000	-1.056159000	5.212981000
C	3.041763000	-1.713268000	3.354437000
C	2.081216000	0.544743000	3.762170000
H	1.643018000	1.317427000	3.130215000
H	3.091723000	0.881225000	4.017966000

C	1.232492000	0.328312000	5.022301000
H	0.326956000	-0.214638000	4.727048000
H	1.774642000	-0.331440000	5.726135000
C	1.697292000	-2.806061000	0.147601000
H	2.158713000	-3.776081000	-0.069734000
C	0.741937000	-3.023965000	-1.965314000
C	1.491503000	-2.649406000	-3.106944000
C	1.276266000	-3.335761000	-4.304487000
H	1.840486000	-3.052976000	-5.187903000
C	0.367389000	-4.385873000	-4.383860000
H	0.214658000	-4.907823000	-5.324790000
C	-0.318066000	-4.781989000	-3.243877000
H	-0.994323000	-5.630893000	-3.296461000
C	-0.146055000	-4.123401000	-2.019292000
C	2.594564000	-1.607829000	-3.013200000
H	2.306318000	-0.894016000	-2.233413000
C	3.907555000	-2.283006000	-2.580629000
H	3.814868000	-2.776561000	-1.609067000
H	4.716289000	-1.547667000	-2.508371000
H	4.207337000	-3.041265000	-3.313103000
C	2.817820000	-0.816409000	-4.304661000
H	3.263156000	-1.435578000	-5.091912000
H	3.512187000	0.008868000	-4.118560000
H	1.887587000	-0.390316000	-4.687971000
C	-0.853096000	-4.669512000	-0.787796000
H	-0.764542000	-3.925701000	0.009219000
C	-2.347881000	-4.925141000	-1.014850000
H	-2.866607000	-4.019243000	-1.340908000
H	-2.815588000	-5.262953000	-0.084570000
H	-2.522266000	-5.704476000	-1.764728000
C	-0.168949000	-5.958639000	-0.302180000
H	-0.230853000	-6.744258000	-1.063846000
H	-0.650890000	-6.332824000	0.607852000
H	0.890717000	-5.798787000	-0.080924000
C	-2.162234000	-1.305222000	0.726947000
H	-2.972951000	-0.650878000	0.359724000
H	-2.087567000	-2.115170000	-0.025605000
Si	-2.831437000	-2.134369000	2.268076000
C	-3.295462000	-0.879353000	3.631899000
H	-2.421375000	-0.370167000	4.050378000
H	-3.802244000	-1.394663000	4.455817000
H	-3.980726000	-0.117467000	3.244435000
C	-4.449922000	-3.097239000	1.939452000
H	-5.236524000	-2.416744000	1.593161000

H	-4.814533000	-3.598057000	2.844164000
H	-4.311843000	-3.859041000	1.165719000
C	-1.582253000	-3.351187000	3.030840000
H	-1.370237000	-4.186596000	2.355099000
H	-1.964892000	-3.773224000	3.967192000
H	-0.630984000	-2.851966000	3.241543000
N	-3.973103000	-1.436600000	-4.693002000
C	-5.277409000	-0.854798000	-4.996021000
H	-5.115970000	0.133962000	-5.442164000
H	-5.871178000	-0.697219000	-4.070310000
C	-6.069814000	-1.738659000	-5.955356000
H	-5.533446000	-1.788400000	-6.911463000
H	-7.045704000	-1.279310000	-6.152469000
C	-6.234464000	-3.146085000	-5.382648000
H	-6.874150000	-3.101418000	-4.489649000
H	-6.740391000	-3.802081000	-6.100615000
C	-4.869035000	-3.713451000	-4.997054000
H	-4.268202000	-3.874443000	-5.901169000
H	-4.975037000	-4.684235000	-4.499012000
C	-4.117827000	-2.753320000	-4.077157000
H	-4.652515000	-2.679009000	-3.105948000
H	-3.122986000	-3.156828000	-3.863947000
C	-4.501933000	3.343916000	-0.172930000
C	-3.968950000	3.164167000	1.087349000
C	-2.748943000	2.456117000	1.232902000
N	-2.110256000	1.917903000	0.163145000
C	-2.656926000	2.126966000	-1.049956000
C	-3.829996000	2.824948000	-1.281326000
H	-5.434332000	3.889563000	-0.291329000
H	-4.475375000	3.566586000	1.954807000
H	-2.108084000	1.697434000	-1.879504000
H	-4.202773000	2.947369000	-2.291688000
N	-2.174978000	2.316497000	2.460710000
C	-2.835702000	2.832650000	3.641468000
H	-3.816918000	2.367450000	3.798478000
H	-2.218529000	2.610535000	4.511177000
H	-2.968754000	3.921523000	3.589572000
C	-0.907560000	1.637931000	2.596035000
H	-0.505567000	1.819017000	3.595717000
H	-0.177128000	2.035126000	1.879315000
H	-1.020072000	0.547942000	2.473695000

TS(A1-A2)

Y	11.127770000	9.471322000	14.417697000

N	10.481428000	9.641693000	10.755824000
N	12.684758000	11.429263000	13.915647000
N	13.486478000	8.880246000	17.279384000
N	12.190359000	11.112050000	20.019160000
C	11.297099000	10.824941000	21.140730000
H	11.814869000	10.225018000	21.919004000
H	10.468855000	10.209008000	20.769950000
C	10.759237000	12.105064000	21.774273000
H	10.147166000	12.637965000	21.035330000
H	10.103509000	11.846753000	22.614058000
C	11.906422000	13.004943000	22.231770000
H	12.441788000	12.517203000	23.058761000
H	11.524466000	13.955882000	22.620915000
C	12.872776000	13.240318000	21.072877000
H	12.379722000	13.835592000	20.294125000
H	13.751447000	13.805656000	21.404922000
C	13.328971000	11.918512000	20.460262000
H	13.972526000	12.125647000	19.600445000
H	13.941465000	11.361765000	21.201617000
N	12.138998000	7.209794000	13.603053000
C	11.072442000	9.972377000	11.944410000
C	11.837245000	11.135253000	11.676288000
C	11.689638000	11.504690000	10.286541000
C	12.187344000	12.518182000	9.456963000
H	12.856410000	13.281375000	9.846619000
C	11.815232000	12.536668000	8.116993000
H	12.195709000	13.319613000	7.466592000
C	10.956906000	11.559436000	7.587540000
H	10.684645000	11.597569000	6.536549000
C	10.447739000	10.542170000	8.389712000
H	9.782917000	9.786731000	7.980715000
C	10.822886000	10.533787000	9.734332000
C	9.593086000	8.514542000	10.523184000
H	9.749166000	7.807481000	11.338968000
H	9.894674000	8.015142000	9.595664000
C	8.123114000	8.946127000	10.395771000
H	7.689677000	9.091659000	11.405688000
H	8.096150000	9.922713000	9.898906000
C	12.618828000	11.793761000	12.659546000
H	13.209907000	12.658851000	12.337148000
C	13.547283000	12.184240000	14.772053000
C	13.062239000	13.344140000	15.419852000
C	13.919789000	14.034432000	16.284119000
H	13.561680000	14.930738000	16.782469000

C	15.221139000	13.604033000	16.509289000
H	15.871894000	14.156321000	17.182263000
C	15.691564000	12.472962000	15.851494000
H	16.716582000	12.151429000	16.011450000
C	14.878012000	11.748605000	14.975415000
C	11.668573000	13.890133000	15.150060000
H	11.063271000	13.069896000	14.750695000
C	11.709933000	14.996875000	14.083404000
H	12.320799000	15.840702000	14.424324000
H	10.701172000	15.370575000	13.875084000
H	12.135943000	14.639224000	13.141667000
C	10.970267000	14.408797000	16.412699000
H	10.995172000	13.668780000	17.217810000
H	9.923824000	14.643257000	16.189439000
H	11.431062000	15.329397000	16.788011000
C	15.458245000	10.580266000	14.195016000
H	14.622151000	9.942404000	13.888444000
C	16.422371000	9.711809000	15.009070000
H	17.351234000	10.241424000	15.249183000
H	16.701147000	8.824509000	14.432196000
H	15.969770000	9.372632000	15.944053000
C	16.152317000	11.096013000	12.923284000
H	15.459835000	11.640284000	12.274054000
H	16.575241000	10.266579000	12.346059000
H	16.970659000	11.778037000	13.181144000
C	12.838145000	8.609267000	16.099787000
C	13.289367000	7.320932000	15.720464000
C	14.226736000	6.817654000	16.696128000
C	14.990265000	5.652060000	16.842433000
H	14.921587000	4.844784000	16.117699000
C	15.847661000	5.539745000	17.930707000
H	16.443873000	4.639728000	18.053956000
C	15.960443000	6.575118000	18.872650000
H	16.644591000	6.466764000	19.709556000
C	15.208077000	7.739286000	18.751749000
H	15.305065000	8.537360000	19.481245000
C	14.337828000	7.839977000	17.663889000
C	13.370366000	10.097456000	18.064804000
H	12.852391000	10.842948000	17.462259000
H	14.380353000	10.478369000	18.251665000
C	12.606837000	9.871517000	19.377557000
H	11.706933000	9.291078000	19.144057000
H	13.208378000	9.242829000	20.061887000
C	12.939090000	6.694150000	14.500568000

H	13.399735000	5.721758000	14.289258000
C	11.977073000	6.453270000	12.397681000
C	12.731439000	6.818389000	11.254856000
C	12.519947000	6.125317000	10.060738000
H	13.087579000	6.402983000	9.177902000
C	11.611029000	5.074975000	9.983262000
H	11.460772000	4.548265000	9.044643000
C	10.925268000	4.683801000	11.124299000
H	10.252424000	3.831637000	11.075657000
C	11.095280000	5.348885000	12.346033000
C	13.835750000	7.858800000	11.343961000
H	13.542733000	8.581363000	12.113582000
C	15.145794000	7.187923000	11.791804000
H	15.047983000	6.704693000	12.767874000
H	15.953409000	7.924719000	11.861243000
H	15.450373000	6.422439000	11.068814000
C	14.069121000	8.635476000	10.045391000
H	14.523193000	8.008031000	9.269732000
H	14.759886000	9.464361000	10.228394000
H	13.141847000	9.055206000	9.648257000
C	10.388011000	4.797057000	13.574811000
H	10.533925000	5.503677000	14.396998000
C	8.877923000	4.632418000	13.369330000
H	8.401613000	5.584960000	13.119693000
H	8.411825000	4.250382000	14.283326000
H	8.650366000	3.920395000	12.568779000
C	11.016856000	3.461257000	14.004744000
H	10.893979000	2.699372000	13.226872000
H	10.543225000	3.087131000	14.919187000
H	12.089271000	3.564099000	14.196683000
C	9.147476000	8.134072000	15.388111000
H	8.369066000	8.540485000	14.722657000
H	9.641054000	7.314381000	14.838387000
Si	8.294612000	7.265100000	16.832083000
C	7.698576000	8.473351000	18.176462000
H	8.526061000	9.002441000	18.658275000
H	7.156137000	7.924113000	18.954365000
H	7.015098000	9.218847000	17.757111000
C	6.729398000	6.338602000	16.267290000
H	6.003575000	7.041157000	15.841910000
H	6.246509000	5.831859000	17.110702000
H	6.948739000	5.586985000	15.503753000
C	9.505118000	6.039789000	17.631295000
H	9.778439000	5.240513000	16.934459000

H	9.070462000	5.572410000	18.521576000
H	10.429541000	6.545836000	17.928404000
N	7.338913000	8.024995000	9.589091000
C	6.030737000	8.590103000	9.271164000
H	6.184738000	9.577454000	8.819556000
H	5.427956000	8.747629000	10.191020000
C	5.256057000	7.690561000	8.311956000
H	5.800674000	7.639963000	7.360606000
H	4.276828000	8.137604000	8.103684000
C	5.102217000	6.285494000	8.893450000
H	4.454266000	6.329224000	9.780538000
H	4.609959000	5.618714000	8.175952000
C	6.470493000	5.736229000	9.294683000
H	7.080733000	5.574988000	8.396994000
H	6.371063000	4.768016000	9.799127000
C	7.203803000	6.711476000	10.213209000
H	6.659533000	6.787266000	11.179408000
H	8.200842000	6.319944000	10.438153000
C	6.883762000	12.894018000	14.075215000
C	7.365372000	12.529618000	15.314083000
C	8.505810000	11.686288000	15.400202000
N	9.130688000	11.228964000	14.278220000
C	8.626316000	11.609577000	13.087632000
C	7.525363000	12.430490000	12.921648000
H	6.011146000	13.538268000	14.004434000
H	6.876671000	12.876305000	16.215445000
H	9.158248000	11.232112000	12.223644000
H	7.187618000	12.697149000	11.926909000
N	9.024982000	11.325114000	16.596922000
C	8.532199000	11.938483000	17.815786000
H	7.500490000	11.638455000	18.036921000
H	9.165139000	11.616395000	18.641698000
H	8.574424000	13.034782000	17.767775000
C	10.225816000	10.510442000	16.615140000
H	10.385579000	10.151839000	17.631388000
H	11.106012000	11.143379000	16.383824000
H	9.796126000	9.291150000	16.042532000

A2

Y	0.578554000	0.621374000	-0.182284000
N	-0.191958000	0.384346000	-3.830025000
N	2.035872000	2.534818000	-0.910135000
N	2.947067000	0.531732000	2.692582000
N	1.560655000	3.174265000	4.988779000

C	0.389461000	3.146514000	5.863559000
H	0.573462000	2.509725000	6.754597000
H	-0.438799000	2.688404000	5.311048000
C	-0.001343000	4.548846000	6.321330000
H	-0.302405000	5.134879000	5.443922000
H	-0.872209000	4.484381000	6.984439000
C	1.168513000	5.237512000	7.023397000
H	1.383646000	4.716209000	7.967102000
H	0.912344000	6.270746000	7.285110000
C	2.407133000	5.194722000	6.129756000
H	2.243523000	5.816380000	5.240709000
H	3.281661000	5.598927000	6.653133000
C	2.705460000	3.766949000	5.678435000
H	3.564051000	3.773926000	5.000191000
H	2.992704000	3.155286000	6.560376000
N	1.322833000	-1.740331000	-0.483342000
C	0.413897000	0.832633000	-2.693390000
C	1.264585000	1.892435000	-3.109666000
C	1.157982000	2.063845000	-4.542596000
C	1.736408000	2.908462000	-5.498310000
H	2.459688000	3.666970000	-5.209243000
C	1.374328000	2.764288000	-6.833799000
H	1.818900000	3.414317000	-7.582523000
C	0.443312000	1.792112000	-7.231887000
H	0.178852000	1.700802000	-8.281593000
C	-0.148291000	0.942427000	-6.300951000
H	-0.870527000	0.192777000	-6.611042000
C	0.220738000	1.093430000	-4.963665000
C	-1.212134000	-0.648357000	-3.894526000
H	-1.101288000	-1.268768000	-3.003915000
H	-1.024542000	-1.285896000	-4.765355000
C	-2.618940000	-0.043380000	-4.014287000
H	-2.920393000	0.377266000	-3.034751000
H	-2.562922000	0.799553000	-4.712040000
C	2.057035000	2.656740000	-2.217191000
H	2.727082000	3.406124000	-2.654427000
C	2.969573000	3.329152000	-0.175157000
C	2.497122000	4.450683000	0.546417000
C	3.415082000	5.220765000	1.265035000
H	3.065300000	6.090705000	1.812941000
C	4.767760000	4.898453000	1.285280000
H	5.468352000	5.512190000	1.845439000
C	5.217490000	3.788977000	0.581230000
H	6.275069000	3.539025000	0.598520000

C	4.340933000	2.983558000	-0.155053000
C	1.033372000	4.855560000	0.492698000
H	0.455264000	3.954390000	0.261912000
C	0.792253000	5.853437000	-0.651166000
H	1.357819000	6.777041000	-0.482857000
H	-0.269978000	6.111811000	-0.721617000
H	1.105947000	5.443437000	-1.616394000
C	0.501534000	5.415081000	1.817104000
H	0.732480000	4.756299000	2.660843000
H	-0.585814000	5.533776000	1.759043000
H	0.918020000	6.404735000	2.037930000
C	4.899821000	1.786248000	-0.911075000
H	4.054125000	1.190475000	-1.267899000
C	5.749154000	0.873635000	-0.016375000
H	6.660458000	1.374287000	0.328645000
H	6.059593000	-0.016361000	-0.574111000
H	5.189363000	0.543098000	0.861875000
C	5.706688000	2.234606000	-2.139894000
H	5.102367000	2.833200000	-2.828634000
H	6.086557000	1.366653000	-2.690156000
H	6.567145000	2.844422000	-1.841951000
C	2.286957000	0.070620000	1.590843000
C	2.673028000	-1.287999000	1.459242000
C	3.599288000	-1.634408000	2.513814000
C	4.313650000	-2.780104000	2.886233000
H	4.219819000	-3.704386000	2.321481000
C	5.153863000	-2.721929000	3.993049000
H	5.712198000	-3.605736000	4.289565000
C	5.295273000	-1.537819000	4.733873000
H	5.960661000	-1.518524000	5.592434000
C	4.594194000	-0.386884000	4.385605000
H	4.706086000	0.526395000	4.962573000
C	3.750616000	-0.453355000	3.276368000
C	2.789401000	1.858970000	3.261253000
H	2.380253000	2.509998000	2.488014000
H	3.780793000	2.245950000	3.518471000
C	1.851531000	1.842676000	4.474314000
H	0.908098000	1.391636000	4.147393000
H	2.262574000	1.177682000	5.258729000
C	2.172879000	-2.129309000	0.438147000
H	2.512509000	-3.171491000	0.422987000
C	0.906513000	-2.711876000	-1.444343000
C	1.595586000	-2.810811000	-2.676711000
C	1.141975000	-3.737687000	-3.619083000

H	1.661194000	-3.827170000	-4.568642000
C	0.044256000	-4.553755000	-3.363661000
H	-0.289700000	-5.269133000	-4.110494000
C	-0.611810000	-4.458479000	-2.143110000
H	-1.455361000	-5.112393000	-1.935826000
C	-0.199250000	-3.545655000	-1.164825000
C	2.842258000	-1.983206000	-2.948881000
H	2.766424000	-1.074824000	-2.340239000
C	4.101646000	-2.744319000	-2.502231000
H	4.073185000	-2.994090000	-1.437810000
H	4.999916000	-2.143307000	-2.682432000
H	4.204634000	-3.681059000	-3.061868000
C	2.985487000	-1.544284000	-4.409601000
H	3.192890000	-2.390575000	-5.074407000
H	3.824937000	-0.848533000	-4.507984000
H	2.087490000	-1.036861000	-4.770568000
C	-0.915326000	-3.515395000	0.177009000
H	-0.511700000	-2.674653000	0.747918000
C	-2.424970000	-3.286115000	0.033723000
H	-2.638459000	-2.353163000	-0.496534000
H	-2.895888000	-3.226693000	1.021216000
H	-2.911771000	-4.102068000	-0.511886000
C	-0.632118000	-4.795149000	0.978332000
H	-1.015083000	-5.681203000	0.459411000
H	-1.111195000	-4.749048000	1.962670000
H	0.441731000	-4.941218000	1.131465000
C	-6.318215000	-4.961884000	3.221556000
H	-6.058191000	-4.250910000	4.013090000
H	-7.141618000	-4.530195000	2.642620000
Si	-6.801962000	-6.646595000	3.950359000
C	-5.340655000	-7.351476000	4.934381000
H	-4.462205000	-7.490354000	4.295288000
H	-5.590924000	-8.323225000	5.373093000
H	-5.055606000	-6.680377000	5.751543000
C	-8.292959000	-6.426389000	5.103616000
H	-8.056025000	-5.744521000	5.927246000
H	-8.601141000	-7.382321000	5.540208000
H	-9.152521000	-6.013162000	4.565168000
C	-7.256644000	-7.838022000	2.545591000
H	-8.102287000	-7.457613000	1.962915000
H	-7.537007000	-8.821498000	2.937390000
H	-6.414922000	-7.979634000	1.859474000
N	-3.594266000	-0.985748000	-4.538633000
C	-4.812233000	-0.302890000	-4.964963000

H	-4.531653000	0.497411000	-5.659736000
H	-5.323121000	0.182436000	-4.105969000
C	-5.780340000	-1.267999000	-5.643621000
H	-5.311013000	-1.650404000	-6.558911000
H	-6.685652000	-0.726544000	-5.942675000
C	-6.122263000	-2.433309000	-4.715733000
H	-6.695981000	-2.056413000	-3.856850000
H	-6.761289000	-3.163459000	-5.225987000
C	-4.837507000	-3.091626000	-4.215011000
H	-4.320847000	-3.576256000	-5.053185000
H	-5.058834000	-3.869847000	-3.475171000
C	-3.898797000	-2.058172000	-3.595710000
H	-4.360355000	-1.650367000	-2.670293000
H	-2.965552000	-2.546062000	-3.297516000
C	-3.769801000	3.641021000	-0.533196000
C	-3.664412000	2.680914000	0.448291000
C	-2.493278000	1.872034000	0.518534000
N	-1.466345000	2.077973000	-0.356349000
C	-1.610520000	3.021051000	-1.309065000
C	-2.725375000	3.823881000	-1.451181000
H	-4.664802000	4.255828000	-0.587334000
H	-4.464193000	2.545661000	1.164977000
H	-0.769119000	3.118820000	-1.988548000
H	-2.774273000	4.565056000	-2.240421000
N	-2.352374000	0.886871000	1.430412000
C	-3.393121000	0.671840000	2.419008000
H	-4.375093000	0.522990000	1.953087000
H	-3.144524000	-0.231816000	2.975796000
H	-3.472952000	1.503748000	3.135864000
C	-1.062980000	0.218518000	1.582580000
H	-1.258366000	-0.847991000	1.768252000
H	-0.589151000	0.590128000	2.511229000
H	-5.453233000	-5.052182000	2.555901000

A3

Y	-0.033502000	-0.072994000	0.129472000
N	-1.114015000	0.229988000	-3.434808000
N	0.951112000	2.200230000	-0.283234000
N	2.596931000	-0.210669000	2.763951000
N	0.993008000	1.618583000	5.638644000
C	-0.080014000	1.205355000	6.541569000
H	0.277456000	0.437002000	7.259456000
H	-0.869132000	0.737340000	5.942075000
C	-0.647751000	2.390219000	7.317346000

H	-1.111003000	3.086905000	6.607455000
H	-1.438180000	2.037799000	7.990661000
C	0.453378000	3.107613000	8.097622000
H	0.827566000	2.444705000	8.890860000
H	0.059722000	4.002218000	8.593972000
C	1.602910000	3.469201000	7.158066000
H	1.268757000	4.228036000	6.439584000
H	2.444101000	3.897597000	7.715726000
C	2.083593000	2.243016000	6.385489000
H	2.868282000	2.542320000	5.684009000
H	2.539770000	1.518024000	7.093151000
N	1.093110000	-2.142117000	-0.686141000
C	-0.487236000	0.570693000	-2.272264000
C	0.093078000	1.845155000	-2.514091000
C	-0.197816000	2.260503000	-3.869290000
C	0.099161000	3.375248000	-4.663332000
H	0.690219000	4.199200000	-4.271201000
C	-0.372647000	3.416857000	-5.971425000
H	-0.146643000	4.277351000	-6.595328000
C	-1.136250000	2.364624000	-6.500857000
H	-1.491283000	2.422594000	-7.525922000
C	-1.446735000	1.246497000	-5.731501000
H	-2.039409000	0.434503000	-6.142715000
C	-0.970139000	1.212938000	-4.420426000
C	-1.917100000	-0.962631000	-3.644729000
H	-1.588279000	-1.706102000	-2.917098000
H	-1.711046000	-1.365201000	-4.642446000
C	-3.418633000	-0.659051000	-3.532766000
H	-3.681123000	-0.499915000	-2.468353000
H	-3.608504000	0.290398000	-4.045872000
C	0.810995000	2.574369000	-1.533677000
H	1.272212000	3.519172000	-1.844155000
C	1.778970000	3.018607000	0.546059000
C	1.168790000	3.858637000	1.507023000
C	1.984071000	4.651160000	2.319059000
H	1.525941000	5.307631000	3.052733000
C	3.369307000	4.618117000	2.200985000
H	3.987984000	5.245037000	2.837775000
C	3.956692000	3.781210000	1.260944000
H	5.039501000	3.757420000	1.170939000
C	3.186916000	2.967078000	0.422029000
C	-0.344024000	3.949234000	1.616871000
H	-0.753436000	3.003227000	1.246206000
C	-0.884985000	5.063241000	0.706911000

H	-0.498240000	6.039597000	1.020655000
H	-1.979009000	5.100051000	0.748574000
H	-0.590723000	4.908640000	-0.335886000
C	-0.845987000	4.134339000	3.053332000
H	-0.404962000	3.400928000	3.736386000
H	-1.935328000	4.023650000	3.082505000
H	-0.617124000	5.134398000	3.439591000
C	3.889998000	2.081424000	-0.597166000
H	3.146656000	1.393150000	-1.011493000
C	4.996294000	1.223336000	0.030731000
H	5.821853000	1.834505000	0.411826000
H	5.416334000	0.545036000	-0.719663000
H	4.612555000	0.617974000	0.855437000
C	4.453233000	2.915547000	-1.758526000
H	3.671309000	3.489406000	-2.265578000
H	4.933391000	2.269320000	-2.501676000
H	5.204407000	3.628593000	-1.399950000
C	1.923567000	-0.582557000	1.636483000
C	2.538201000	-1.787342000	1.208670000
C	3.616016000	-2.129972000	2.109362000
C	4.563676000	-3.157590000	2.196763000
H	4.585715000	-3.959881000	1.463396000
C	5.485544000	-3.139082000	3.238123000
H	6.224670000	-3.932004000	3.313919000
C	5.478663000	-2.110828000	4.193984000
H	6.211283000	-2.119358000	4.996106000
C	4.545701000	-1.079899000	4.130181000
H	4.542953000	-0.287870000	4.873242000
C	3.622983000	-1.105827000	3.084117000
C	2.257734000	0.926745000	3.601562000
H	1.675959000	1.628132000	3.002583000
H	3.184862000	1.436174000	3.883966000
C	1.448693000	0.495217000	4.830694000
H	0.566134000	-0.040531000	4.464453000
H	2.032379000	-0.232667000	5.427436000
C	2.095302000	-2.511309000	0.077427000
H	2.617448000	-3.443282000	-0.168802000
C	0.765727000	-2.987894000	-1.790065000
C	1.329496000	-2.722077000	-3.060745000
C	0.958327000	-3.534129000	-4.135770000
H	1.383452000	-3.344527000	-5.116945000
C	0.061527000	-4.585661000	-3.974127000
H	-0.212096000	-5.205446000	-4.823866000
C	-0.468172000	-4.848306000	-2.717068000

H	-1.148437000	-5.686593000	-2.587414000
C	-0.130221000	-4.064925000	-1.606879000
C	2.369963000	-1.628625000	-3.244770000
H	2.196377000	-0.883572000	-2.459905000
C	3.785968000	-2.196155000	-3.050129000
H	3.915027000	-2.646311000	-2.061673000
H	4.537228000	-1.406247000	-3.160622000
H	3.996897000	-2.969393000	-3.797802000
C	2.275409000	-0.906561000	-4.592510000
H	2.561136000	-1.556788000	-5.427218000
H	2.959413000	-0.051880000	-4.605892000
H	1.267036000	-0.530085000	-4.781277000
C	-0.685490000	-4.429539000	-0.238410000
H	-0.388022000	-3.641697000	0.458981000
C	-2.217432000	-4.499208000	-0.220851000
H	-2.663866000	-3.551282000	-0.535865000
H	-2.575969000	-4.719611000	0.790716000
H	-2.598131000	-5.286616000	-0.880752000
C	-0.074401000	-5.745846000	0.266397000
H	-0.339625000	-6.583741000	-0.388306000
H	-0.437118000	-5.978924000	1.273693000
H	1.018090000	-5.690467000	0.305029000
N	-4.245348000	-1.674867000	-4.164598000
C	-5.612847000	-1.202010000	-4.356857000
H	-5.573799000	-0.244541000	-4.889578000
H	-6.112264000	-1.007406000	-3.383773000
C	-6.438916000	-2.208884000	-5.153105000
H	-6.005956000	-2.300951000	-6.157282000
H	-7.461017000	-1.830168000	-5.271912000
C	-6.439133000	-3.574377000	-4.466158000
H	-6.983603000	-3.501071000	-3.513692000
H	-6.968502000	-4.316551000	-5.075106000
C	-5.003146000	-4.020462000	-4.192779000
H	-4.490781000	-4.219469000	-5.142626000
H	-4.986749000	-4.951072000	-3.613257000
C	-4.228990000	-2.941322000	-3.438987000
H	-4.662917000	-2.819182000	-2.422759000
H	-3.191627000	-3.263516000	-3.305845000
C	-4.910570000	1.950975000	0.652723000
C	-4.514401000	0.878417000	1.420348000
C	-3.204532000	0.341184000	1.256865000
N	-2.336752000	0.913337000	0.372704000
C	-2.764453000	1.955776000	-0.368026000
C	-4.024991000	2.512913000	-0.278114000

H	-5.910733000	2.358491000	0.777434000
H	-5.191931000	0.450389000	2.147807000
H	-2.036398000	2.349210000	-1.071249000
H	-4.302330000	3.353267000	-0.903844000
N	-2.774360000	-0.733119000	1.952122000
C	-3.638902000	-1.331278000	2.952877000
H	-4.618617000	-1.600370000	2.539295000
H	-3.160413000	-2.245084000	3.305522000
H	-3.798871000	-0.672235000	3.820399000
C	-1.366567000	-1.117390000	1.892013000
H	-1.317889000	-2.216277000	1.886788000
H	-0.885057000	-0.813195000	2.841112000

TS(A3-A4)

Y	0.139917000	-0.133049000	-0.028546000
N	-1.059245000	0.169107000	-3.586814000
N	0.857619000	2.203586000	-0.422479000
N	2.400072000	-0.577638000	2.859894000
N	2.732188000	2.337476000	5.232150000
C	1.811515000	3.092143000	6.076278000
H	1.460684000	2.483457000	6.937501000
H	0.926555000	3.341354000	5.480114000
C	2.459422000	4.371522000	6.599388000
H	2.685660000	5.021212000	5.744587000
H	1.746424000	4.906973000	7.237783000
C	3.746562000	4.060108000	7.362047000
H	3.498914000	3.511513000	8.282135000
H	4.249598000	4.983755000	7.671456000
C	4.668020000	3.201760000	6.496671000
H	5.019503000	3.786093000	5.637072000
H	5.553504000	2.886600000	7.061174000
C	3.930323000	1.968507000	5.980331000
H	4.594705000	1.392319000	5.328274000
H	3.673531000	1.309931000	6.838079000
N	0.648496000	-2.340144000	-0.552852000
C	-0.484006000	0.554739000	-2.410937000
C	-0.012037000	1.875570000	-2.643525000
C	-0.305643000	2.269179000	-4.003653000
C	-0.083323000	3.402555000	-4.795508000
H	0.426467000	4.275009000	-4.394392000
C	-0.523005000	3.396971000	-6.115436000
H	-0.354124000	4.270762000	-6.739044000
C	-1.181266000	2.281499000	-6.658227000
H	-1.512531000	2.307076000	-7.692649000

C	-1.417354000	1.143061000	-5.892324000
H	-1.936556000	0.279630000	-6.300548000
C	-0.969665000	1.159529000	-4.570530000
C	-1.711572000	-1.103206000	-3.851297000
H	-1.476270000	-1.764837000	-3.017735000
H	-1.265465000	-1.538400000	-4.752345000
C	-3.233109000	-0.954010000	-4.072942000
H	-3.781505000	-1.349975000	-3.195695000
H	-3.470370000	0.113521000	-4.135150000
C	0.633170000	2.635030000	-1.645457000
H	0.965175000	3.647315000	-1.902833000
C	1.533465000	3.102184000	0.457428000
C	0.772613000	3.837827000	1.395684000
C	1.439435000	4.719151000	2.249767000
H	0.869649000	5.302214000	2.967875000
C	2.820316000	4.874200000	2.188213000
H	3.321684000	5.564774000	2.860085000
C	3.554760000	4.143152000	1.263685000
H	4.633345000	4.270125000	1.218831000
C	2.937080000	3.245441000	0.386222000
C	-0.745684000	3.741219000	1.418291000
H	-1.020285000	2.794243000	0.936398000
C	-1.371300000	4.866396000	0.578862000
H	-1.117694000	5.847065000	0.996914000
H	-2.463453000	4.777780000	0.558996000
H	-1.010898000	4.841967000	-0.453895000
C	-1.342343000	3.725917000	2.829407000
H	-0.898096000	2.938337000	3.446440000
H	-2.422136000	3.548535000	2.779680000
H	-1.197544000	4.679636000	3.348145000
C	3.786213000	2.474873000	-0.615279000
H	3.129395000	1.777016000	-1.143353000
C	4.876873000	1.639380000	0.068655000
H	5.584501000	2.268267000	0.619816000
H	5.449323000	1.079845000	-0.679190000
H	4.444872000	0.919747000	0.769395000
C	4.395679000	3.415879000	-1.665714000
H	3.622762000	3.976969000	-2.200828000
H	4.973390000	2.848146000	-2.403241000
H	5.070512000	4.144160000	-1.202208000
C	1.512679000	-0.867427000	1.793440000
C	1.653149000	-2.336776000	1.627941000
C	2.410184000	-2.864097000	2.749283000
C	2.777473000	-4.144316000	3.163324000

H	2.431526000	-5.020175000	2.619347000
C	3.605079000	-4.294941000	4.280845000
H	3.893219000	-5.290611000	4.607129000
C	4.065449000	-3.176361000	4.976639000
H	4.708629000	-3.306210000	5.843050000
C	3.704176000	-1.882286000	4.581826000
H	4.066831000	-1.020738000	5.133787000
C	2.870651000	-1.738916000	3.474728000
C	2.787516000	0.737493000	3.320410000
H	2.576359000	1.459626000	2.529430000
H	3.875140000	0.743763000	3.471939000
C	2.088233000	1.182539000	4.619596000
H	1.056354000	1.460890000	4.378363000
H	2.026620000	0.326760000	5.319840000
C	1.256091000	-2.982727000	0.487758000
H	1.461689000	-4.050209000	0.375021000
C	0.507179000	-3.092841000	-1.747551000
C	1.346183000	-2.795923000	-2.854227000
C	1.199757000	-3.529716000	-4.033275000
H	1.841291000	-3.311072000	-4.882005000
C	0.259999000	-4.551778000	-4.138949000
H	0.170017000	-5.119702000	-5.061287000
C	-0.551217000	-4.845949000	-3.050574000
H	-1.278031000	-5.651406000	-3.129441000
C	-0.450924000	-4.131638000	-1.850214000
C	2.445239000	-1.751265000	-2.736273000
H	2.099048000	-0.999283000	-2.014918000
C	3.721056000	-2.379936000	-2.153985000
H	3.534510000	-2.818940000	-1.170136000
H	4.510371000	-1.627391000	-2.044961000
H	4.095354000	-3.169704000	-2.815573000
C	2.749330000	-1.013592000	-4.042684000
H	3.225976000	-1.667053000	-4.781951000
H	3.445434000	-0.189855000	-3.852754000
H	1.843952000	-0.593283000	-4.490020000
C	-1.370819000	-4.500997000	-0.695670000
H	-1.192367000	-3.779856000	0.107707000
C	-2.852231000	-4.402765000	-1.084999000
H	-3.104630000	-3.400903000	-1.445378000
H	-3.490908000	-4.619732000	-0.221472000
H	-3.112489000	-5.117238000	-1.873784000
C	-1.053021000	-5.900528000	-0.147720000
H	-1.217048000	-6.671596000	-0.909062000
H	-1.695121000	-6.138026000	0.708469000

H	-0.011455000	-5.977156000	0.178850000
N	-3.683151000	-1.576148000	-5.310084000
C	-5.016866000	-1.116912000	-5.686493000
H	-5.006462000	-0.020904000	-5.713119000
H	-5.773861000	-1.415666000	-4.930261000
C	-5.425138000	-1.669461000	-7.049622000
H	-4.743711000	-1.266031000	-7.809233000
H	-6.433823000	-1.318821000	-7.297899000
C	-5.359864000	-3.196660000	-7.060325000
H	-6.132121000	-3.598043000	-6.388520000
H	-5.579181000	-3.587395000	-8.060727000
C	-3.985202000	-3.664525000	-6.583828000
H	-3.220977000	-3.374282000	-7.315847000
H	-3.952679000	-4.756729000	-6.495080000
C	-3.635079000	-3.035251000	-5.237437000
H	-4.336429000	-3.410052000	-4.461530000
H	-2.631033000	-3.344502000	-4.928207000
C	-4.705681000	-1.578852000	1.046620000
C	-3.686930000	-1.879768000	1.924025000
C	-2.402572000	-1.318574000	1.711392000
N	-2.166325000	-0.519871000	0.631372000
C	-3.187326000	-0.241109000	-0.209579000
C	-4.465186000	-0.734070000	-0.050981000
H	-5.698803000	-1.984532000	1.218964000
H	-3.873471000	-2.498396000	2.793133000
H	-2.929877000	0.399087000	-1.049342000
H	-5.246678000	-0.474942000	-0.755469000
N	-1.366684000	-1.506747000	2.561936000
C	-1.415957000	-2.519172000	3.600569000
H	-1.921975000	-3.417918000	3.240010000
H	-0.391313000	-2.798110000	3.853217000
H	-1.922166000	-2.157914000	4.507566000
C	-0.240798000	-0.595943000	2.566699000
H	0.176283000	-0.610754000	3.569708000
H	-0.619046000	0.432636000	2.398348000

A4

Y	0.353613000	-0.180059000	-0.192530000
N	-1.041660000	0.401819000	-3.616514000
N	1.441025000	2.015548000	-0.599454000
N	1.403960000	-0.571403000	3.329107000
N	0.298936000	1.588081000	6.224017000
C	-0.423808000	1.269751000	7.452151000
H	0.236868000	0.772355000	8.193589000

H	-1.219133000	0.554946000	7.208889000
C	-1.025728000	2.524425000	8.079707000
H	-1.766589000	2.942063000	7.385937000
H	-1.555979000	2.254665000	9.000870000
C	0.058414000	3.564566000	8.360156000
H	0.727839000	3.186979000	9.146351000
H	-0.382463000	4.493145000	8.741179000
C	0.869543000	3.827670000	7.091851000
H	0.237411000	4.324519000	6.345177000
H	1.714237000	4.495055000	7.299750000
C	1.390719000	2.520175000	6.499752000
H	1.926688000	2.725292000	5.568181000
H	2.125135000	2.068657000	7.200829000
N	0.524691000	-2.350617000	-0.717672000
C	-0.376697000	0.702693000	-2.462484000
C	0.380827000	1.867923000	-2.757842000
C	0.147446000	2.266157000	-4.128481000
C	0.600467000	3.291189000	-4.968231000
H	1.301437000	4.040176000	-4.608274000
C	0.141671000	3.339854000	-6.280593000
H	0.486281000	4.132422000	-6.939215000
C	-0.757012000	2.379686000	-6.771609000
H	-1.095210000	2.439421000	-7.802214000
C	-1.221149000	1.349707000	-5.957899000
H	-1.915347000	0.606391000	-6.339241000
C	-0.759442000	1.311420000	-4.641769000
C	-1.953924000	-0.714246000	-3.801620000
H	-1.735327000	-1.440877000	-3.017439000
H	-1.740697000	-1.191152000	-4.765268000
C	-3.423107000	-0.263880000	-3.792353000
H	-3.749774000	-0.093823000	-2.746340000
H	-3.482902000	0.704654000	-4.301706000
C	1.220238000	2.490643000	-1.805133000
H	1.709347000	3.429741000	-2.087631000
C	2.246989000	2.804623000	0.281346000
C	1.605761000	3.663747000	1.204820000
C	2.399127000	4.412693000	2.077373000
H	1.924564000	5.081263000	2.789481000
C	3.787339000	4.324647000	2.045026000
H	4.387703000	4.916887000	2.730469000
C	4.402339000	3.481641000	1.128980000
H	5.486795000	3.422064000	1.103062000
C	3.654463000	2.706302000	0.235805000
C	0.092607000	3.824048000	1.203962000

H	-0.334748000	2.876124000	0.853551000
C	-0.339403000	4.916944000	0.212135000
H	0.087098000	5.884595000	0.499689000
H	-1.430570000	5.017671000	0.199234000
H	-0.010810000	4.697903000	-0.807559000
C	-0.505620000	4.112138000	2.584905000
H	-0.175817000	3.390015000	3.336720000
H	-1.598379000	4.068375000	2.530351000
H	-0.244842000	5.115351000	2.940556000
C	4.369912000	1.829039000	-0.780523000
H	3.628039000	1.146056000	-1.209187000
C	5.475709000	0.970407000	-0.155309000
H	6.304589000	1.581570000	0.218377000
H	5.892295000	0.291405000	-0.907543000
H	5.099201000	0.368230000	0.675491000
C	4.932021000	2.676737000	-1.932907000
H	4.147401000	3.248684000	-2.438175000
H	5.420672000	2.040719000	-2.679390000
H	5.674911000	3.392385000	-1.562697000
C	0.729487000	-0.991084000	2.099438000
C	1.753105000	-1.759789000	1.337018000
C	3.009355000	-1.644620000	2.081495000
C	4.293852000	-2.124671000	1.835012000
H	4.502898000	-2.713129000	0.945247000
C	5.323992000	-1.826340000	2.730184000
H	6.327401000	-2.198658000	2.545341000
C	5.068255000	-1.028825000	3.848577000
H	5.879264000	-0.780530000	4.528450000
C	3.786782000	-0.546183000	4.117026000
H	3.608587000	0.067632000	4.993913000
C	2.746229000	-0.892204000	3.247284000
C	0.984152000	0.625192000	4.039035000
H	0.042137000	0.961800000	3.601440000
H	1.718489000	1.429795000	3.879709000
C	0.760057000	0.386876000	5.537402000
H	-0.008406000	-0.385561000	5.641340000
H	1.671217000	-0.031042000	6.004455000
C	1.645054000	-2.390987000	0.098938000
H	2.534950000	-2.903009000	-0.272924000
C	0.432039000	-3.246543000	-1.809552000
C	1.297049000	-3.168557000	-2.930584000
C	1.115306000	-4.067075000	-3.988991000
H	1.778639000	-4.010811000	-4.848837000
C	0.104908000	-5.018191000	-3.972882000

H	-0.020428000	-5.700664000	-4.809310000
C	-0.743497000	-5.091511000	-2.872249000
H	-1.527413000	-5.843045000	-2.855799000
C	-0.593950000	-4.229873000	-1.783825000
C	2.420874000	-2.148489000	-3.039524000
H	2.338755000	-1.467203000	-2.183707000
C	3.799871000	-2.821937000	-2.962611000
H	3.912158000	-3.417240000	-2.051020000
H	4.599859000	-2.073322000	-2.983112000
H	3.953018000	-3.496002000	-3.812932000
C	2.316667000	-1.292369000	-4.309174000
H	2.446652000	-1.896241000	-5.213777000
H	3.097117000	-0.523625000	-4.315276000
H	1.348255000	-0.790639000	-4.373753000
C	-1.470680000	-4.380983000	-0.550800000
H	-1.634654000	-3.370776000	-0.158204000
C	-2.844889000	-5.000000000	-0.819633000
H	-3.380897000	-4.473942000	-1.615730000
H	-3.458119000	-4.953358000	0.086933000
H	-2.774284000	-6.056892000	-1.101181000
C	-0.729725000	-5.183513000	0.531153000
H	-0.521816000	-6.199790000	0.177079000
H	-1.333032000	-5.261162000	1.443765000
H	0.223080000	-4.714195000	0.790439000
N	-4.295507000	-1.186522000	-4.498967000
C	-5.613749000	-0.600603000	-4.721582000
H	-5.478702000	0.371487000	-5.210616000
H	-6.135070000	-0.406615000	-3.759663000
C	-6.482867000	-1.506733000	-5.589357000
H	-6.019146000	-1.593319000	-6.580129000
H	-7.466850000	-1.043690000	-5.729001000
C	-6.615763000	-2.893193000	-4.960119000
H	-7.187734000	-2.813562000	-4.024415000
H	-7.178663000	-3.566543000	-5.616938000
C	-5.230206000	-3.462412000	-4.658422000
H	-4.699583000	-3.660650000	-5.598217000
H	-5.306261000	-4.415090000	-4.121455000
C	-4.402993000	-2.480738000	-3.831017000
H	-4.861271000	-2.368723000	-2.824392000
H	-3.398515000	-2.888938000	-3.680632000
C	-4.279115000	1.354622000	1.672577000
C	-3.580752000	0.497251000	2.495309000
C	-2.379694000	-0.110602000	2.035615000
N	-1.909265000	0.169425000	0.786170000

C	-2.631095000	1.003068000	0.002404000
C	-3.804966000	1.621885000	0.383957000
H	-5.198174000	1.810745000	2.030931000
H	-3.951923000	0.285208000	3.488432000
H	-2.207904000	1.172168000	-0.985662000
H	-4.325042000	2.282591000	-0.299648000
N	-1.697818000	-0.979047000	2.825536000
C	-2.240126000	-1.322697000	4.126599000
H	-3.219286000	-1.816809000	4.051509000
H	-1.551509000	-2.009139000	4.618125000
H	-2.345799000	-0.438825000	4.766051000
C	-0.560706000	-1.761094000	2.313417000
H	-0.855869000	-2.231960000	1.365870000
H	-0.414590000	-2.584304000	3.026476000

TS(A4-A5)

Y	0.569125000	0.123731000	-0.663282000
N	-1.191052000	1.013101000	-3.820523000
N	2.420680000	1.427393000	-1.660749000
N	0.383959000	0.681211000	3.003304000
N	-2.062837000	0.189591000	5.829663000
C	-2.400227000	-0.993982000	6.617605000
H	-1.616699000	-1.211550000	7.373469000
H	-2.437040000	-1.856609000	5.941930000
C	-3.744117000	-0.825224000	7.321550000
H	-4.529850000	-0.733112000	6.560880000
H	-3.963211000	-1.723985000	7.909944000
C	-3.739471000	0.419610000	8.208564000
H	-3.035108000	0.270169000	9.039201000
H	-4.726269000	0.582207000	8.657352000
C	-3.305667000	1.637584000	7.393692000
H	-4.067652000	1.867091000	6.637992000
H	-3.205172000	2.521558000	8.034411000
C	-1.979341000	1.371119000	6.685498000
H	-1.712888000	2.238060000	6.072188000
H	-1.175146000	1.254658000	7.442880000
N	1.399135000	-1.987456000	-0.384082000
C	-0.165248000	0.950343000	-2.920431000
C	0.883039000	1.718140000	-3.491782000
C	0.464788000	2.234609000	-4.776196000
C	1.046427000	3.014924000	-5.782952000
H	2.061115000	3.391730000	-5.681745000
C	0.307521000	3.300642000	-6.926672000
H	0.751127000	3.903869000	-7.714080000

C	-1.001690000	2.819487000	-7.083458000
H	-1.554776000	3.055095000	-7.988321000
C	-1.603708000	2.043686000	-6.096094000
H	-2.617908000	1.673942000	-6.218810000
C	-0.855830000	1.764071000	-4.951869000
C	-2.511481000	0.438818000	-3.646139000
H	-2.429554000	-0.305882000	-2.852849000
H	-2.806363000	-0.075208000	-4.569623000
C	-3.570446000	1.506647000	-3.325357000
H	-3.516452000	1.766932000	-2.250898000
H	-3.314297000	2.414362000	-3.881815000
C	2.123634000	1.916853000	-2.843410000
H	2.880681000	2.518089000	-3.359114000
C	3.727451000	1.720030000	-1.152921000
C	3.928210000	2.890732000	-0.389936000
C	5.212994000	3.161516000	0.090671000
H	5.384691000	4.062104000	0.673318000
C	6.272947000	2.300379000	-0.163431000
H	7.264940000	2.527665000	0.217909000
C	6.058988000	1.146215000	-0.909004000
H	6.892207000	0.478353000	-1.107612000
C	4.794736000	0.831311000	-1.416415000
C	2.797877000	3.874917000	-0.130009000
H	1.857292000	3.344739000	-0.322269000
C	2.865258000	5.057446000	-1.109526000
H	3.804250000	5.608098000	-0.983430000
H	2.039197000	5.756602000	-0.935310000
H	2.813110000	4.726008000	-2.151026000
C	2.756948000	4.377466000	1.317632000
H	2.746961000	3.550566000	2.032344000
H	1.859330000	4.985623000	1.479134000
H	3.617228000	5.014127000	1.551129000
C	4.603158000	-0.406466000	-2.279482000
H	3.544978000	-0.686299000	-2.220819000
C	5.424219000	-1.614310000	-1.812102000
H	6.495604000	-1.477303000	-1.997800000
H	5.110559000	-2.510782000	-2.355165000
H	5.291226000	-1.810122000	-0.744141000
C	4.926060000	-0.097248000	-3.750751000
H	4.289476000	0.696619000	-4.151864000
H	4.784262000	-0.987280000	-4.373354000
H	5.968033000	0.226347000	-3.855677000
C	0.379851000	-0.294731000	1.951869000
C	1.766258000	-0.563549000	1.587691000

C	2.572137000	0.280073000	2.471020000
C	3.948726000	0.459339000	2.599838000
H	4.634750000	-0.044411000	1.925445000
C	4.439244000	1.299692000	3.598766000
H	5.510125000	1.441717000	3.706688000
C	3.556614000	1.963972000	4.458611000
H	3.951874000	2.611015000	5.237466000
C	2.175972000	1.818270000	4.337183000
H	1.505611000	2.340025000	5.013478000
C	1.687208000	0.975564000	3.330825000
C	-0.739074000	0.961865000	3.864698000
H	-1.663655000	0.925470000	3.280575000
H	-0.645535000	1.995087000	4.215600000
C	-0.850906000	-0.013495000	5.047901000
H	-0.873441000	-1.031527000	4.642008000
H	0.066009000	0.051485000	5.664252000
C	2.232536000	-1.367087000	0.550697000
H	3.311321000	-1.504901000	0.457126000
C	1.783422000	-3.244650000	-0.863606000
C	1.677399000	-3.535462000	-2.258369000
C	2.149518000	-4.753982000	-2.746017000
H	2.083473000	-4.958148000	-3.810851000
C	2.712779000	-5.710754000	-1.907478000
H	3.087729000	-6.647476000	-2.310600000
C	2.756068000	-5.457426000	-0.543500000
H	3.147941000	-6.220603000	0.125534000
C	2.280632000	-4.262720000	0.004864000
C	1.020959000	-2.555695000	-3.207934000
H	1.223499000	-1.542383000	-2.827206000
C	1.551440000	-2.595497000	-4.644136000
H	2.643577000	-2.535293000	-4.671315000
H	1.150229000	-1.750172000	-5.212656000
H	1.251325000	-3.509454000	-5.169261000
C	-0.502058000	-2.754598000	-3.204315000
H	-0.751547000	-3.761523000	-3.558544000
H	-0.993233000	-2.028378000	-3.860094000
H	-0.913858000	-2.648660000	-2.195180000
C	2.216333000	-4.167869000	1.526074000
H	1.779428000	-3.203565000	1.794038000
C	1.290034000	-5.251120000	2.102809000
H	0.294643000	-5.202800000	1.648744000
H	1.178801000	-5.124751000	3.186347000
H	1.682361000	-6.258674000	1.926260000
C	3.600793000	-4.234376000	2.184179000

H	4.104732000	-5.182982000	1.966478000
H	3.518081000	-4.145345000	3.273395000
H	4.247894000	-3.427075000	1.828092000
N	-4.907452000	1.103816000	-3.734458000
C	-5.834464000	2.231473000	-3.705736000
H	-5.398668000	3.047298000	-4.294148000
H	-5.967750000	2.616775000	-2.672432000
C	-7.195935000	1.843246000	-4.276691000
H	-7.070987000	1.581633000	-5.334939000
H	-7.870293000	2.706454000	-4.231530000
C	-7.782126000	0.652462000	-3.518783000
H	-8.018307000	0.957449000	-2.489081000
H	-8.724268000	0.326289000	-3.974141000
C	-6.770890000	-0.492699000	-3.487543000
H	-6.625405000	-0.883991000	-4.502183000
H	-7.135660000	-1.321021000	-2.868742000
C	-5.422244000	-0.015774000	-2.952997000
H	-5.526572000	0.262947000	-1.881660000
H	-4.702627000	-0.840645000	-2.999928000
C	-3.668780000	2.509730000	1.042301000
C	-3.440540000	1.155183000	0.859456000
C	-2.174169000	0.735078000	0.413683000
N	-1.178372000	1.629396000	0.160479000
C	-1.412031000	2.936490000	0.369820000
C	-2.632159000	3.425061000	0.802582000
H	-4.643611000	2.857713000	1.372105000
H	-4.222480000	0.429006000	1.051958000
H	-0.585158000	3.608837000	0.156171000
H	-2.777499000	4.491614000	0.935157000
N	-1.744928000	-0.566388000	0.243793000
C	-2.769110000	-1.587226000	0.100962000
H	-3.443444000	-1.345689000	-0.725816000
H	-2.288161000	-2.544169000	-0.116975000
H	-3.374987000	-1.719526000	1.011665000
C	-0.765543000	-1.087152000	1.628385000
H	-0.511946000	-2.074736000	1.249651000
H	-1.553256000	-1.119157000	2.383890000

A5

Y	-0.136026000	-0.244511000	-0.262441000
N	-1.632615000	0.609647000	-3.506984000
N	1.938824000	0.965382000	-1.264678000
N	0.283462000	0.301853000	3.600105000
N	-2.111414000	-0.240071000	6.448202000

C	-2.445902000	-1.444978000	7.203442000
H	-1.654103000	-1.689844000	7.942499000
H	-2.497322000	-2.285732000	6.501982000
C	-3.779638000	-1.288749000	7.929187000
H	-4.573648000	-1.170702000	7.180971000
H	-3.996709000	-2.202795000	8.494378000
C	-3.756834000	-0.069933000	8.851321000
H	-3.044505000	-0.247114000	9.669801000
H	-4.737627000	0.085675000	9.315504000
C	-3.324937000	1.168857000	8.067257000
H	-4.093689000	1.424344000	7.327108000
H	-3.211824000	2.033182000	8.732253000
C	-2.008789000	0.915431000	7.335513000
H	-1.745473000	1.798277000	6.743676000
H	-1.195651000	0.773278000	8.079200000
N	1.207878000	-2.242639000	0.177159000
C	-0.632195000	0.544462000	-2.576056000
C	0.468486000	1.212200000	-3.161607000
C	0.116585000	1.675164000	-4.483680000
C	0.767036000	2.360863000	-5.517588000
H	1.799393000	2.684723000	-5.411404000
C	0.071518000	2.621928000	-6.693348000
H	0.567094000	3.152094000	-7.502152000
C	-1.262087000	2.211963000	-6.855050000
H	-1.780265000	2.430790000	-7.784538000
C	-1.932497000	1.532097000	-5.842257000
H	-2.967744000	1.224212000	-5.961554000
C	-1.225021000	1.272959000	-4.666877000
C	-2.990642000	0.118530000	-3.359746000
H	-2.993964000	-0.541953000	-2.494014000
H	-3.252598000	-0.458797000	-4.255453000
C	-4.014065000	1.260476000	-3.201251000
H	-4.189451000	1.453519000	-2.125879000
H	-3.575984000	2.174202000	-3.615561000
C	1.692388000	1.394243000	-2.480314000
H	2.484007000	1.940833000	-3.004919000
C	3.257639000	1.285100000	-0.793625000
C	3.457107000	2.481732000	-0.069760000
C	4.754832000	2.819752000	0.323768000
H	4.921525000	3.742101000	0.872151000
C	5.835252000	1.998844000	0.025381000
H	6.838053000	2.278730000	0.337189000
C	5.625748000	0.818718000	-0.678133000
H	6.474264000	0.183699000	-0.916635000

C	4.347717000	0.438998000	-1.104411000
C	2.301141000	3.424395000	0.223087000
H	1.384048000	2.826796000	0.159720000
C	2.203803000	4.526334000	-0.843889000
H	3.113615000	5.137325000	-0.852052000
H	1.354530000	5.188475000	-0.640483000
H	2.071930000	4.111745000	-1.847371000
C	2.362551000	4.041834000	1.624386000
H	2.463351000	3.278061000	2.399646000
H	1.451448000	4.618608000	1.821785000
H	3.201040000	4.739590000	1.725389000
C	4.179743000	-0.823046000	-1.938165000
H	3.132252000	-1.133379000	-1.858846000
C	5.047549000	-1.992338000	-1.455354000
H	6.110201000	-1.824049000	-1.663361000
H	4.755042000	-2.912367000	-1.969967000
H	4.942426000	-2.166719000	-0.380711000
C	4.476376000	-0.547831000	-3.421986000
H	3.808004000	0.207841000	-3.843653000
H	4.363261000	-1.463659000	-4.012732000
H	5.504775000	-0.190631000	-3.548633000
C	0.251074000	-0.646131000	2.582155000
C	1.593435000	-0.684284000	1.992762000
C	2.430168000	0.175455000	2.823687000
C	3.789448000	0.475648000	2.828541000
H	4.449430000	0.075566000	2.064596000
C	4.296944000	1.318900000	3.821749000
H	5.357228000	1.552925000	3.832941000
C	3.454212000	1.869939000	4.787809000
H	3.863932000	2.523568000	5.552870000
C	2.081752000	1.596332000	4.788520000
H	1.434257000	2.022329000	5.548858000
C	1.588954000	0.747707000	3.803241000
C	-0.827619000	0.579672000	4.482730000
H	-1.755693000	0.559527000	3.904403000
H	-0.713202000	1.604239000	4.848678000
C	-0.918737000	-0.427838000	5.636746000
H	-0.960172000	-1.429230000	5.194348000
H	0.012723000	-0.385203000	6.234414000
C	2.023741000	-1.583832000	1.017442000
H	3.104310000	-1.727033000	0.913659000
C	1.719146000	-3.413223000	-0.419110000
C	1.489730000	-3.656098000	-1.800872000
C	2.060879000	-4.776255000	-2.402078000

H	1.907560000	-4.947024000	-3.463048000
C	2.828600000	-5.679008000	-1.670580000
H	3.277901000	-6.539615000	-2.158230000
C	2.978229000	-5.484437000	-0.305789000
H	3.528422000	-6.218215000	0.278171000
C	2.418754000	-4.382184000	0.351916000
C	0.578150000	-2.742020000	-2.592781000
H	0.781516000	-1.705476000	-2.276712000
C	0.800876000	-2.749197000	-4.106165000
H	1.850915000	-2.576406000	-4.359494000
H	0.207148000	-1.955984000	-4.569846000
H	0.491480000	-3.698505000	-4.557716000
C	-0.888573000	-3.074530000	-2.272987000
H	-1.123639000	-4.086631000	-2.620366000
H	-1.568210000	-2.374744000	-2.768138000
H	-1.085691000	-3.058287000	-1.194313000
C	2.487283000	-4.364606000	1.876820000
H	1.965273000	-3.476481000	2.243201000
C	1.743066000	-5.575880000	2.462584000
H	0.709755000	-5.614718000	2.104049000
H	1.722426000	-5.518469000	3.556725000
H	2.226649000	-6.519708000	2.188219000
C	3.924986000	-4.303419000	2.409768000
H	4.506401000	-5.178341000	2.098152000
H	3.928500000	-4.276556000	3.504853000
H	4.451440000	-3.413924000	2.050063000
N	-5.249638000	0.999507000	-3.926719000
C	-6.068316000	2.203164000	-4.039846000
H	-5.447833000	3.000479000	-4.465079000
H	-6.405810000	2.555413000	-3.042219000
C	-7.286892000	1.957832000	-4.926764000
H	-6.940112000	1.732670000	-5.943237000
H	-7.888275000	2.872823000	-4.982658000
C	-8.119309000	0.790005000	-4.397398000
H	-8.566476000	1.070873000	-3.433021000
H	-8.950356000	0.565627000	-5.076105000
C	-7.231535000	-0.438814000	-4.202063000
H	-6.881063000	-0.800337000	-5.177033000
H	-7.791991000	-1.256219000	-3.733268000
C	-6.016324000	-0.097504000	-3.343825000
H	-6.351930000	0.157207000	-2.315154000
H	-5.367967000	-0.976388000	-3.256327000
C	-3.821291000	2.667086000	1.585392000
C	-3.847447000	1.397560000	1.048555000

C	-2.645787000	0.838953000	0.518678000
N	-1.473789000	1.563679000	0.603838000
C	-1.483670000	2.793516000	1.134372000
C	-2.622957000	3.401507000	1.630589000
H	-4.737853000	3.101224000	1.978648000
H	-4.767989000	0.826222000	1.016348000
H	-0.523988000	3.302390000	1.164347000
H	-2.580367000	4.402426000	2.044115000
N	-2.486344000	-0.361760000	-0.046875000
C	-3.595842000	-1.281022000	-0.018393000
H	-4.480859000	-0.905239000	-0.557300000
H	-3.306231000	-2.223306000	-0.492764000
H	-3.922958000	-1.519530000	1.007553000
C	-0.844847000	-1.377856000	2.209297000
H	-0.709642000	-2.235965000	1.560408000
H	-1.796489000	-1.274367000	2.714633000

5d

Y	8.218913000	22.780973000	18.132381000
N	10.883221000	19.428045000	17.886552000
N	10.502490000	17.076647000	14.972684000
N	8.422584000	21.920727000	20.477937000
N	12.460210000	23.004909000	17.910462000
N	14.281008000	24.872068000	20.621490000
N	8.685695000	23.340279000	15.754231000
N	6.842115000	24.728209000	18.863777000
C	6.791000000	25.932557000	19.437516000
H	7.742199000	26.336994000	19.776001000
C	5.616075000	26.650294000	19.602729000
H	5.623258000	27.624243000	20.078160000
C	4.432538000	26.066777000	19.126711000
H	3.488417000	26.597329000	19.228795000
C	4.451498000	24.823919000	18.522268000
H	3.541297000	24.371943000	18.145319000
C	5.692003000	24.137387000	18.403254000
N	5.918184000	22.921410000	17.873224000
C	9.806857000	20.051103000	18.472802000
C	10.168945000	20.352725000	19.824279000
C	11.484613000	19.791892000	20.051182000
C	12.348701000	19.733667000	21.148284000
H	12.057315000	20.148663000	22.109526000
C	13.595629000	19.126102000	20.999733000
H	14.265625000	19.065158000	21.853054000
C	13.994204000	18.591068000	19.769452000

H	14.969306000	18.121685000	19.675606000
C	13.151891000	18.647423000	18.657171000
H	13.464999000	18.234271000	17.703533000
C	11.907263000	19.246131000	18.818219000
C	10.944958000	18.971382000	16.512440000
H	11.966797000	19.133565000	16.158629000
H	10.304242000	19.609244000	15.900472000
C	10.509385000	17.509651000	16.362984000
H	11.146622000	16.867603000	17.001657000
H	9.489435000	17.423754000	16.754574000
C	9.677355000	15.884363000	14.788892000
H	8.683145000	16.086819000	15.203745000
H	10.090772000	15.020514000	15.350690000
C	9.560967000	15.514037000	13.313011000
H	8.944131000	14.613390000	13.211269000
H	9.041897000	16.325599000	12.787578000
C	10.942496000	15.301183000	12.694254000
H	11.405308000	14.408177000	13.138162000
H	10.861596000	15.111565000	11.617655000
C	11.828153000	16.516731000	12.966146000
H	11.442935000	17.385269000	12.417256000
H	12.852642000	16.340510000	12.617888000
C	11.851619000	16.851871000	14.455849000
H	12.351661000	16.029108000	15.009797000
H	12.450872000	17.753685000	14.615511000
C	8.570843000	20.322229000	17.822397000
H	7.720062000	20.212315000	18.506865000
H	8.394038000	19.814047000	16.877865000
C	9.425900000	21.107909000	20.748842000
H	9.737933000	21.020490000	21.795566000
C	7.790680000	22.540475000	21.603378000
C	6.448174000	22.193437000	21.892139000
C	5.815109000	22.804790000	22.975745000
H	4.787146000	22.545340000	23.208916000
C	6.477466000	23.735110000	23.770324000
H	5.967718000	24.198320000	24.610858000
C	7.794591000	24.061951000	23.483470000
H	8.313096000	24.784387000	24.108964000
C	8.476130000	23.483646000	22.405803000
C	5.734722000	21.118757000	21.086281000
H	6.099980000	21.195595000	20.055896000
C	6.096680000	19.720065000	21.611782000
H	7.175973000	19.545044000	21.583558000
H	5.612715000	18.941936000	21.010208000

H	5.763469000	19.600591000	22.649134000
C	4.213808000	21.290284000	21.036451000
H	3.744476000	21.097926000	22.008010000
H	3.782496000	20.574229000	20.328932000
H	3.933398000	22.298357000	20.715918000
C	9.922435000	23.892642000	22.163090000
H	10.247555000	23.432486000	21.225706000
C	10.850388000	23.390582000	23.280180000
H	10.592356000	23.849652000	24.241145000
H	11.891652000	23.644645000	23.053369000
H	10.782324000	22.305894000	23.410914000
C	10.084368000	25.409943000	21.996564000
H	9.450499000	25.791605000	21.191527000
H	11.126221000	25.651799000	21.759236000
H	9.820598000	25.950096000	22.912174000
C	11.226750000	23.440422000	17.481197000
C	11.067437000	23.001587000	16.124643000
C	12.309952000	22.370697000	15.729877000
C	12.774249000	21.778226000	14.552313000
H	12.155119000	21.753806000	13.659512000
C	14.052225000	21.218604000	14.530979000
H	14.424755000	20.770703000	13.613746000
C	14.861772000	21.230358000	15.672498000
H	15.853975000	20.789854000	15.635003000
C	14.413963000	21.806771000	16.863147000
H	15.043455000	21.809982000	17.747358000
C	13.142760000	22.370289000	16.871228000
C	13.023025000	23.251518000	19.222363000
H	13.642142000	22.388985000	19.482353000
H	12.213475000	23.280767000	19.954333000
C	13.812262000	24.564776000	19.277794000
H	14.637128000	24.530234000	18.539919000
H	13.140124000	25.368563000	18.957141000
C	14.602723000	26.291295000	20.762721000
H	13.730779000	26.873969000	20.443707000
H	15.443699000	26.580179000	20.098029000
C	14.961965000	26.636201000	22.205356000
H	15.204022000	27.703196000	22.275372000
H	14.083101000	26.458675000	22.838040000
C	16.128985000	25.778854000	22.694579000
H	16.337636000	25.972624000	23.753081000
H	17.037436000	26.051535000	22.138648000
C	15.821524000	24.299620000	22.464493000
H	14.996339000	23.987626000	23.117034000

H	16.687558000	23.676323000	22.716392000
C	15.421390000	24.044809000	21.013140000
H	16.292524000	24.239918000	20.352184000
H	15.157984000	22.989707000	20.888629000
C	10.311396000	24.186053000	18.267354000
H	9.739236000	24.907373000	17.673811000
H	10.681651000	24.614487000	19.194253000
C	9.914115000	23.109322000	15.328916000
H	10.059455000	22.962610000	14.252541000
C	7.680579000	23.485718000	14.745396000
C	7.287539000	22.396337000	13.932557000
C	6.294893000	22.609567000	12.967983000
H	5.988575000	21.781108000	12.333998000
C	5.694022000	23.849180000	12.804460000
H	4.924883000	23.990604000	12.049829000
C	6.087902000	24.912175000	13.611498000
H	5.621589000	25.883148000	13.474494000
C	7.078357000	24.757297000	14.583008000
C	7.890603000	21.003627000	14.053240000
H	8.566705000	21.003752000	14.912625000
C	6.822774000	19.933617000	14.322326000
H	6.241155000	20.168086000	15.218305000
H	7.294291000	18.955008000	14.464679000
H	6.121780000	19.841907000	13.485739000
C	8.714941000	20.625328000	12.813156000
H	8.079611000	20.551401000	11.923349000
H	9.203035000	19.655762000	12.962050000
H	9.489349000	21.368812000	12.598215000
C	7.559123000	25.951749000	15.392232000
H	7.889917000	25.570179000	16.364344000
C	6.474062000	26.996301000	15.665583000
H	6.173445000	27.526739000	14.754880000
H	6.852448000	27.749878000	16.363696000
H	5.583420000	26.543637000	16.110776000
C	8.774648000	26.604572000	14.713776000
H	9.594762000	25.892371000	14.583104000
H	9.147653000	27.443947000	15.311822000
H	8.502785000	26.989161000	13.724153000
C	4.802423000	22.202307000	17.306970000
H	4.378937000	22.708920000	16.426105000
H	3.985351000	22.053372000	18.030015000
H	5.131847000	21.210536000	16.985933000

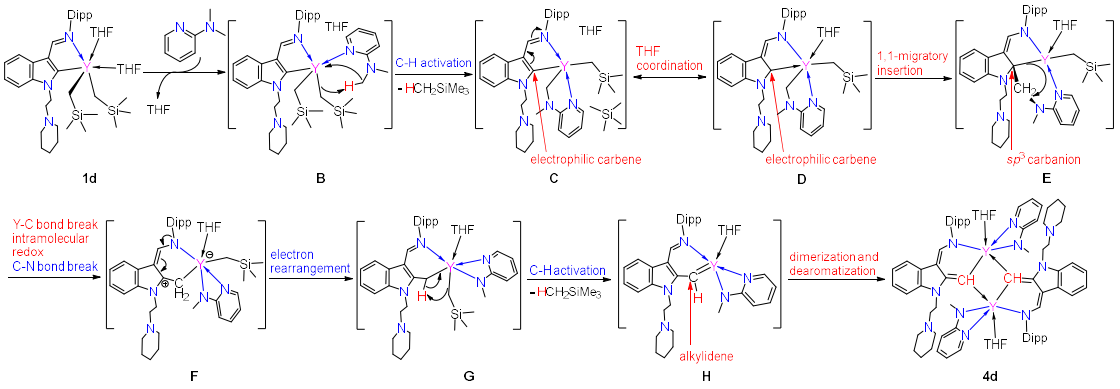
6d

Y	8.269063000	23.039537000	18.212229000
N	10.299033000	20.005144000	17.650419000
N	10.023529000	18.486062000	14.212442000
N	8.058097000	22.154095000	20.560191000
N	11.865843000	23.999450000	18.348384000
N	13.055332000	25.322067000	21.670765000
N	8.401780000	23.979221000	15.898935000
N	6.782132000	24.796616000	19.031565000
C	6.650508000	25.944809000	19.702542000
H	7.573654000	26.375036000	20.083846000
C	5.434074000	26.574475000	19.906313000
H	5.375590000	27.504089000	20.460282000
C	4.294423000	25.967586000	19.353699000
H	3.319346000	26.433248000	19.478452000
C	4.396825000	24.788601000	18.642853000
H	3.521118000	24.325200000	18.203650000
C	5.675320000	24.175757000	18.497717000
N	5.966308000	23.017198000	17.881772000
C	9.428783000	20.824736000	18.316143000
C	9.573797000	20.493713000	19.687488000
C	10.564724000	19.453587000	19.833583000
C	11.133439000	18.758458000	20.909029000
H	10.814576000	18.952411000	21.930068000
C	12.122030000	17.814908000	20.654445000
H	12.569103000	17.269396000	21.480978000
C	12.558600000	17.559593000	19.344201000
H	13.339540000	16.824023000	19.173129000
C	12.008409000	18.235974000	18.260004000
H	12.354591000	18.036215000	17.250477000
C	11.009263000	19.175806000	18.521256000
C	10.454549000	19.931881000	16.208438000
H	11.523750000	19.971215000	15.973701000
H	9.993947000	20.820300000	15.774068000
C	9.800960000	18.662913000	15.642023000
H	10.141931000	17.784045000	16.221074000
H	8.721737000	18.745916000	15.813631000
C	9.083160000	17.512867000	13.656893000
H	8.067113000	17.827738000	13.919929000
H	9.235460000	16.511150000	14.110573000
C	9.219371000	17.404968000	12.140786000
H	8.508381000	16.659610000	11.765310000
H	8.947103000	18.368652000	11.692593000
C	10.650451000	17.039924000	11.746883000
H	10.870842000	16.017408000	12.085171000

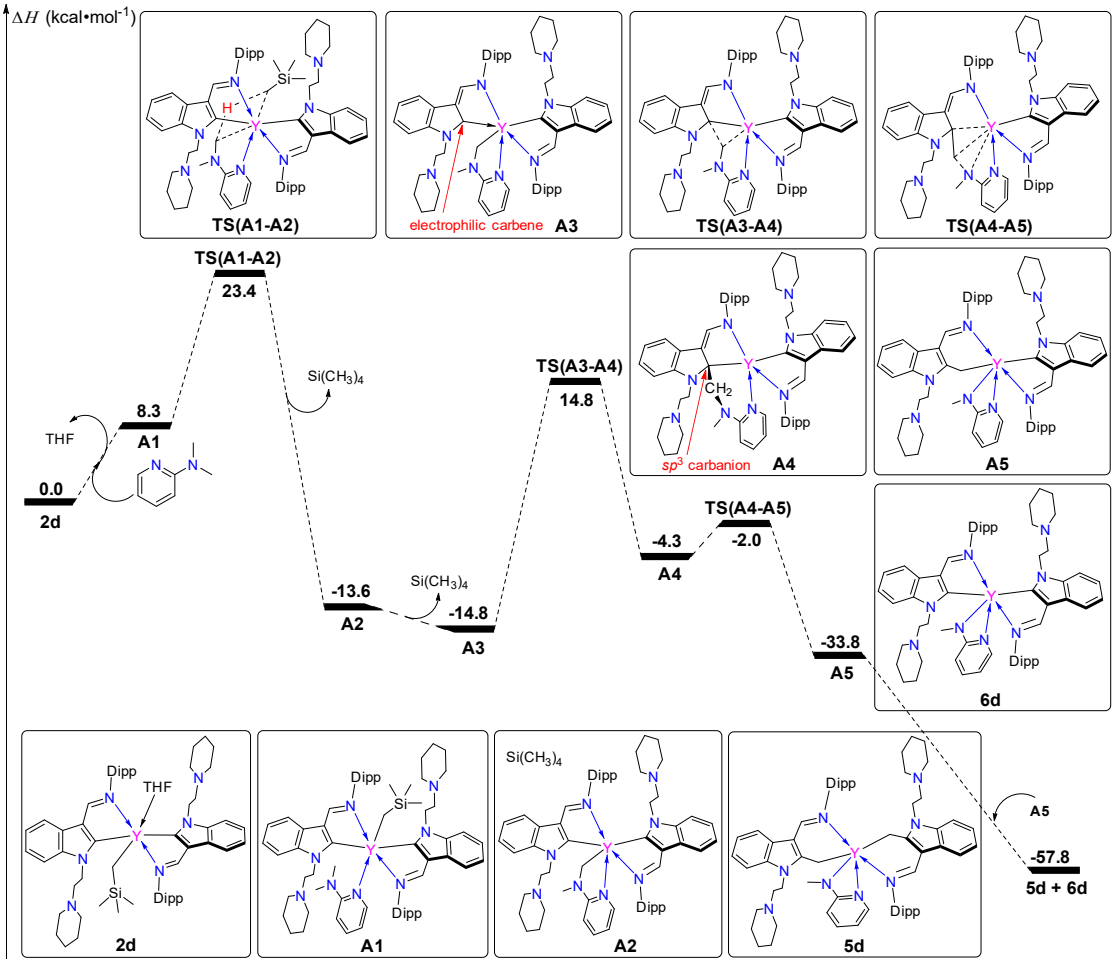
H	10.766780000	17.043142000	10.656980000
C	11.633078000	18.010457000	12.400669000
H	11.505497000	19.012602000	11.972627000
H	12.668978000	17.705567000	12.211603000
C	11.398340000	18.090159000	13.907154000
H	11.632905000	17.107547000	14.368805000
H	12.087963000	18.819556000	14.342732000
C	8.821986000	21.103407000	20.725285000
H	8.877373000	20.650517000	21.722070000
C	7.244058000	22.524051000	21.679970000
C	6.010608000	21.866079000	21.884330000
C	5.246207000	22.218147000	23.001777000
H	4.299994000	21.714599000	23.178776000
C	5.670582000	23.198452000	23.889151000
H	5.062199000	23.456095000	24.752017000
C	6.877238000	23.850357000	23.664677000
H	7.203408000	24.617146000	24.361216000
C	7.680985000	23.532298000	22.566428000
C	5.512880000	20.780667000	20.941063000
H	6.053762000	20.897538000	19.996075000
C	5.814758000	19.377611000	21.490296000
H	6.887022000	19.218596000	21.637686000
H	5.454333000	18.606303000	20.800201000
H	5.320815000	19.223252000	22.456599000
C	4.017107000	20.914586000	20.628345000
H	3.392276000	20.682125000	21.497875000
H	3.734761000	20.213728000	19.835340000
H	3.769861000	21.927461000	20.297548000
C	9.022052000	24.219164000	22.378508000
H	9.257965000	24.181096000	21.306937000
C	10.137394000	23.471481000	23.127161000
H	9.936982000	23.473195000	24.205019000
H	11.106885000	23.950848000	22.949785000
H	10.208626000	22.427184000	22.808109000
C	9.013833000	25.693693000	22.796423000
H	8.170000000	26.235740000	22.359648000
H	9.941799000	26.176466000	22.475400000
H	8.956335000	25.808098000	23.884374000
C	10.591596000	23.984715000	17.851279000
C	10.735676000	24.177158000	16.451864000
C	12.135023000	24.301637000	16.117213000
C	12.869871000	24.477979000	14.937579000
H	12.369393000	24.572966000	13.977183000
C	14.257624000	24.525173000	15.008765000

H	14.837332000	24.663184000	14.100175000
C	14.924130000	24.390511000	16.237372000
H	16.009686000	24.422204000	16.264668000
C	14.215918000	24.214422000	17.422280000
H	14.738930000	24.107797000	18.367930000
C	12.822560000	24.175987000	17.344955000
C	12.222743000	23.935955000	19.754601000
H	13.036210000	23.212146000	19.874276000
H	11.361170000	23.553884000	20.303594000
C	12.619551000	25.322691000	20.280025000
H	13.385309000	25.760497000	19.611988000
H	11.735673000	25.965510000	20.198774000
C	13.052308000	26.683375000	22.208111000
H	12.058762000	27.115516000	22.043646000
H	13.774353000	27.325909000	21.661795000
C	13.390609000	26.699475000	23.695442000
H	13.385660000	27.734390000	24.057227000
H	12.607158000	26.159667000	24.241840000
C	14.744953000	26.039860000	23.949390000
H	14.954900000	25.981342000	25.023583000
H	15.538439000	26.657795000	23.505414000
C	14.773139000	24.649999000	23.315168000
H	14.072682000	23.988771000	23.840431000
H	15.769400000	24.200530000	23.400486000
C	14.374743000	24.713410000	21.841992000
H	15.144031000	25.282384000	21.277890000
H	14.358966000	23.700786000	21.427286000
C	9.635801000	24.264359000	15.562565000
H	9.833698000	24.609548000	14.541021000
C	7.379448000	24.308342000	14.953481000
C	6.835560000	23.300508000	14.125933000
C	5.828817000	23.648853000	13.221973000
H	5.405630000	22.886014000	12.575332000
C	5.366127000	24.956805000	13.125833000
H	4.585288000	25.209173000	12.413313000
C	5.911636000	25.938304000	13.942754000
H	5.551771000	26.960284000	13.862012000
C	6.916471000	25.640605000	14.869713000
C	7.386982000	21.885679000	14.156214000
H	7.766875000	21.707540000	15.171198000
C	6.338567000	20.808337000	13.860807000
H	5.445367000	20.928249000	14.480487000
H	6.758771000	19.816291000	14.053305000
H	6.024791000	20.821856000	12.811243000

C	8.573239000	21.746914000	13.187455000
H	8.240012000	21.913499000	12.156373000
H	9.021362000	20.748943000	13.255959000
H	9.354520000	22.482461000	13.401732000
C	7.495741000	26.754225000	15.730875000
H	8.040842000	26.285579000	16.556560000
C	6.412966000	27.644879000	16.352360000
H	5.883501000	28.234947000	15.595806000
H	6.867367000	28.353359000	17.053088000
H	5.675511000	27.052110000	16.899591000
C	8.495529000	27.607261000	14.934216000
H	9.321654000	27.007029000	14.541242000
H	8.922661000	28.393504000	15.566808000
H	8.003630000	28.090407000	14.082186000
C	4.903533000	22.309217000	17.210189000
H	4.514639000	22.861357000	16.340762000
H	4.053444000	22.090301000	17.873637000
H	5.281356000	21.348924000	16.848679000



Scheme S5. Possible mechanism of the reaction of **1d** with 2-*N,N*-dimethylaminopyridine.



Scheme S6. Computed enthalpy profile for the formation of **5d** and **6d** from **2d** at room temperature. The enthalpy is given in kcal·mol^{-1}.

5. Olex2 Drawing of Complexes

Diagrams of complexes **1a-1e**

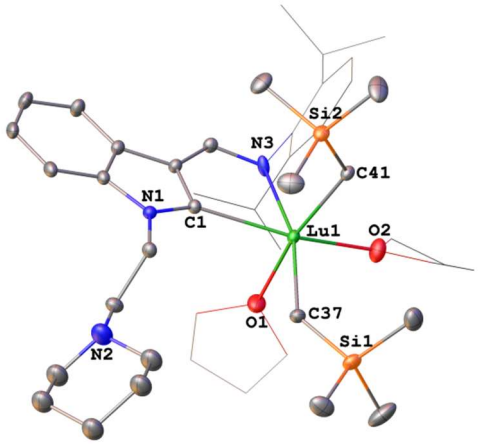


Fig. S54. Diagram of complex **1a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Lu(1)-C(1), 2.432(5); Lu(1)-C(37), 2.370(6); Lu(1)-C(41), 2.345(6); Lu(1)-N(3), 2.541(10); Selected bond angles (deg): C(1)-Lu(1)-N(3),

71.5(3); C(1)-Lu(1)-C(37), 98.6(2); C(1)-Lu(1)-C(41), 102.84(19); C(37)-Lu(1)-C(41), 96.1(2).

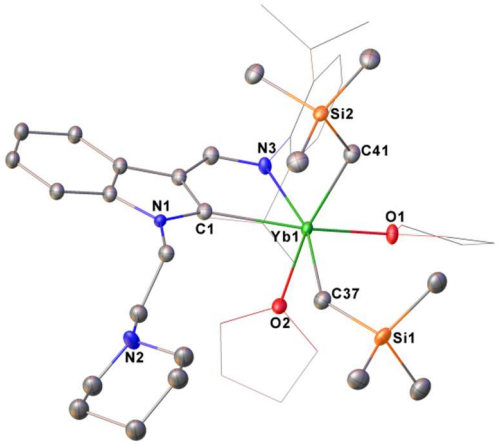


Fig. S55. Diagram of complex **1b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Yb(1)-C(1), 2.445(9); Yb(1)-C(37), 2.378(10); Yb(1)-C(41), 2.361(10); Yb(1)-N(3), 2.599(7); Selected bond angles (deg): C(1)-Yb(1)-N(3), 70.8(3); C(1)-Yb(1)-C(37), 98.5(3); C(1)-Yb(1)-C(41), 102.2(3); C(37)-Yb(1)-C(41), 94.9(4).

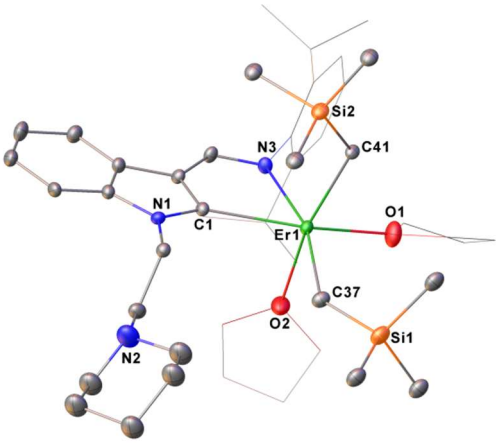


Fig. S56. Diagram of complex **1c** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-C(1), 2.472(8); Er(1)-C(37), 2.387(8); Er(1)-C(41), 2.380(8); Er(1)-N(3), 2.617(6); Selected bond angles (deg): C(1)-Er(1)-N(3), 70.2(3); C(1)-Er(1)-C(37), 98.7(3); C(1)-Er(1)-C(41), 103.3(3); C(37)-Er(1)-C(41), 95.3(3).

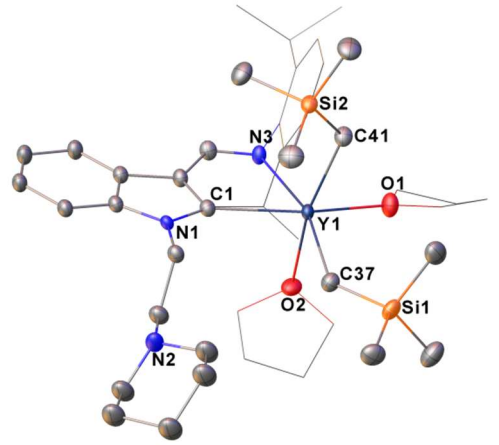


Fig. S57. Diagram of complex **1d** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Y(1)-C(1), 2.469(6); Y(1)-C(37), 2.393(7); Y(1)-C(41), 2.382(6); Y(1)-N(3), 2.606(5); Selected bond angles (deg): C(1)-Y(1)-N(3), 69.77(17); C(1)-Y(1)-C(37), 98.1(2); C(1)-Y(1)-C(41), 103.7(2); C(37)-Y(1)-C(41), 95.4(2).

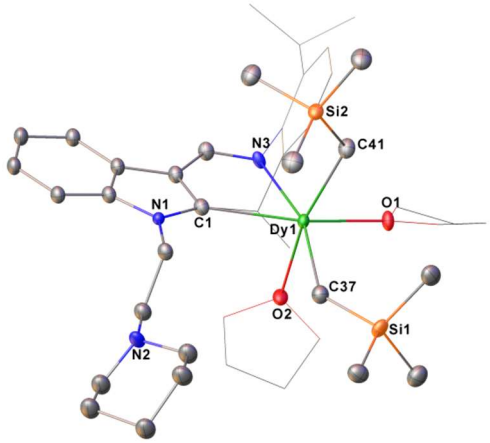


Fig. S58. Diagram of complex **1e** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Dy(1)-C(1), 2.498(10); Dy(1)-C(37), 2.427(11); Dy(1)-C(41), 2.399(11); Dy(1)-N(3), 2.626(8); Selected bond angles (deg): C(1)-Dy(1)-N(3), 69.6(3); C(1)-Dy(1)-C(37), 98.5(4); C(1)-Dy(1)-C(41), 103.4(3); C(37)-Dy(1)-C(41), 95.1(4).
Diagrams of complexes **2a-2e**

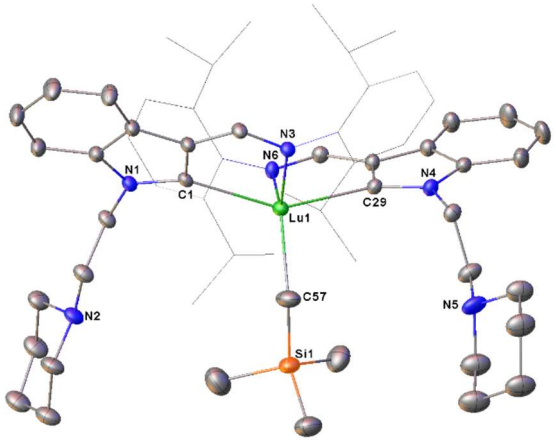


Fig. S59. Diagram of complex **2a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Lu(1)-C(1), 2.421(4); Lu(1)-C(29), 2.417(4); Lu(1)-C(57), 2.285(6); Lu(1)-N(3), 2.339(3); Lu(1)-N(6), 2.382(3); Selected bond angles (deg): C(1)-Lu(1)-N(3), 73.96(12); C(1)-Lu(1)-C(29), 150.88(14); C(1)-Lu(1)-C(57), 105.7(2).

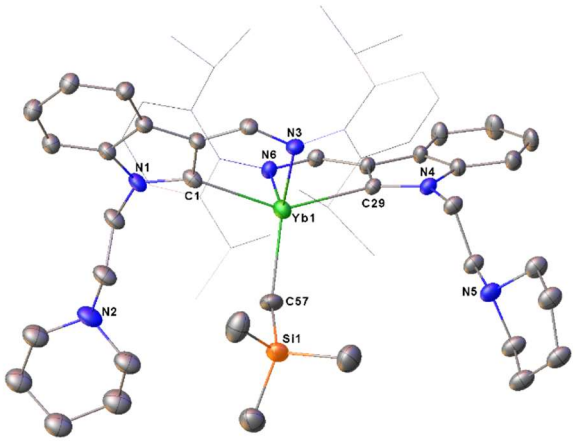


Fig. S60. Diagram of complex **2b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Yb(1)-C(1), 2.429(9); Yb(1)-C(29), 2.440(8); Yb(1)-C(57), 2.318(13); Yb(1)-N(3), 2.444(6); Yb(1)-N(6), 2.382(6); Selected bond angles (deg): C(1)-Yb(1)-N(3), 72.5(2); C(1)-Yb(1)-C(29), 148.5(3); C(1)-Yb(1)-C(57), 104.0(6).

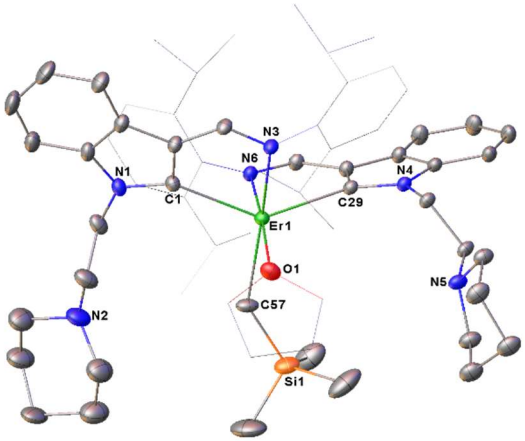


Fig. S61. Diagram of complex **2c** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-C(1), 2.456(3); Er(1)-C(29), 2.442(3); Er(1)-C(57), 2.389(6); Er(1)-N(3), 2.606(3); Er(1)-N(6), 2.474(2); Er(1)-O(1), 2.385(3); Selected bond angles (deg): C(1)-Er(1)-N(3), 69.73(10); C(1)-Er(1)-C(29), 141.24(10); C(1)-Er(1)-C(57), 106.3(2).

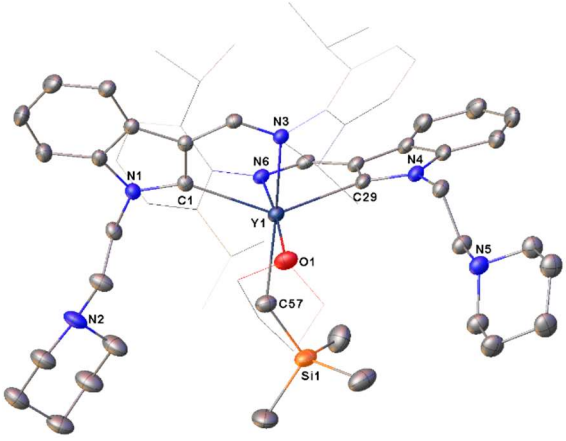


Fig. S62. Diagram of complex **2d** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Y(1)-C(1), 2.485(6); Y(1)-C(29), 2.488(5); Y(1)-C(57), 2.424(6); Y(1)-N(3), 2.634(5); Y(1)-N(6), 2.485(5); Y(1)-O(1), 2.403(4); Selected bond angles (deg): C(1)-Y(1)-N(3), 69.29(12); C(1)-Y(1)-C(29), 141.74(14); C(1)-Y(1)-C(57), 106.39(15).

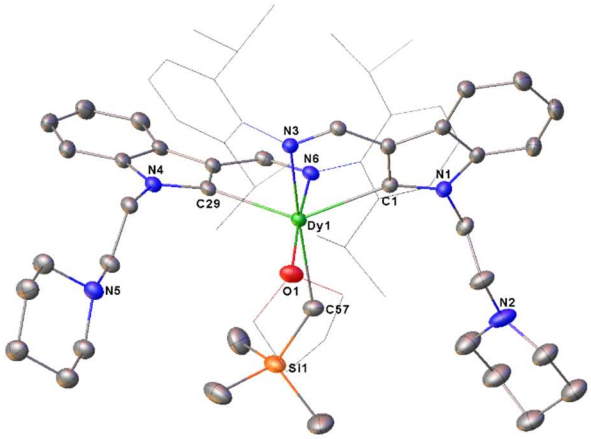


Fig. S63. Diagram of complex **2e** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Dy(1)-C(1), 2.500(4); Dy(1)-C(29), 2.502(4); Dy(1)-C(57), 2.435(4); Dy(1)-N(3), 2.653(3); Dy(1)-N(6), 2.493(3); Dy(1)-O(1), 2.385(3); Selected bond angles (deg): C(1)-Dy(1)-N(3), 69.54(11); C(1)-Dy(1)-C(29), 141.92(13); C(1)-Dy(1)-C(57), 106.31(15).

Diagrams of complexes **3a-3e**

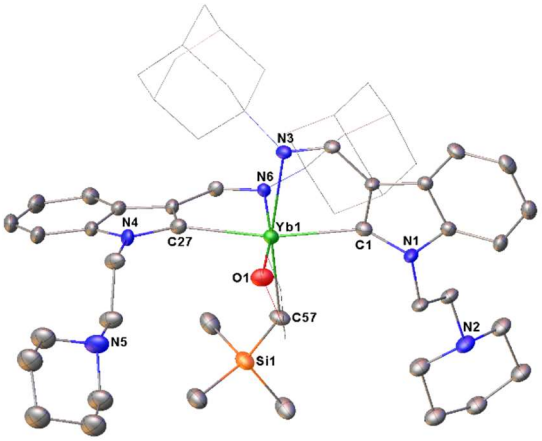


Fig. S64. Diagram of complex **3a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the adamantyl (Ad) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Yb(1)-C(1), 2.456(10); Yb(1)-C(27), 2.415(10); Yb(1)-C(57), 2.369(8); Yb(1)-N(3), 2.546(7); Yb(1)-N(6), 2.414(7); Yb(1)-O(1), 2.362(7); Selected bond angles (deg): C(1)-Yb(1)-N(3), 71.5(3); C(1)-Yb(1)-C(27), 168.0(3); C(1)-Yb(1)-C(57), 95.5(3).

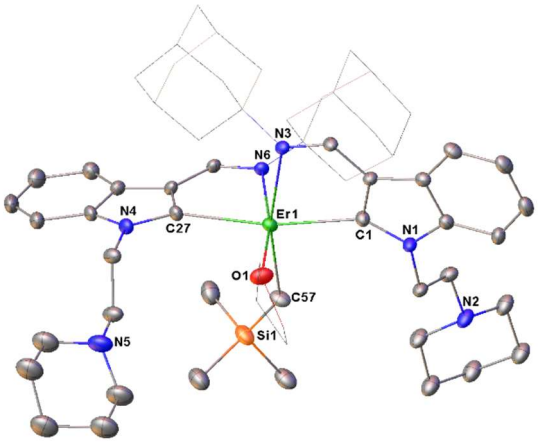


Fig. S65. Diagram of complex **3b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the adamantyl (Ad) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-C(1), 2.474(8); Er(1)-C(27), 2.459(8); Er(1)-C(57), 2.354(10); Er(1)-N(3), 2.560(6); Er(1)-N(6), 2.435(6); Er(1)-O(1), 2.392(7); Selected bond angles (deg): C(1)-Er(1)-N(3), 70.5(2); C(1)-Er(1)-C(27), 167.7(3); C(1)-Er(1)-C(57), 95.8(4).

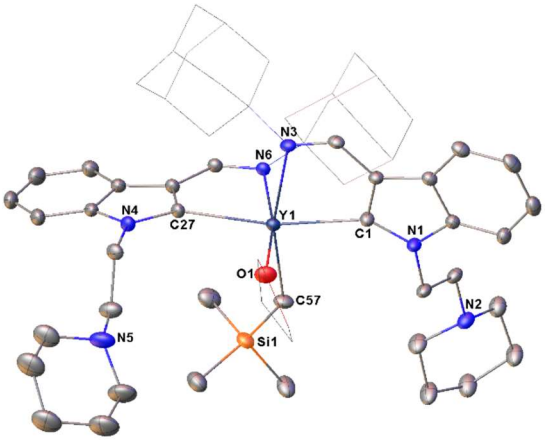


Fig. S66. Diagram of complex **3c** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the adamantyl (Ad) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Y(1)-C(1), 2.490(4); Y(1)-C(27), 2.500(4); Y(1)-C(57), 2.412(3); Y(1)-N(3), 2.458(5); Y(1)-N(6), 2.591(3); Y(1)-O(1), 2.393(2); Selected bond angles (deg): C(1)-Y(1)-N(3), 73.11(15); C(1)-Y(1)-C(27), 166.45(12); C(1)-Y(1)-C(57), 98.66(14).

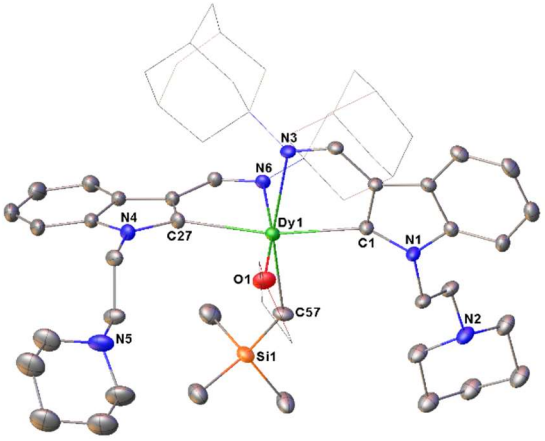


Fig. S67. Diagram of complex **3d** with 30% probability thermal ellipsoids. All hydrogen atoms were

omitted and the adamantyl (Ad) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Dy(1)-C(1), 2.507(4); Dy(1)-C(27), 2.491(4); Dy(1)-C(57), 2.419(4); Dy(1)-N(3), 2.607(3); Dy(1)-N(6), 2.470(3); Dy(1)-O(1), 2.419(3); Selected bond angles (deg): C(1)-Dy(1)-N(3), 69.60(12); C(1)-Dy(1)-C(27), 166.41(14); C(1)-Dy(1)-C(57), 94.81(16).

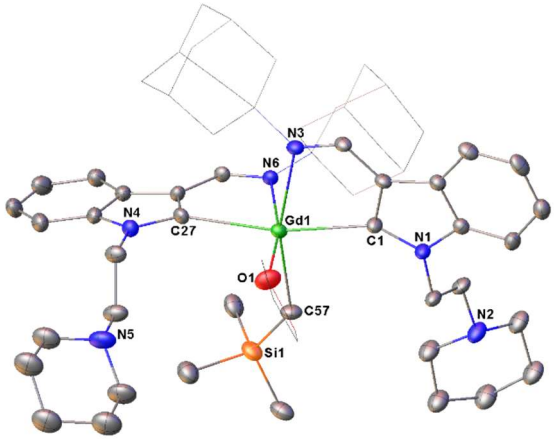


Fig. S68. Diagram of complex **3e** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the adamantyl (Ad) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Gd(1)-C(1), 2.533(6); Gd(1)-C(27), 2.533(7); Gd(1)-C(57), 2.442(7); Gd(1)-N(3), 2.641(5); Gd(1)-N(6), 2.489(7); Gd(1)-O(1), 2.440(5); Selected bond angles (deg): C(1)-Gd(1)-N(3), 68.49(19); C(1)-Gd(1)-C(27), 165.7(2); C(1)-Gd(1)-C(57), 94.8(2).
Diagrams of complexes **4a-4d**

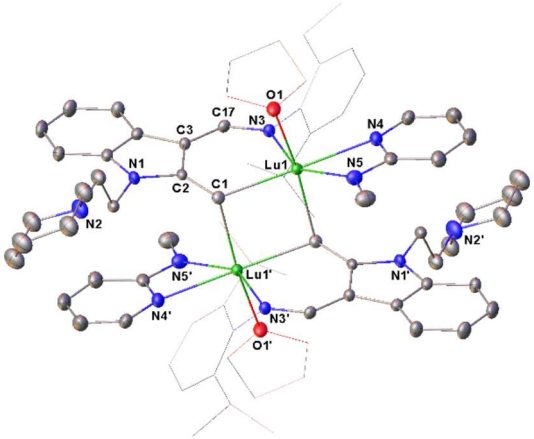


Fig. S69. Diagram of complex **4a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Lu(1)-C(1), 2.393(5); Lu(1)-N(3), 2.330(5); Lu(1)-N(4), 2.432(5); Lu(1)-N(5), 2.299(5); Lu(1)-O(1), 2.367(4); C(1)-C(2), 1.385(7); C(2)-C(3), 1.463(8); C(3)-C(17), 1.374(7); C(17)-N(3), 1.330(7); Selected bond angles (deg): C(1)-Lu(1)-N(3), 84.85(17); C(1)-Lu(1)-N(4), 178.80(19); C(1)-Lu(1)-N(5), 125.0(2); C(1)-Lu(1)-O(1), 86.07(17).

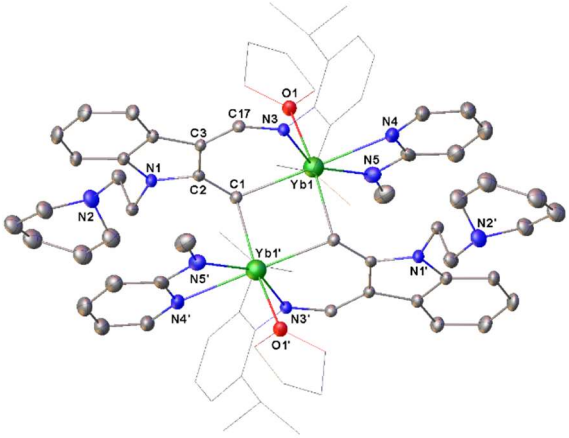


Fig. S70. Diagram of complex **4b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Yb(1)-C(1), 2.402(5); Yb(1)-N(3), 2.347(4); Yb(1)-N(4), 2.450(5); Yb(1)-N(5), 2.328(5); Yb(1)-O(1), 2.384(4); C(1)-C(2), 1.384(7); C(2)-C(3), 1.459(7); C(3)-C(17), 1.377(7); C(17)-N(3), 1.331(6); Selected bond angles (deg): C(1)-Yb(1)-N(3), 84.14(15); C(1)-Yb(1)-N(4), 178.75(18); C(1)-Yb(1)-N(5), 125.51(19); C(1)-Yb(1)-O(1), 85.99(15).

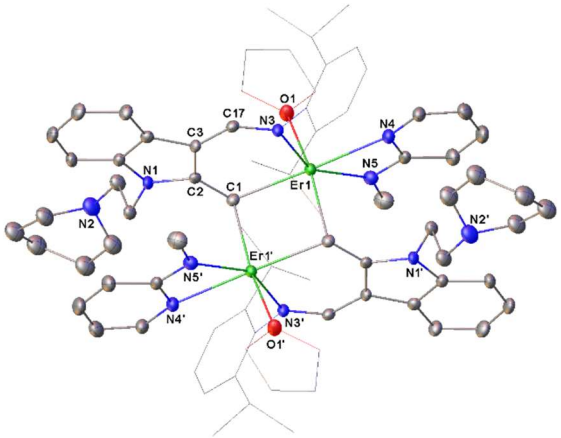


Fig. S71. Diagram of complex **4c** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-C(1), 2.404(6); Er(1)-N(3), 2.352(5); Er(1)-N(4), 2.470(5); Er(1)-N(5), 2.324(6); Er(1)-O(1), 2.399(5); C(1)-C(2), 1.375(8); C(2)-C(3), 1.466(8); C(3)-C(17), 1.373(8); C(17)-N(3), 1.336(7); Selected bond angles (deg): C(1)-Er(1)-N(3), 83.08(19); C(1)-Er(1)-N(4), 177.7(2); C(1)-Er(1)-N(5), 126.6(2); C(1)-Er(1)-O(1), 85.35(19).

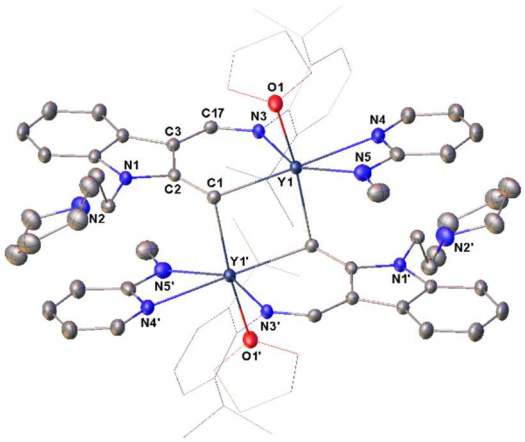


Fig. S72. Diagram of complex **4d** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Y(1)-C(1), 2.446(4); Y(1)-N(3), 2.374(4); Y(1)-N(4), 2.486(4); Y(1)-N(5), 2.350(4); Y(1)-O(1), 2.401(3); C(1)-C(2), 1.376(6); C(2)-C(3), 1.456(6); C(3)-C(17), 1.366(6); C(17)-N(3), 1.342(5); Selected bond angles (deg): C(1)-Y(1)-N(3), 82.59(13); C(1)-Y(1)-N(4), 177.75(15); C(1)-Y(1)-N(5), 127.36(16); C(1)-Y(1)-O(1), 85.66(13).

Diagrams of complexes **5a-5d**

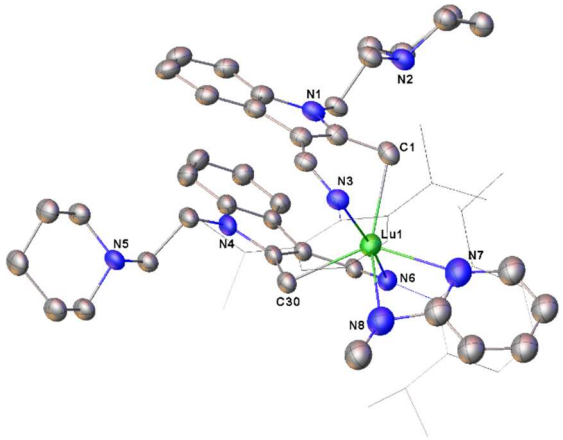


Fig. S73. Diagram of complex **5a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Lu(1)-C(1), 2.457(15); Lu(1)-C(30), 2.406(13); Lu(1)-N(3), 2.404(11); Lu(1)-N(6), 2.395(11); Lu(1)-N(7), 2.39(3); Lu(1)-N(8), 2.31(2); Selected bond angles (deg): C(1)-Lu(1)-N(3), 78.6(4); C(1)-Lu(1)-C(30), 119.4(5); C(1)-Lu(1)-N(6), 95.9(4); C(1)-Lu(1)-N(7), 86.2(7); C(1)-Lu(1)-N(8), 141.8(7).

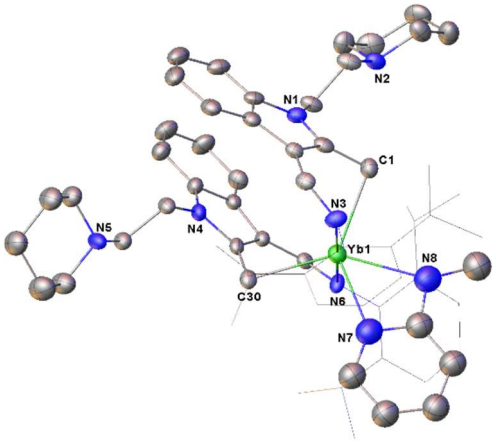


Fig. S74. Diagram of complex **5b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Yb(1)-C(1), 2.495(9); Yb(1)-C(30), 2.507(8); Yb(1)-N(3), 2.413(7); Yb(1)-N(6), 2.424(6); Yb(1)-N(7), 2.526(16); Yb(1)-N(8), 2.433(12); Selected bond angles (deg): C(1)-Yb(1)-N(3), 77.4(3); C(1)-Yb(1)-C(30), 123.9(3); C(1)-Yb(1)-N(6), 99.1(3); C(1)-Yb(1)-N(7), 136.9(5); C(1)-Yb(1)-N(8), 85.5(4).

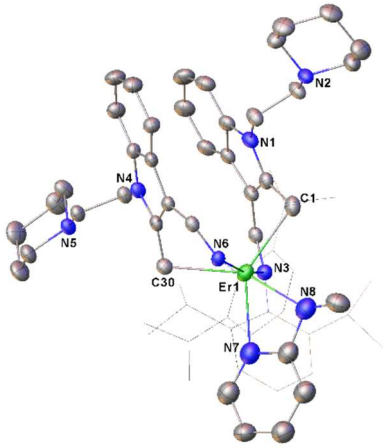


Fig. S75. Diagram of complex **5c** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-C(1), 2.469(8); Er(1)-C(30), 2.461(7); Er(1)-N(3), 2.431(5); Er(1)-N(6), 2.430(5); Er(1)-N(7), 2.433(11); Er(1)-N(8), 2.327(17); Selected bond angles (deg): C(1)-Er(1)-N(3), 78.2(2); C(1)-Er(1)-C(30), 119.7(3); C(1)-Er(1)-N(6), 96.3(2); C(1)-Er(1)-N(7), 141.4(4); C(1)-Er(1)-N(8), 87.5(5).

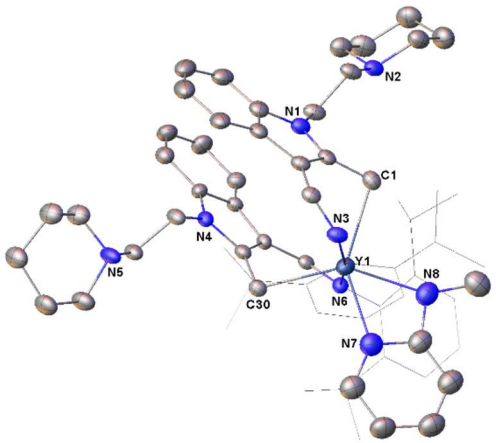


Fig. S76. Diagram of complex **5d** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Y(1)-C(1), 2.484(6); Y(1)-C(30), 2.487(6); Y(1)-N(3), 2.431(5); Y(1)-N(6), 2.449(4); Y(1)-N(7), 2.384(9); Y(1)-N(8), 2.354(12); Selected bond angles (deg): C(1)-Y(1)-N(3), 77.72(19); C(1)-Y(1)-C(30), 119.4(2); C(1)-Y(1)-N(6), 96.27(18); C(1)-Y(1)-N(7), 143.4(4); C(1)-Y(1)-N(8), 91.3(4).

Diagrams of complexes **6a-6d**

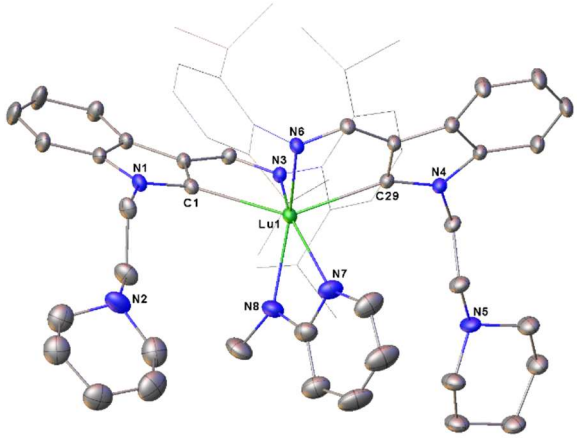


Fig. S77. Diagram of complex **6a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Lu(1)-C(1), 2.435(4); Lu(1)-C(29), 2.430(4); Lu(1)-N(3), 2.385(3); Lu(1)-N(6), 2.402(3); Lu(1)-N(7), 2.411(5); Lu(1)-N(8), 2.261(5); Selected bond angles (deg): C(1)-Lu(1)-N(3), 72.64(12); C(1)-Lu(1)-C(29), 143.50(13); C(1)-Lu(1)-N(6), 86.85(13); C(1)-Lu(1)-N(7), 129.70(17); C(1)-Lu(1)-N(8), 95.12(17).

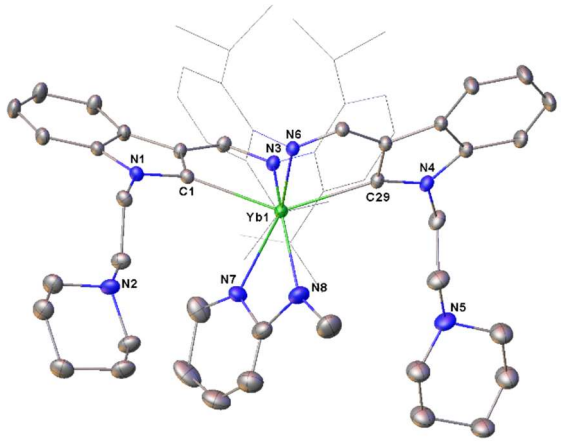


Fig. S78. Diagram of complex **6b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Yb(1)-C(1), 2.442(4); Yb(1)-C(29), 2.450(4); Yb(1)-N(3), 2.430(3); Yb(1)-N(6), 2.404(3); Yb(1)-N(7), 2.427(5); Yb(1)-N(8), 2.266(5); Selected bond angles (deg): C(1)-Yb(1)-N(3), 72.64(11); C(1)-Yb(1)-C(29), 141.92(12); C(1)-Yb(1)-N(6), 86.65(11); C(1)-Yb(1)-N(7), 81.74(16); C(1)-Yb(1)-N(8), 121.1(2).

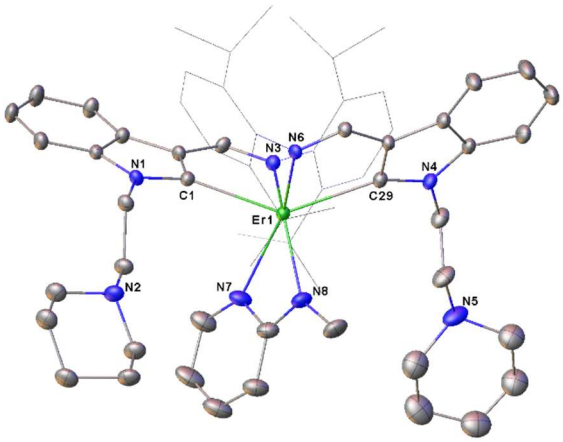


Fig. S79. Diagram of complex **6c** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-C(1), 2.463(6); Er(1)-C(29), 2.481(6); Er(1)-N(3), 2.456(5); Er(1)-N(6), 2.424(5); Er(1)-N(7), 2.454(7); Er(1)-N(8), 2.295(7); Selected bond angles (deg): C(1)-Er(1)-N(3), 72.54(18); C(1)-Er(1)-C(29), 141.0(2); C(1)-Er(1)-N(6), 86.40(18); C(1)-Er(1)-N(7), 82.6(2); C(1)-Er(1)-N(8), 120.4(2).

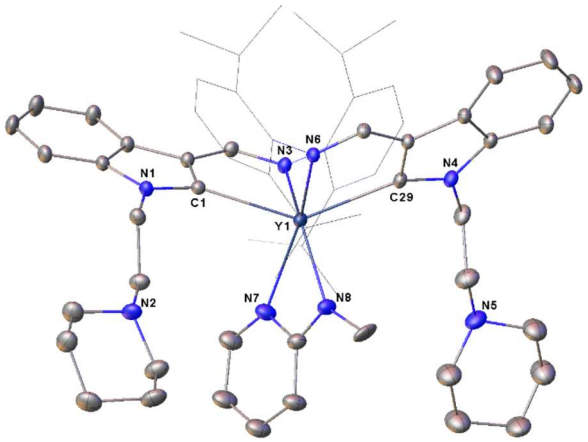


Fig. S80. Diagram of complex **6d** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Y(1)-C(1), 2.480(2); Y(1)-C(29), 2.488(2); Y(1)-N(3), 2.455(2); Y(1)-N(6), 2.440(2); Y(1)-N(7), 2.440(10); Y(1)-N(8), 2.289(11); Selected bond angles (deg): C(1)-Y(1)-N(3), 72.23(7); C(1)-Y(1)-C(29), 140.67(8); C(1)-Y(1)-N(6), 86.31(7); C(1)-Y(1)-N(7), 87.0(4); C(1)-Y(1)-N(8), 121.6(6).

Diagrams of complexes **7a-7b**

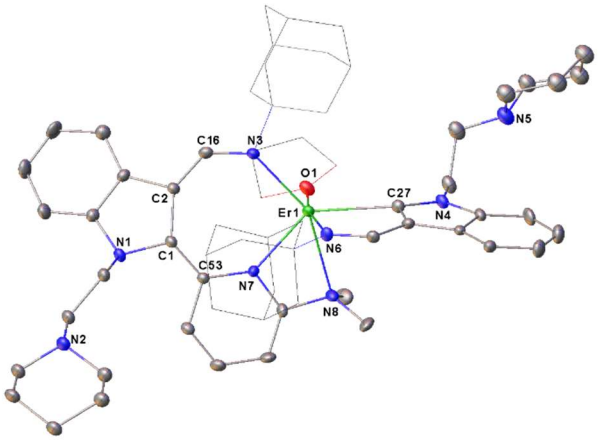


Fig. S81. Diagram of complex **7a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the adamantyl (Ad) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-C(27), 2.515(9); Er(1)-N(3), 2.252(7); Er(1)-N(6), 2.415(7); Er(1)-N(7), 2.297(7); Er(1)-N(8), 2.562(7); Er(1)-O(1), 2.408(6); C(1)-C(2), 1.498(12); C(1)-C(53), 1.360(11); C(2)-C(16), 1.367(12); C(16)-N(3), 1.383(11); Selected bond angles (deg): C(27)-Er(1)-N(3), 128.8(3); C(27)-Er(1)-N(6), 73.8(6); C(27)-Er(1)-N(7), 135.6(3); C(27)-Er(1)-N(8), 79.6(3); C(27)-Er(1)-O(1), 95.0(3); C(1)-C(53)-N(7), 123.8(8); C(2)-C(1)-C(53), 134.6(8); C(16)-C(2)-C(1), 136.9(8).

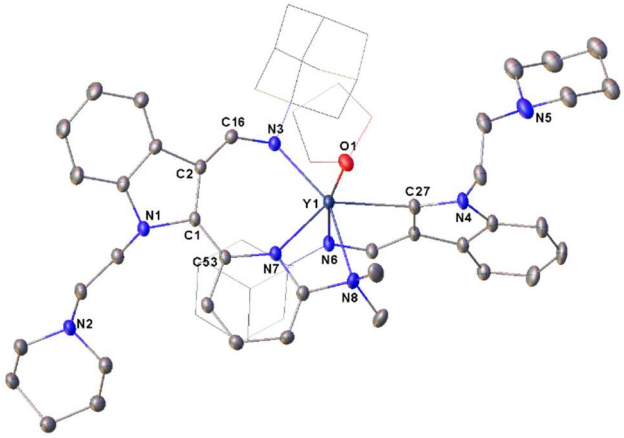


Fig. S82. Diagram of complex **7b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the adamantyl (Ad) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Y(1)-C(27), 2.507(3); Y(1)-N(3), 2.250(3); Y(1)-N(6), 2.428(3); Y(1)-N(7), 2.296(3); Y(1)-N(8), 2.549(3); Y(1)-O(1), 2.412(2); C(1)-C(2), 1.470(5); C(1)-C(53), 1.362(5); C(2)-C(16), 1.363(5); C(16)-N(3), 1.373(4); Selected bond angles (deg): C(27)-Y(1)-N(3), 129.01(11); C(27)-Y(1)-N(6), 73.53(10); C(27)-Y(1)-N(7), 135.53(12); C(27)-Y(1)-N(8), 80.10(11); C(27)-Y(1)-O(1), 94.95(10); C(1)-C(53)-N(7), 122.8(3); C(2)-C(1)-C(53), 135.6(3); C(16)-C(2)-C(1), 136.8(3).

Diagrams of complexes **8-9**

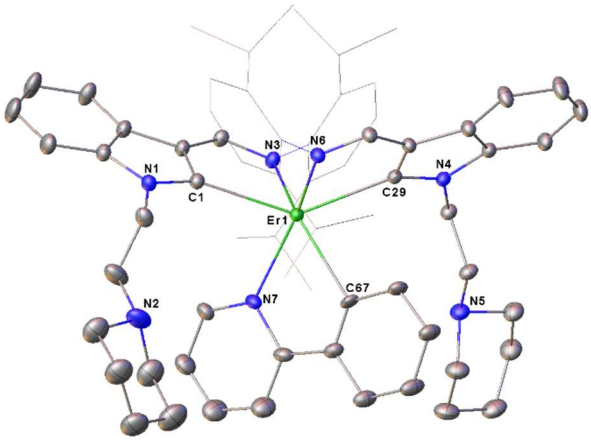


Fig. S83. Diagram of complex **8a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-C(1), 2.472(3); Er(1)-C(29), 2.466(3); Er(1)-C(67), 2.544(19); Er(1)-N(3), 2.444(2); Er(1)-N(6), 2.440(2); Er(1)-N(7), 2.381(16); Selected bond angles (deg): C(1)-Er(1)-N(3), 72.10(8); C(1)-Er(1)-C(29), 140.46(9); C(1)-Er(1)-C(67), 132.6(4); C(1)-Er(1)-N(6), 86.14(18); C(1)-Er(1)-N(7), 84.2(4).

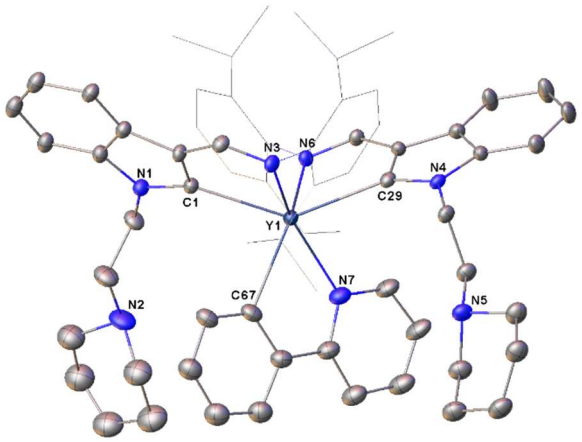


Fig. S84. Diagram of complex **8b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Y(1)-C(1), 2.487(6); Y(1)-C(29), 2.477(6); Y(1)-C(67), 2.53(3); Y(1)-N(3), 2.460(5); Y(1)-N(6), 2.439(4); Y(1)-N(7), 2.40(3); Selected bond angles (deg): C(1)-Y(1)-N(3), 71.47(18); C(1)-Y(1)-C(29), 140.66(19); C(1)-Y(1)-C(67), 86.0(7); C(1)-Y(1)-N(6), 86.98(17); C(1)-Y(1)-N(7), 86.4(5).

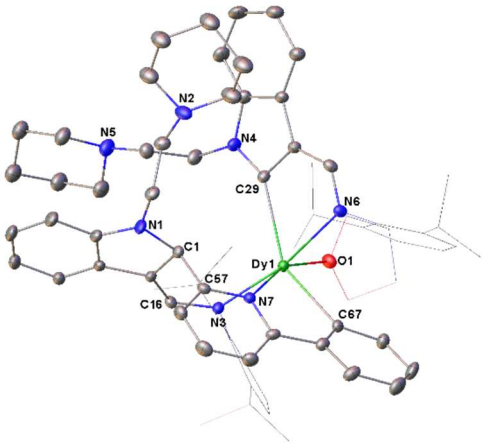


Fig. S85. Diagram of complex **9** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and the carbon atoms of THF were drawn in wireframe style for clarity. Selected bond lengths (Å): Dy(1)-C(29), 2.575(5); Dy(1)-C(67), 2.462(5); Dy(1)-N(3), 2.333(4); Dy(1)-N(6), 2.596(4); Dy(1)-N(7), 2.428(4); Dy(1)-O(1), 2.370(4); C(1)-C(57), 1.523(7); C(1)-N(1), 1.460(6); C(16)-N(3), 1.357(6); Selected bond angles (deg): C(29)-Dy(1)-C(67), 147.31(17); C(29)-Dy(1)-N(7), 112.61(16); C(29)-Dy(1)-N(6), 68.31(16); C(1)-C(57)-N(7), 116.0(5); N(1)-C(1)-C(57), 112.1(5).

Diagrams of complexes **10-11**

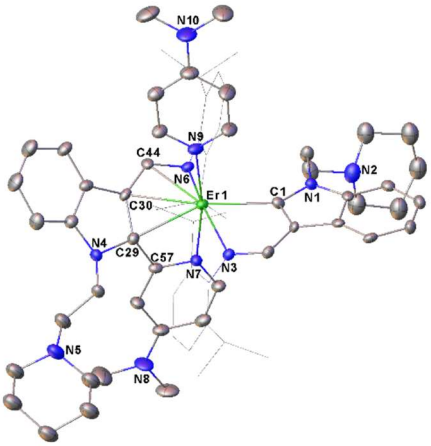


Fig. S86. Diagram of complex **10a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-C(1), 2.461(8); Er(1)-C(29), 2.530(8); Er(1)-C(30), 2.616(8); Er(1)-C(44), 2.588(8); Er(1)-N(3), 2.550(6); Er(1)-N(6), 2.230(6); Er(1)-N(7), 2.350(6); Er(1)-N(9), 2.440(7); C(29)-C(30), 1.485(11); C(29)-C(57), 1.479(10); C(30)-C(44), 1.367(10); C(44)-N(6), 1.380(9); Selected bond angles (deg): C(1)-Er(1)-N(3), 70.3(2); C(1)-Er(1)-C(29), 153.1(3); C(1)-Er(1)-C(30), 162.3(3); C(1)-Er(1)-C(44), 133.1(3); C(1)-Er(1)-N(6), 102.4(3); C(1)-Er(1)-N(7), 83.6(2); C(1)-Er(1)-N(9), 97.7(2).

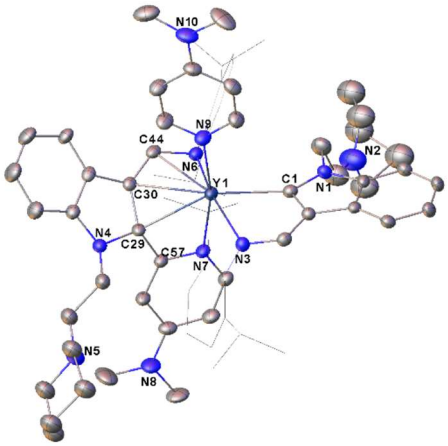


Fig. S87. Diagram of complex **10b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Y(1)-C(1), 2.465(6); Y(1)-C(29), 2.565(6); Y(1)-C(30), 2.656(6); Y(1)-C(44), 2.597(6); Y(1)-N(3), 2.568(5); Y(1)-N(6), 2.229(5); Y(1)-N(7), 2.376(5); Y(1)-N(9), 2.459(5); C(29)-C(30), 1.491(8); C(29)-C(57), 1.468(8); C(30)-C(44), 1.386(8); C(44)-N(6), 1.392(7); Selected bond angles (deg): C(1)-Y(1)-N(3), 70.98(19); C(1)-Y(1)-C(29), 151.78(18); C(1)-Y(1)-C(30), 159.0(2); C(1)-Y(1)-C(44), 130.4(2); C(1)-Y(1)-N(6), 98.9(2); C(1)-Y(1)-N(7), 95.34(18); C(1)-Y(1)-N(9), 97.1(2).

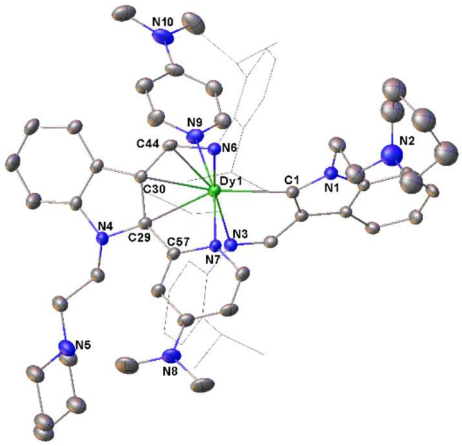


Fig. S88. Diagram of complex **10c** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Dy(1)-C(1), 2.469(6); Dy(1)-C(29), 2.586(6); Dy(1)-C(30), 2.664(6); Dy(1)-C(44), 2.588(6); Dy(1)-N(3), 2.571(5); Dy(1)-N(6), 2.229(5); Dy(1)-N(7), 2.368(5); Dy(1)-N(9), 2.471(6); C(29)-C(30), 1.497(8); C(29)-C(57), 1.472(8); C(30)-C(44), 1.379(8); C(44)-N(6), 1.395(8); Selected bond angles (deg): C(1)-Dy(1)-N(3), 70.8(2); C(1)-Dy(1)-C(29), 151.05(19); C(1)-Dy(1)-C(30), 158.3(2); C(1)-Dy(1)-C(44), 130.1(2); C(1)-Dy(1)-N(6), 98.4(2); C(1)-Dy(1)-N(7), 94.79(19); C(1)-Dy(1)-N(9), 98.0(2).

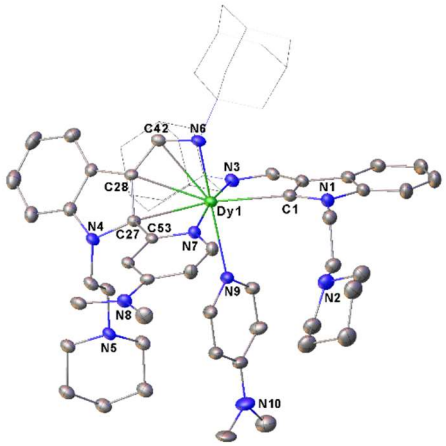


Fig. S89. Diagram of complex **11** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the adamantyl (Ad) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Dy(1)-C(1), 2.501(5); Dy(1)-C(27), 2.586(4); Dy(1)-C(28), 2.655(6); Dy(1)-C(42), 2.584(4); Dy(1)-N(3), 2.485(3); Dy(1)-N(6), 2.234(3); Dy(1)-N(7), 2.404(3); Dy(1)-N(9), 2.534(4); C(27)-C(28), 1.500(5); C(27)-C(53), 1.459(5); C(28)-C(42), 1.385(5); C(42)-N(6), 1.375(5); Selected bond angles (deg): C(1)-Dy(1)-N(3), 70.90(14); C(1)-Dy(1)-C(27), 162.84(14); C(1)-Dy(1)-C(28), 156.14(13); C(1)-Dy(1)-C(42), 125.53(14); C(1)-Dy(1)-N(6), 97.06(14); C(1)-Dy(1)-N(7), 106.11(14); C(1)-Dy(1)-N(9), 81.85(13).

Diagrams of complexes **12-13**

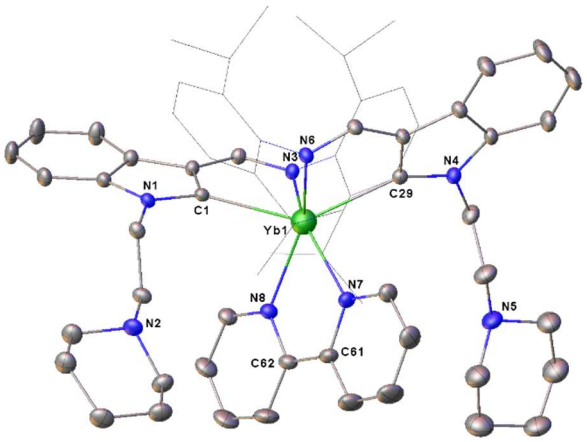


Fig. S90. Diagram of complex **12a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Yb(1)-C(1), 2.433(3); Yb(1)-C(29), 2.445(3); Yb(1)-N(3), 2.423(2); Yb(1)-N(6), 2.421(2); Yb(1)-N(7), 2.330(3); Yb(1)-N(8), 2.358(3); C(61)-C(62), 1.414(5); Selected bond angles (deg): C(1)-Yb(1)-C(29), 140.10(10); C(1)-Yb(1)-N(3), 72.54(9); C(1)-Yb(1)-N(6), 85.76(9); C(1)-Yb(1)-N(7), 130.12(10); C(1)-Yb(1)-N(8), 82.31(10).

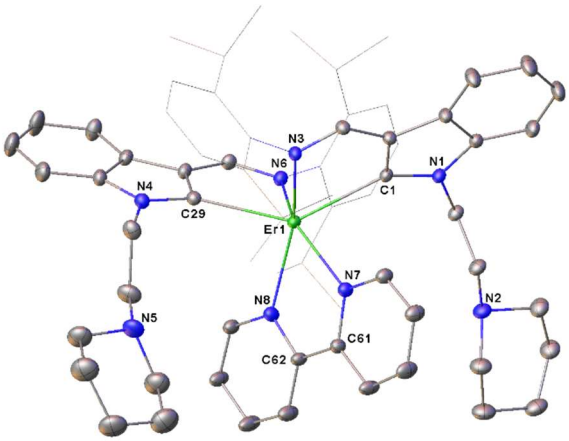


Fig. S91. Diagram of complex **12b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-C(1), 2.459(3); Er(1)-C(29), 2.465(3); Er(1)-N(3), 2.439(3); Er(1)-N(6), 2.432(3); Er(1)-N(7), 2.382(7); Er(1)-N(8), 2.349(7); C(61)-C(62), 1.413(8); Selected bond angles (deg): C(1)-Er(1)-C(29), 139.61(11); C(1)-Er(1)-N(3), 71.89(9); C(1)-Er(1)-N(6), 85.84(10); C(1)-Er(1)-N(7), 81.2(3); C(1)-Er(1)-N(8), 129.1(2).

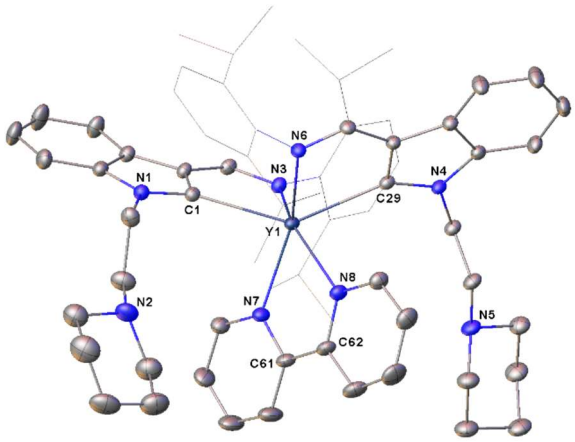


Fig. S92. Diagram of complex **12c** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Y(1)-C(1), 2.492(4); Y(1)-C(29), 2.476(4); Y(1)-N(3), 2.453(3); Y(1)-N(6), 2.454(3); Y(1)-N(7), 2.365(3); Y(1)-N(8), 2.393(3); C(61)-C(62), 1.412(6); Selected bond angles (deg): C(1)-Y(1)-C(29), 139.56(11); C(1)-Y(1)-N(3), 71.54(11); C(1)-Y(1)-N(6), 85.86(11); C(1)-Y(1)-N(7), 86.58(11); C(1)-Y(1)-N(8), 133.80(11).

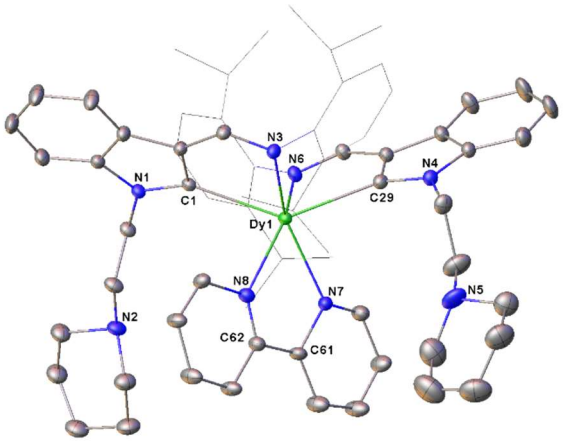


Fig. S93. Diagram of complex **12d** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Dy(1)-C(1), 2.487(3); Dy(1)-C(29), 2.495(3); Dy(1)-N(3), 2.461(2); Dy(1)-N(6), 2.458(2); Dy(1)-N(7), 2.370(9); Dy(1)-N(8), 2.406(9); C(61)-C(62), 1.407(9); Selected bond angles (deg): C(1)-Dy(1)-C(29), 139.39(9); C(1)-Dy(1)-N(3), 71.56(8); C(1)-Dy(1)-N(6), 86.21(8); C(1)-Dy(1)-N(7), 132.5(3); C(1)-Dy(1)-N(8), 83.9(5).

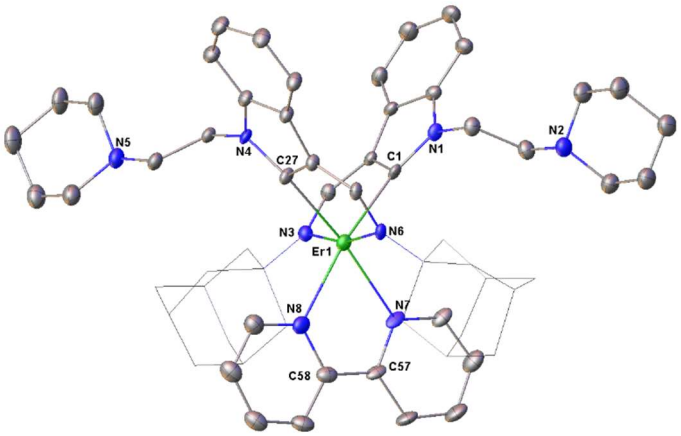
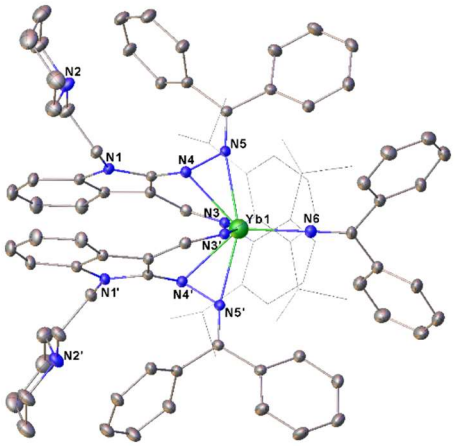


Fig. S94. Diagram of complex **13** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the adamantyl (Ad) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-C(1), 2.378(14); Er(1)-C(27), 2.402(13); Er(1)-N(3), 2.463(11); Er(1)-N(6), 2.441(10); Er(1)-N(7), 2.352(11); Er(1)-N(8), 2.365(13); C(57)-C(58), 1.41(2); Selected bond angles (deg): C(1)-Er(1)-C(27), 91.3(5); C(1)-Er(1)-N(3), 73.3(4); C(1)-Er(1)-N(6), 98.7(4); C(1)-Er(1)-N(7), 100.1(4); C(1)-Er(1)-N(8), 167.3(4).



Diagrams of complexes **14a-14c**

Fig. S95. Diagram of complex **14a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Yb(1)-N(3), 2.480(3); Yb(1)-N(4), 2.338(2); Yb(1)-N(5), 2.398(2); Yb(1)-N(6), 2.172(4); Selected bond angles (deg): N(3)-Yb(1)-N(4), 81.69(8); N(3)-Yb(1)-N(5), 75.87(8); N(3)-Yb(1)-N(6), 99.81(5).

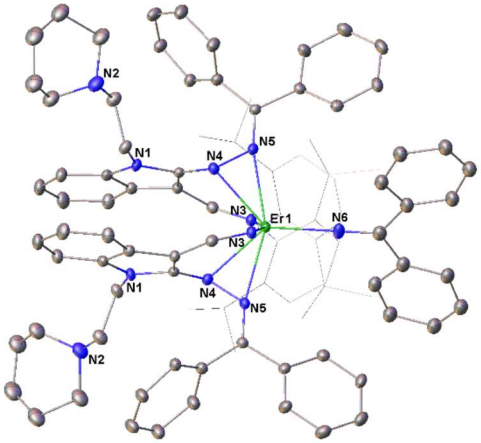


Fig. S96. Diagram of complex **14b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Er(1)-N(3), 2.475(5); Er(1)-N(4), 2.364(5); Er(1)-N(5), 2.421(5); Er(1)-N(6), 2.221(8); Selected bond angles (deg): N(3)-Er(1)-N(4), 81.55(16); N(3)-Er(1)-N(5), 75.44(16); N(3)-Er(1)-N(6), 100.02(11).

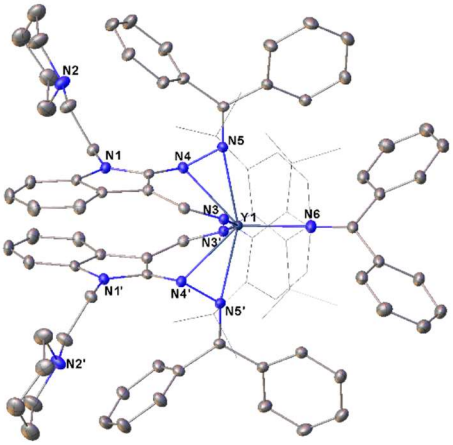


Fig. S97. Diagram of complex **14c** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group was drawn in wireframe style for clarity. Selected bond lengths (Å): Y(1)-N(3), 2.488(3); Y(1)-N(4), 2.393(3); Y(1)-N(5), 2.427(3); Y(1)-N(6), 2.193(5); Selected bond angles (deg): N(3)-Y(1)-N(4), 81.17(9); N(3)-Y(1)-N(5), 75.03(9); N(3)-Y(1)-N(6), 99.96(6).

6. Electron Paramagnetic Resonance and UV/vis Absorption Spectra

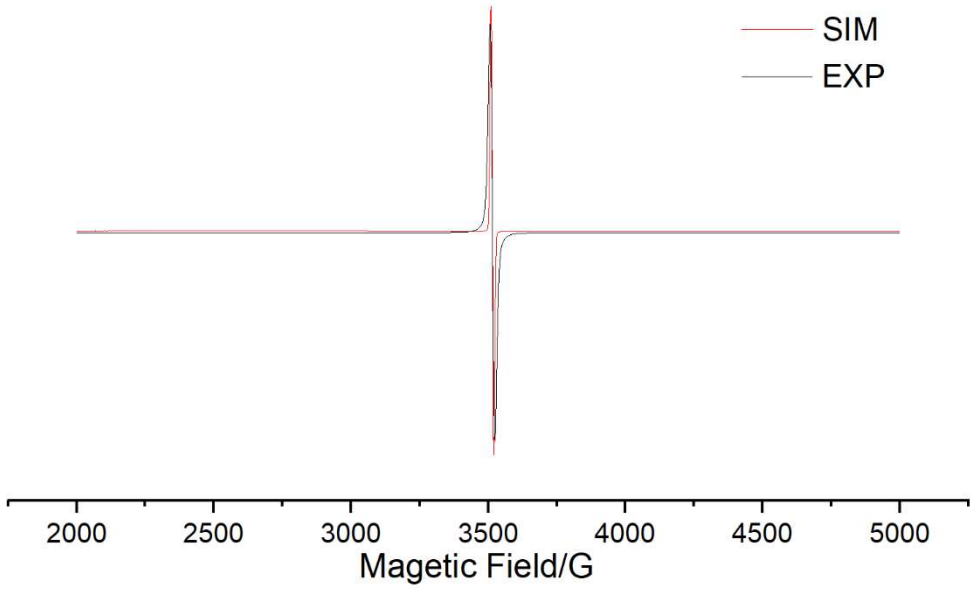


Fig. S98. Continuous-wave X-Band EPR spectrum (perpendicular mode) of **12c** (298 K)

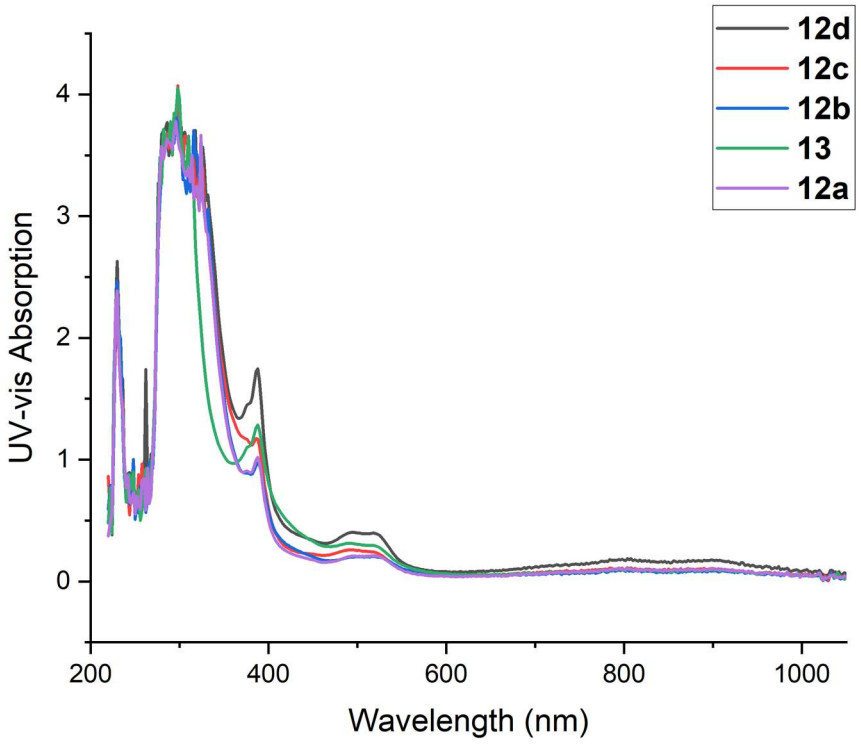


Fig. S99. UV/vis absorption spectrum of complexes **12-13** (298 K, 0.30 mM/L in THF)

7. GC-MS

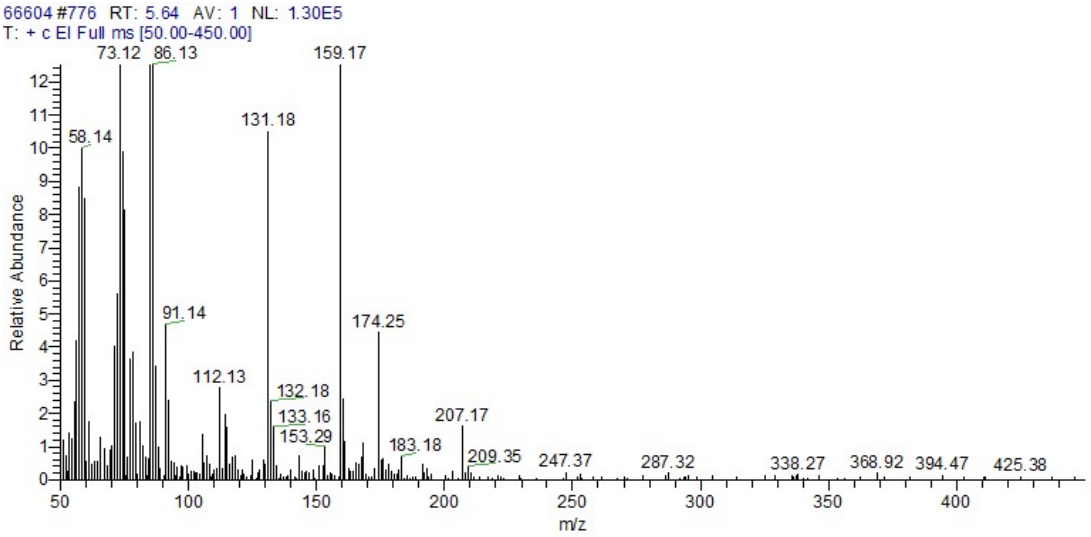


Fig. S100. GC-MS (EI) analyses of the coupling product $(Me_3SiCH_2)_2$ from the hydrolysis of reaction mixtures of the corresponding reactions in the formation of **12c**.

8. Tables of Crystal Data and Structure Refinement

Table S22. Selected bond lengths (Å) and angles (deg) for the indolyl rare-earth metal alkyl complexes **1-3**

Compd (RE)	RE–C(1)	RE–C(29)	RE–C(27)	RE–C(37)	RE–C(41)	RE–C(57)	RE–N(3)	RE–N(6)
1a(Lu)	2.432(5)	/	/	2.370(6)	2.345(6)	/	2.541(10)	
1b(Yb)	2.445(9)	/	/	2.378(10)	2.361(10)	/	2.599(7)	
1c(Er)	2.472(8)	/	/	2.387(8)	2.380(8)	/	2.617(6)	
1d(Y)	2.469(6)	/	/	2.393(7)	2.382(6)	/	2.606(5)	
1e(Dy)	2.498(10)	/	/	2.427(11)	2.399(11)	/	2.626(8)	
2a(Lu)	2.421(4)	2.417(4)	/	/	/	2.285(6)	2.339(3)	2.382(3)
2b(Yb)	2.429(9)	2.440(8)	/	/	/	2.318(13)	2.444(6)	2.382(6)
2c(Er)	2.456(3)	2.442(3)	/	/	/	2.389(6)	2.606(3)	2.474(2)
2d(Y)	2.485(6)	2.488(5)	/	/	/	2.424(6)	2.634(5)	2.485(5)
2e(Dy)	2.500(4)	2.502(4)	/	/	/	2.435(4)	2.653(6)	2.493(3)
3a(Yb)	2.456(10)	/	2.415(10)	/	/	2.369(8)	2.546(7)	2.414(7)
3b(Er)	2.474(8)	/	2.459(8)	/	/	2.354(10)	2.560(6)	2.435(6)
3c(Y)	2.500(4)	/	2.490(4)	/	/	2.412(3)	2.591(5)	2.458(3)
3d(Dy)	2.507(4)	/	2.491(4)	/	/	2.419(4)	2.607(3)	2.470(3)
3e(Gd)	2.533(6)	/	2.533(7)	/	/	2.442(7)	2.641(5)	2.489(7)

Table S23. Crystal data and structure refinement for **1a-1e**

	1a	**1b**	**1c**	**1d**	**1e**
Formula	$C_{44}H_{74}LuN_3O_2Si_2$	$C_{44}H_{74}YbN_3O_2Si_2$	$C_{44}H_{74}ErN_3O_2Si_2$	$C_{44}H_{74}YN_3O_2Si_2$	$C_{44}H_{74}DyN_3O_2Si_2$
FW	908.21	906.28	900.50	822.15	895.74
T (K)	300	300	300	300	300
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	12.8893(7)	12.887(3)	12.905(4)	12.860(3)	12.958(3)
b (Å)	39.791(2)	39.892(9)	39.957(11)	39.772(8)	40.101(8)
c (Å)	10.5197(6)	10.500(2)	10.506(3)	10.405(2)	10.503(2)
α (deg)	90	90	90	90	90
β (deg)	113.687(1)	113.607(6)	113.507(4)	113.53(3)	113.45(3)
γ (deg)	90	90	90	90	90
V (Å^3)	4940.7(5)	4946.2(19)	4968(3)	4879(2)	5007(2)
Z	4	4	4	4	4
ρ_{calc} (g·cm^{-3})	1.221	1.217	1.204	1.119	1.188
μ (mm^{-1})	2.080	1.973	1.771	1.279	1.573
F (000)	1896.0	1892.0	1884.0	1768.0	1876.0
θ range (deg)	1.023 to 27.499	2.942 to 27.532	1.795 to 27.492	2.959 to 27.661	2.932 to 27.546
Reflections collected	57484	182884	42868	195277	188539
Independent reflections	11359	11407	11403	11397	11551
R_{int}	0.0493	0.0564	0.1263	0.0993	0.0558
Data / restraints / parameters	11359 / 1099 / 810	11407 / 1018 / 799	11403 / 1176 / 791	11397 / 1170 / 792	11551 / 1160 / 790
Goodness-of-fit on F2	1.179	1.351	1.092	1.210	1.294
R1, *w*R2 [I>=2σ(I)]	0.0563, 0.1060	0.0894, 0.1768	0.0829, 0.1247	0.1053, 0.1986	0.1031, 0.2108
R1, *w*R2 (all data)	0.0743, 0.1113	0.0959, 0.1847	0.1819, 0.1528	0.1429, 0.2116	0.1139, 0.2149
Largest diff. peak and hole e.Å^{-3}	1.16, -2.34	1.69, -4.45	1.25, -1.62	0.64, -1.40	2.21, -5.05

Table S24. Crystal data and structure refinement for **2a-2e**

	(2a)$_2$·C$_7$H$_8$	**2b**	**2c**	**2d**	**2e**
Formula	$(C_{60}H_{83}LuN_6Si)_2·C_7H_8$	$C_{60}H_{83}YbN_6Si$	$C_{64}H_{91}ErN_6OSi$	$C_{64}H_{91}YN_6OSi$	$C_{64}H_{91}DyN_6OSi$
FW	2274.91	1089.46	1155.78	1077.43	1151.02
T (K)	300	300	300	300	300
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic	Monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	$P2_1/c$
a (Å)	13.4249(7)	13.372(5)	13.1343(18)	16.63(3)	16.598(3)
b (Å)	13.4551(7)	13.624(6)	13.9845(19)	19.68(4)	19.476(3)
c (Å)	18.955(1)	18.823(8)	18.709(3)	19.37(4)	19.325(3)
α (deg)	73.095(1)	72.565(5)	73.486(2)	90	90
β (deg)	84.897(1)	84.873(5)	84.862(2)	94.60(3)	94.720(2)
γ (deg)	70.203(1)	70.974(5)	71.051(2)	90	90
V (Å^3)	3082.2(3)	3093(2)	3116.1(8)	6319(22)	6225.9(18)

Z	1	2	2	4	4
ρ_{calc} (g·cm^{-3})	1.226	1.170	1.232	1.133	1.228
μ (mm^{-1})	1.662	1.569	1.409	0.985	1.263
F (000)	1190.0	1138.0	1214.0	2312.0	2420.0
θ range (deg)	1.123 to 27.502	1.134 to 25.398	1.135 to 27.481	1.228 to 24.998	1.231 to 27.487
Reflections collected	36378	30465	36406	57841	72329
Independent reflections	14175	11393	14277	11127	14284
R_{int}	0.0494	0.0543	0.0307	0.1114	0.0766
Data / restraints / parameters	14175 / 628 / 818	11393 / 1468 / 1037	14277 / 1227 / 985	11127 / 791 / 864	14284 / 692 / 856
Goodness-of-fit on F2	0.992	1.073	1.026	1.016	1.002
R1, *w*R2 [I>=2σ(I)]	0.0490, 0.1023	0.0674, 0.1523	0.0373, 0.0924	0.0562, 0.1272	0.0455, 0.0894
R1, *w*R2 (all data)	0.0775, 0.1120	0.1066, 0.1698	0.0472, 0.0972	0.1252, 0.1583	0.0879, 0.1035
Largest diff. peak and hole e.Å^{-3}	1.31, -0.65	2.02, -1.47	1.765, -0.90	0.32, -0.53	2.11, -0.63

Table S25. Crystal data and structure refinement for **3a-3e**

	3a·(C_6H_{14})$_{0.5}$	**3b·(C_6H_{14})$_{0.5}$**	**3c·(C_6H_{14})$_{0.5}$**	**3d·(C_6H_{14})$_{0.5}$**	**3e·(C_6H_{14})$_{0.5}$**
Formula	$C_{60}H_{87}YbN_6OSi\cdot(C_6H_{14})_{0.5}$	$C_{60}H_{87}ErN_6OSi\cdot(C_6H_{14})_{0.5}$	$C_{60}H_{87}YN_6OSi\cdot(C_6H_{14})_{0.5}$	$C_{60}H_{87}DyN_6OSi\cdot(C_6H_{14})_{0.5}$	$C_{60}H_{87}GdN_6OSi\cdot(C_6H_{14})_{0.5}$
FW	1152.57	1146.79	1068.44	1142.03	1136.78
T (K)	300	300	300	300	300
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	10.5491(9)	10.554(9)	10.5911(5)	10.6118(4)	10.6574(12)
b (Å)	12.7578(12)	12.716(12)	12.7677(7)	12.7636(5)	12.7730(14)
c (Å)	23.367(2)	23.25(2)	23.3687(13)	23.3508(10)	23.381(3)
α (deg)	103.217(4)	103.08(4)	102.763(2)	102.801(2)	102.815(2)
β (deg)	95.149(4)	94.75(4)	94.670(2)	94.606(2)	94.392(2)
γ (deg)	94.504(4)	94.70(3)	94.644(2)	94.785(2)	94.981(2)
V (Å^3)	3033.2(5)	3013(5)	3055.7(3)	3057.5(2)	3076.7(6)
Z	2	2	2	2	2
ρ_{calc} (g·cm^{-3})	1.262	1.264	1.161	1.240	1.227
μ (mm^{-1})	1.605	1.457	1.017	1.285	1.140
F (000)	1212.0	1208.0	1150.0	1204.0	1200.0
θ range (deg)	2.911 to 25.000	2.885 to 25.000	2.877 to 24.999	2.879 to 27.559	2.885 to 27.611
Reflections collected	99814	95245	124009	127330	27147
Independent reflections	10701	10629	10765	14137	14305
R_{int}	0.1437	0.1155	0.1177	0.0780	0.0515
Data / restraints / parameters	10701 / 1574 / 1040	10629 / 1214 / 921	10765 / 1613 / 1050	14137 / 1560 / 1032	14305 / 1587 / 1040
Goodness-of-fit on F2	1.121	1.184	1.059	1.097	1.044
R1, *w*R2	0.0744,	0.0776,	0.0559,	0.0545,	0.0691, 0.1495

[I>=2σ(I)]	0.1337	0.1477	0.1477	0.1028	
R1, wR2 (all data)	0.1090, 0.1468	0.1006, 0.1589	0.1006, 0.1410	0.0729, 0.1102	0.1202, 0.1752
Largest diff. peak and hole e.Å^{-3}	1.32, -1.42	1.59, -1.59	0.59, -0.44	1.70, -1.05	1.85, -1.34

Table S26. Crystal data and structure refinement for **4a-4d**

	4a	**4b**	**4c**	**4d**
Formula	$C_{78}H_{104}Lu_2N_{10}O_2$	$C_{78}H_{104}Yb_2N_{10}O_2$	$C_{78}H_{104}Er_2N_{10}O_2$	$C_{78}H_{104}Y_2N_{10}O_2$
FW	1563.65	1559.79	1548.23	1391.53
T (K)	300	300	300	300
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*C2/c*	*C2/c*	*C2/c*	*C2/c*
a (Å)	13.6267(10)	13.6308(8)	13.6472(7)	13.6694(7)
b (Å)	20.1993(15)	20.2415(11)	20.2383(10)	20.2490(11)
c (Å)	26.817(2)	26.8881(15)	26.8628(14)	26.9122(14)
α (deg)	90	90	90	90
β (deg)	91.110(1)	91.364(1)	91.340(1)	91.415(1)
γ (deg)	90	90	90	90
V (Å^3)	7380.0(9)	7416.5(7)	7417.4(7)	7446.8(7)
Z	4	4	4	4
ρ_{calc} (g·cm^{-3})	1.407	1.397	1.386	1.241
μ (mm^{-1})	2.711	2.558	2.299	1.602
F (000)	3200.0	3192.0	3176.0	2944.0
θ range (deg)	1.519 to 24.998	1.515 to 25.000	1.517 to 25.000	1.514 to 24.999
Reflections collected	35887	35942	36004	36188
Independent reflections	6507	6534	6539	6569
R_{int}	0.0748	0.0394	0.0887	0.0800
Data / restraints / parameters	6507 / 749 / 616	6534 / 757 / 625	6539 / 781 / 625	6569 / 786 / 616
Goodness-of-fit on F2	1.032	1.113	1.053	1.026
R1, wR2 [I>=2σ(I)]	0.0415, 0.0824	0.0385, 0.0935	0.0485, 0.0888	0.0568, 0.1280
R1, wR2 (all data)	0.0702 0.0916	0.0468 0.0978	0.0878 0.1015	0.1030 0.1497
Largest diff. peak and hole e.Å^{-3}	0.69, -0.62	1.08, -0.40	1.42, -0.55	0.56, -0.26

Table S27. Crystal data and structure refinement for **5a-5d**

	5a	**5b**	**5c**	**5d**
Formula	$C_{64}H_{83}LuN_8$	$C_{64}H_{83}YbN_8$	$C_{64}H_{83}ErN_8$	$C_{64}H_{83}YN_8$
FW	1139.36	1137.43	1131.65	1053.30
T (K)	300	300	300	300
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Triclinic	Triclinic
Space group	*P*$\bar{1}$	*P*2$_1$/*c*	*P*$\bar{1}$	*P*$\bar{1}$
a (Å)	13.584(5)	24.140(4)	13.665(6)	13.6160(16)
b (Å)	18.222(7)	13.516(2)	18.226(8)	18.253(2)

c (Å)	25.76(1)	18.231(3)	25.786(12)	25.838(3)
α (deg)	70.931(5)	90	71.040(6)	71.129(2)
β (deg)	81.514(5)	91.093(2)	81.488(6)	81.630(2)
γ (deg)	89.800(5)	90	89.511(7)	89.722(2)
V (Å^3)	5954(4)	5947.3(16)	6002(5)	6005.6(12)
Z	4	4	4	4
ρ_{calc} (g·cm^{-3})	1.271	1.270	1.252	1.165
μ (mm^{-1})	1.703	1.617	1.442	1.015
F (000)	2376.0	2372.0	2364.0	2248.0
θ range (deg)	1.684 to 24.737	1.727 to 24.999	1.682 to 25.000	1.68 to 25.000
Reflections collected	20349	56385	59247	58706
Independent reflections	20349	10456	21146	21167
R_{int}	/	0.1097	0.0500	0.0823
Data / restraints / parameters	20349 / 1490 / 1430	10456 / 669 / 715	21146 / 1255 / 1477	21167 / 1201 / 1479
Goodness-of-fit on F2	1.034	1.023	1.025	1.018
R1, *w*R2 [I>=2σ(I)]	0.0995, 0.2720	0.0640, 0.1489	0.0567, 0.1324	0.0811, 0.2044
R1, *w*R2 (all data)	0.2217, 0.3381	0.1310, 0.1803	0.1129, 0.1585	0.1901, 0.2621
Largest diff. peak and hole e.Å^{-3}	1.79, -1.61	1.18, -1.63	1.23, -1.31	1.33, -0.47

Table S28. Crystal data and structure refinement for **6a-6d**

	6a	**6b**	**6c**	**6d**
Formula	$C_{62}H_{79}LuN_8$	$C_{62}H_{79}YbN_8$	$C_{62}H_{79}ErN_8$	$C_{62}H_{79}YN_8$
FW	1111.30	1109.38	1102.59	1025.24
T (K)	300	300	300	300
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	13.2585(12)	13.2252(8)	13.255(10)	13.210(2)
b (Å)	13.3239(12)	13.3516(9)	13.375(10)	13.311(2)
c (Å)	18.7854(18)	18.7595(11)	18.831(14)	18.771(3)
α (deg)	84.057(3)	83.489(2)	83.839(10)	83.749(2)
β (deg)	71.876(3)	71.436(2)	71.754(10)	71.645(2)
γ (deg)	69.550(3)	69.008(2)	69.498(10)	69.345(2)
V (Å^3)	2955.1(5)	2931.7(3)	2970(4)	2931.4(8)
Z	2	2	2	2
ρ_{calc} (g·cm^{-3})	1.249	1.257	1.233	1.161
μ (mm^{-1})	1.714	1.639	1.456	1.038
F (000)	1156.0	1154.0	1148.0	1092.0
θ range (deg)	2.582 to 24.999	2.571 to 27.549	1.139 to 24.999	1.143 to 27.433
Reflections collected	133141	108290	28901	33972
Independent reflections	10386	13557	10446	13384
R_{int}	0.0893	0.0802	0.0580	0.0467
Data / restraints / parameters	10386 / 1139 / 975	13557 / 783 / 850	10446 / 692 / 833	13384 / 795 / 851
Goodness-of-	1.084	1.039	1.002	1.034

fit on F2				
R1, *w*R2 [$I>=2\sigma(I)$]	0.0352, 0.0801	0.0383, 0.0914	0.0506, 0.1331	0.0489, 0.1159
R1, *w*R2 (all data)	0.0478, 0.0867	0.0546, 0.0994	0.0711, 0.1455	0.0848, 0.1281
Largest diff. peak and hole e.Å^{-3}	0.82, -0.76	1.34, -0.85	1.82, -1.29	0.34, -0.52

Table S29. Crystal data and structure refinement for **7a-7b**

	7a	**7b**
Formula	$C_{63}H_{85}ErN_8O$	$C_{63}H_{85}YN_8O$
FW	1137.65	1059.30
T (K)	300	300
λ (Å)	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	*P*$\bar{1}$	*P*$\bar{1}$
a (Å)	11.152(3)	11.1074(3)
b (Å)	14.224(4)	14.1540(3)
c (Å)	19.011(5)	18.9061(5)
α (deg)	74.607(3)	74.549(1)
β (deg)	86.798(3)	86.700(2)
γ (deg)	80.220(3)	80.292(1)
V (Å^3)	2865.0(13)	2823.61(12)
Z	2	2
ρ_{calc} (g·cm^{-3})	1.319	1.246
μ (mm^{-1})	1.513	1821
F (000)	1190.0	1132.0
θ range (deg)	1.505 to 25.000	2.425 to 68.437
Reflections collected	27272	52987
Independent reflections	10096	10385
R_{int}	0.1396	0.0911
Data / restraints / parameters	10096 / 1490 / 1007	10385 / 1276 / 980
Goodness-of-fit on F2	0.982	1.079
R1, *w*R2 [$I>=2\sigma(I)$]	0.0735, 0.1307	0.0535, 0.1322
R1, *w*R2 (all data)	0.1556, 0.1569	0.0820, 0.1520
Largest diff. peak and hole e.Å^{-3}	1.67, -1.76	1.07, -1.22

Table S30. Crystal data and structure refinement for **8-9**

	8a	**8b**	**9**
Formula	$C_{67}H_{80}ErN_7$	$C_{67}H_{80}YN_7$	$C_{71}H_{88}DyN_7O$
FW	1150.64	1072.29	1217.99
T (K)	300	300	300
λ (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic
Space group	*P*$\bar{1}$	*P*$\bar{1}$	*P*$\bar{1}$
a (Å)	13.3096(11)	13.338(4)	13.5582(10)

b (Å)	13.3936(11)	13.409(4)	20.4707(15)
c (Å)	19.2327(16)	19.202(6)	23.6618(17)
α (deg)	82.266(1)	82.575(4)	100.406(1)
β (deg)	72.456(1)	72.696(4)	90.275(1)
γ (deg)	68.290(1)	68.602(4)	99.791(1)
V (Å^3)	3036.1(4)	3052.0(16)	6360.9(8)
Z	2	2	4
ρ_{calc} (g·cm^{-3})	1.259	1.167	1.272
μ (mm^{-1})	1.427	1.000	1.223
F (000)	1198.0	1140.0	6360.9(8)
θ range (deg)	1.111 to 27.459	1.631 to 25.000	1.221 to 27.601
Reflections collected	35673	29678	29539
Independent reflections	13904	10734	29539
R_{int}	0.0311	0.1247	/
Data / restraints / parameters	13904 / 1351 / 1035	10734 / 1964 / 1183	29539 / 757 / 1682
Goodness-of-fit on F2	1.027	1.018	1.005
R1, *w*R2 [I>=2σ(I)]	0.0324, 0.0777	0.0837, 0.1565	0.0586, 0.1163
R1, *w*R2 (all data)	0.0400, 0.0808	0.1878, 0.1952	0.1124, 0.1356
Largest diff. peak and hole e.Å^{-3}	1.03, -0.57	0.53, -0.48	2.19, -1.13

Table S31. Crystal data and structure refinement for **10-11**

	(10a)$_2$·C$_7$H$_8$	**(10b)$_4$·(C$_7$H$_8$)$_2$·C$_6$H$_{14}$**	**(10c)$_4$·(C$_7$H$_8$)$_2$·C$_6$H$_{14}$**	**11·(C$_4$H$_8$O)$_2$**
Formula	$(C_{70}H_{91}ErN_{10})_2·C_7H_8$	$(C_{70}H_{91}YN_{10})_4·(C_7H_8)_2·C_6H_{14}$	$(C_{70}H_{91}DyN_{10})_4·(C_7H_8)_2·C_6H_{14}$	$C_{66}H_{87}DyN_{10}·(C_4H_8O)_2$
FW	2571.72	4916.20	5210.56	1327.17
T (K)	300	300	300	300
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P*2$_1$/*c*	*C2/c*	*C2/c*	*P*2$_1$/*c*
a (Å)	21.640(3)	30.880(2)	30.753(3)	12.8231(6)
b (Å)	23.137(3)	22.9324(15)	22.844(2)	23.6040(11)
c (Å)	29.409(4)	21.5684(14)	21.5677(19)	23.0899(10)
α (deg)	90	90	90	90
β (deg)	98.576(2)	95.594(1)	95.600(1)	93.653(1)
γ (deg)	90	90	90	90
V (Å^3)	14560(3)	15201.0(17)	15080(2)	6974.6(6)
Z	4	2	2	4
ρ_{calc} (g·cm^{-3})	1.173	1.074	1.148	1.264
μ (mm^{-1})	1.198	0.812	1.036	1.123
F (000)	5392.0	5260.0	5476.0	2796.0
θ range (deg)	1.125 to 25.000	1.108 to 25.000	1.112 to 24.999	1.235 to 24.999
Reflections collected	139385	74054	71987	67930
Independent reflections	25642	13390	13295	12289

R_{int}	0.1643	0.1229	0.1104	0.0771
Data / restraints / parameters	25642 / 1483 / 1881	13390 / 1332 / 1124	13295 / 1379 / 1152	12289 / 1581 / 1184
Goodness-of-fit on F2	1.040	1.027	1.020	1.018
R1, *w*R2 [$I>=2\sigma(I)$]	0.0703, 0.1315	0.0848, 0.2184	0.0556, 0.1348	0.0422, 0.0763
R1, *w*R2 (all data)	0.1611, 0.1653	0.1791, 0.2827	0.1186, 0.1651	0.0795, 0.0890
Largest diff. peak and hole e.Å^{-3}	1.69, -1.14	0.53, -0.83	0.68, -0.68	0.42, -0.35

Table S32. Crystal data and structure refinement for **12a-12d**

	12a	**12b**	**12c**	**12d**
Formula	$C_{66}H_{80}YbN_8$	$C_{66}H_{80}ErN_8$	$C_{66}H_{80}YN_8$	$C_{66}H_{80}DyN_8$
FW	1158.42	1152.64	1074.29	1147.88
T (K)	300	300	300	300
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	*P*ī	*P*ī	*P*ī	*P*ī
a (Å)	13.2678(7)	13.2828(10)	13.275(4)	13.2834(8)
b (Å)	13.3947(7)	13.3925(10)	13.391(4)	13.4042(8)
c (Å)	19.2204(10)	19.2277(14)	19.241(6)	19.2405(11)
α (deg)	82.493(1)	82.472(1)	82.481(4)	82.430(1)
β (deg)	72.318(1)	72.475(1)	72.614(4)	72.629(1)
γ (deg)	67.954(1)	68.097(1)	68.205(4)	68.145(1)
V (Å^3)	3016.0(3)	3025.6(4)	3030.0(16)	3033.8(3)
Z	2	2	2	2
ρ_{calc} (g·cm^{-3})	1.276	1.265	1.178	1.257
μ (mm^{-1})	2.596	1.432	1.008	1.277
F (000)	1204.0	1200.0	1142.0	1196.0
θ range (deg)	1.112 to 27.488	1.639 to 27.607	1.638 to 27.488	1.109 to 27.488
Reflections collected	35678	35144	35200	35735
Independent reflections	13855	14064	13915	13927
R_{int}	0.0432	0.0498	0.0829	0.0358
Data / restraints / parameters	13855 / 551 / 833	14064 / 1751 / 1137	13915 / 550 / 845	13927 / 1036 / 963
Goodness-of-fit on F2	1.007	0.997	0.986	1.036
R1, *w*R2 [$I>=2\sigma(I)$]	0.0370, 0.0729	0.0414, 0.0776	0.0682, 0.1601	0.0348, 0.0807
R1, *w*R2 (all data)	0.0527 0.0776	0.0642 0.0843	0.1186 0.1871	0.0452 0.0845
Largest diff. peak and hole e.Å^{-3}	1.07, -0.65	1.62, -1.48	1.38, -0.89	1.12, -0.61

Table S33. Crystal data and structure refinement for **13-14**

	13·C_7H_8	**14a C_6H_{14}**	**14b C_6H_{14}**	**14c C_6H_{14}**
Formula	$C_{62}H_{76}ErN_8·C_7H_8$	$C_{95}H_{102}YbN_{11}·C_6H_{14}$	$C_{95}H_{102}ErN_{11}·C_6H_{14}$	$C_{95}H_{102}YN_{11}·C_6H_{14}$
FW	1100.57	1657.09	1651.31	1572.96

T (K)	300	300	300	300
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P*$\bar{1}$	*C2/c*	*C2/c*	*C2/c*
a (Å)	14.584(9)	22.488(9)	22.4080(19)	22.4825(13)
b (Å)	14.899(9)	20.758(8)	20.7325(18)	20.7751(12)
c (Å)	15.053(9)	21.613(8)	21.4331(18)	21.4740(12)
α (deg)	75.276(6)	90	90	90
β (deg)	84.282(6)	114.787(5)	114.672(1)	115.007(1)
γ (deg)	74.311(6)	90	90	90
V (Å^3)	3044(3)	9160(6)	9048.3(13)	9089.7(9)
Z	2	4	4	4
ρ_{calc} (g·cm^{-3})	1.201	1.202	1.212	1.149
μ (mm^{-1})	1.420	1.072	0.979	0.693
F (000)	1144.0	3476.0	3468.0	3352.0
θ range (deg)	1.399 to 25.433	1.399 to 27.502	1.402 to 24.999	1.400 to 24.998
Reflections collected	11236	36960	43793	44084
Independent reflections	11236	10512	7975	8019
R_{int}	/	0.0396	0.1268	0.0848
Data / restraints / parameters	11236 / 493 / 640	10512 / 920 / 756	7975 / 1178 / 821	8019 / 884 / 744
Goodness-of-fit on F2	0.957	1.022	1.059	1.059
R1, *w*R2 [I>=2σ(I)]	0.1203, 0.2409	0.0370, 0.0916	0.0607, 0.1277	0.0598, 0.1405
R1, *w*R2 (all data)	0.2281 0.2770	0.0492 0.0992	0.0979 0.1448	0.0960 0.1576
Largest diff. peak and hole e.Å^{-3}	2.18, -1.31	1.65, -1.05	1.69, -1.04	0.70, -0.35

9. IR Spectra

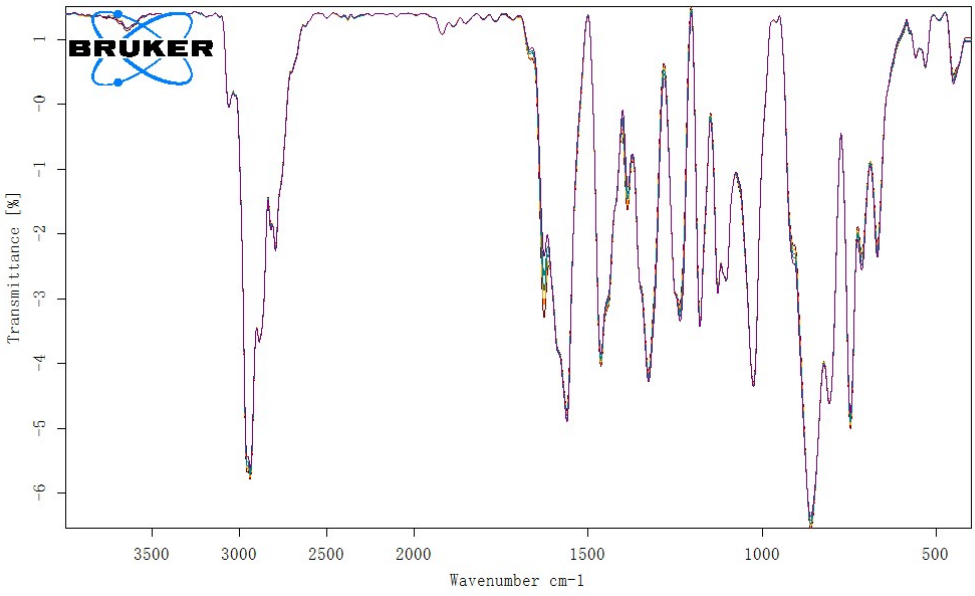


Fig. S101. IR spectrum of complexes **1a-1e**

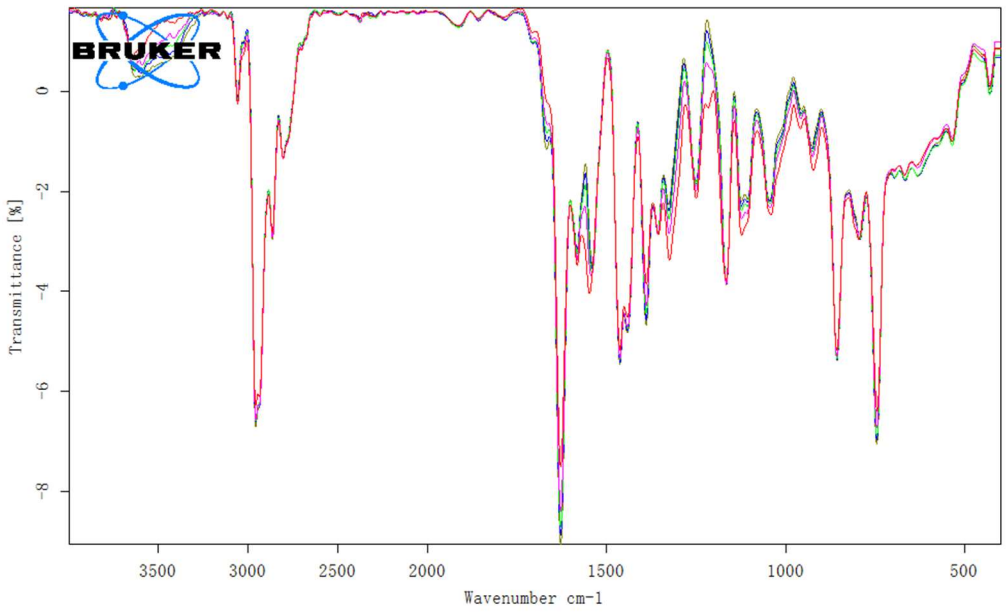


Fig. S102. IR spectrum of complexes **2a-2e**

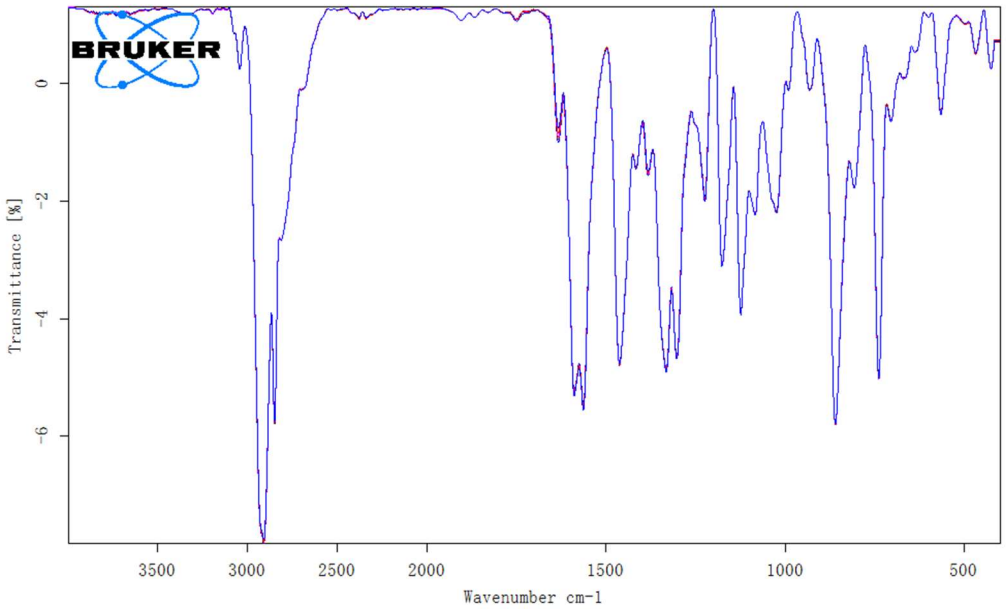


Fig. S103. IR spectrum of complexes **3a-3e**

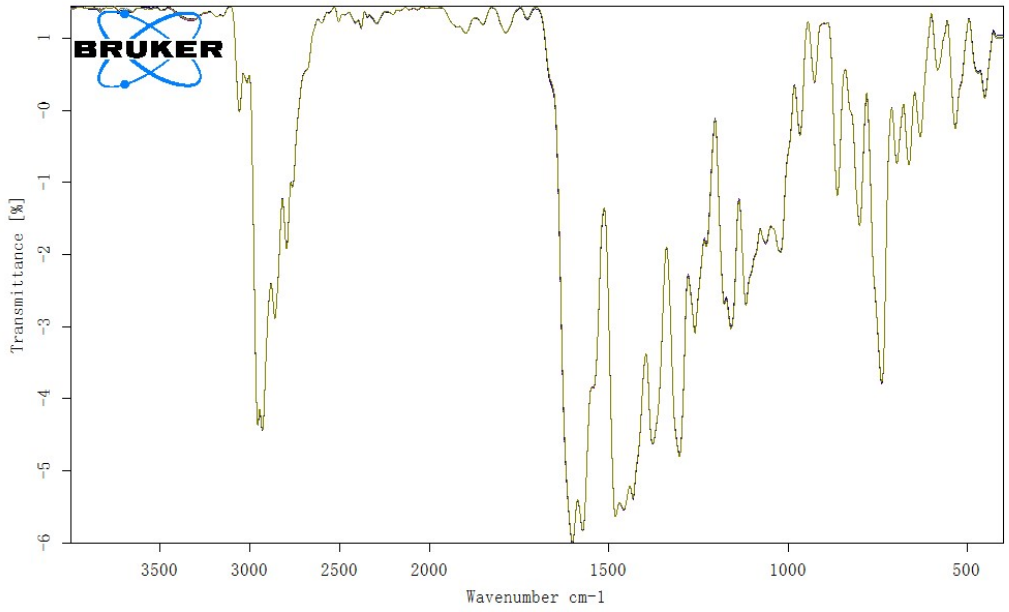


Fig. S104. IR spectrum of complexes **4a-4d**

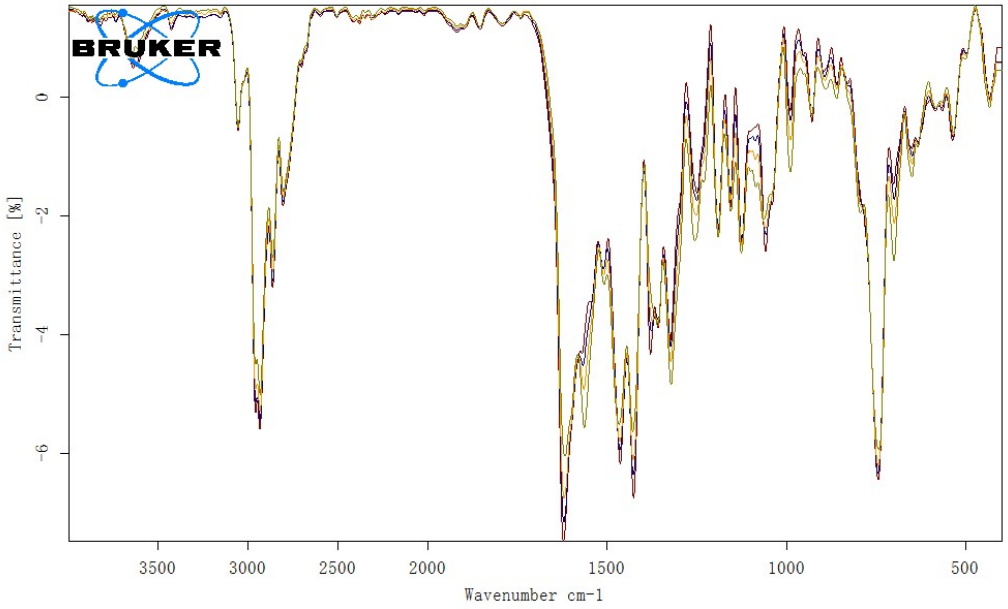


Fig. S105. IR spectrum of complexes **5a-5d**

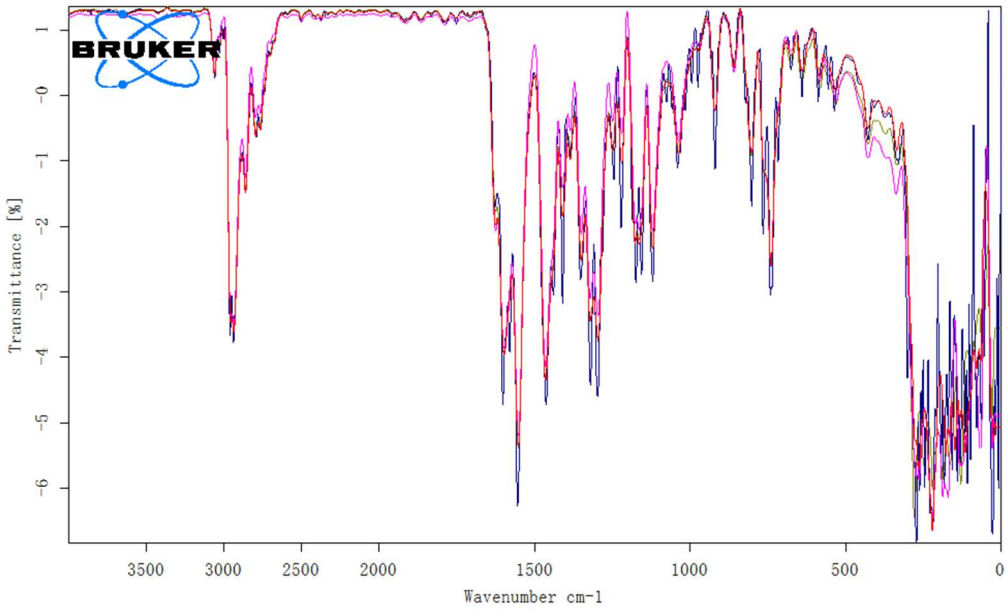


Fig. S106. IR spectrum of complexes **6a-6d**

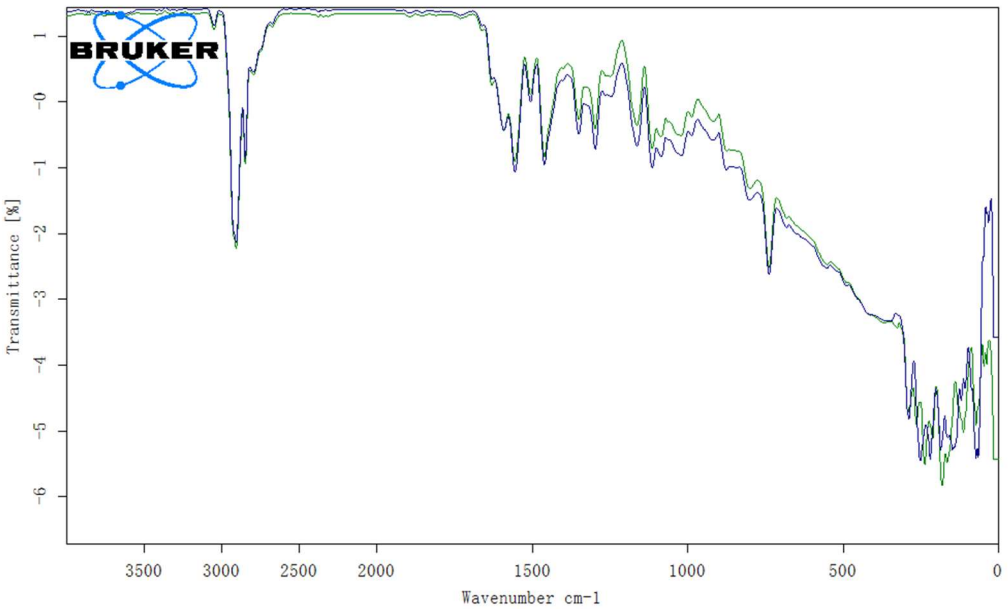


Fig. S107. IR spectrum of complexes **7a-7b**

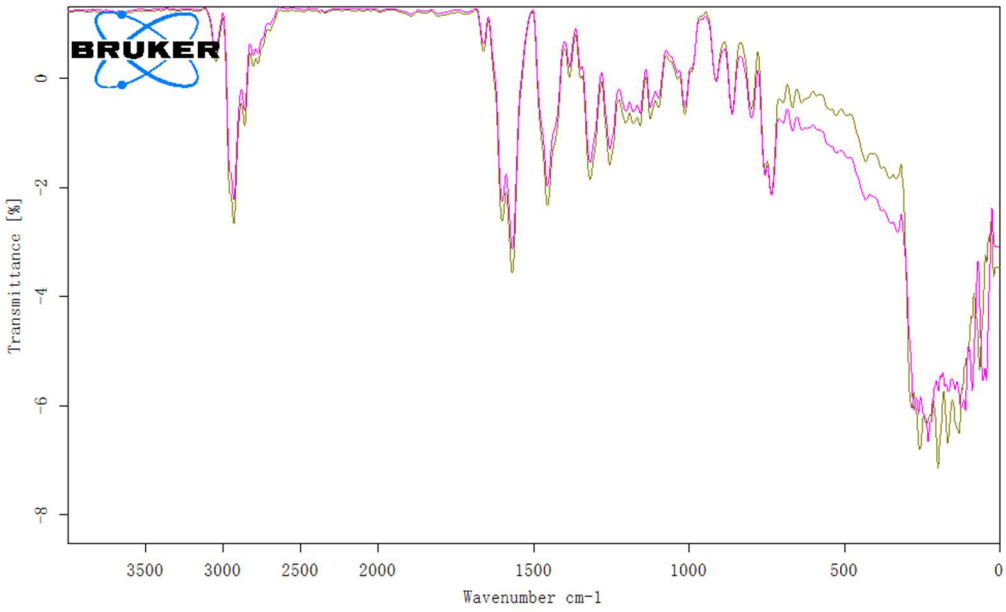


Fig. S108. IR spectrum of complexes **8a-8b**

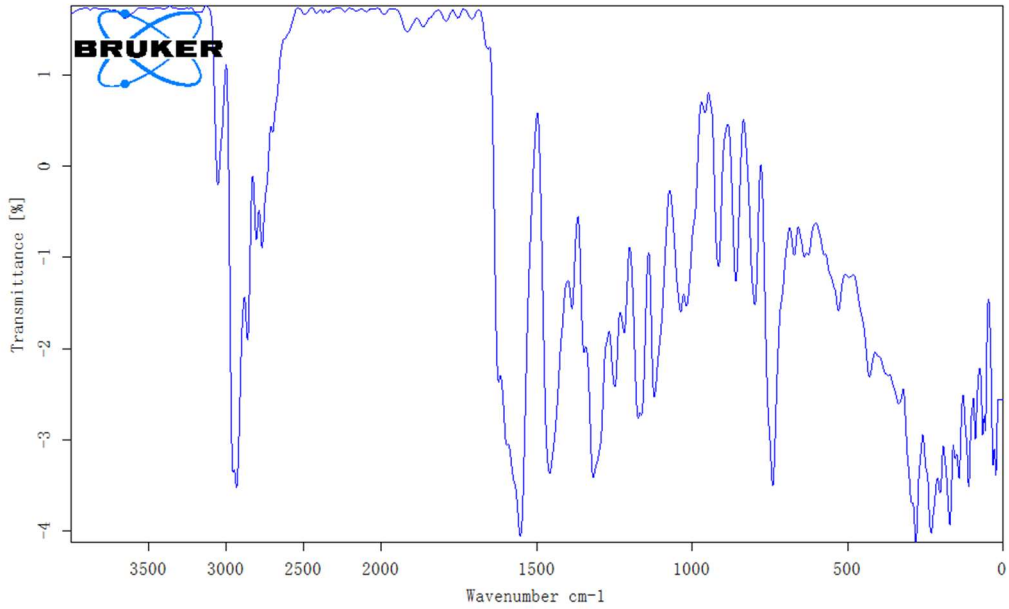


Fig. S109. IR spectrum of complex **9**

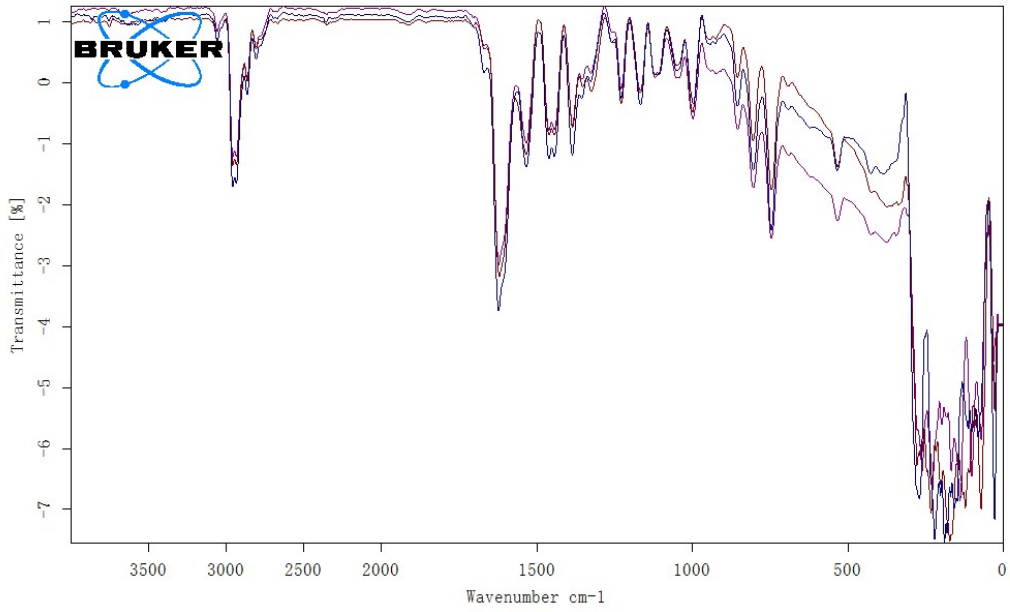


Fig. S110. IR spectrum of complexes **10a-10c**

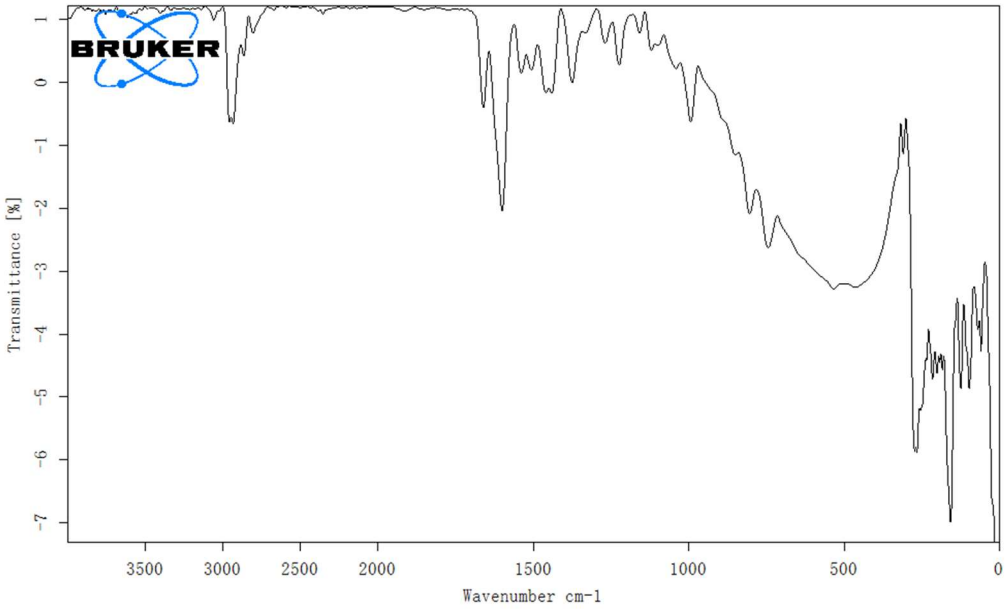


Fig. S111. IR spectrum of complex **11**

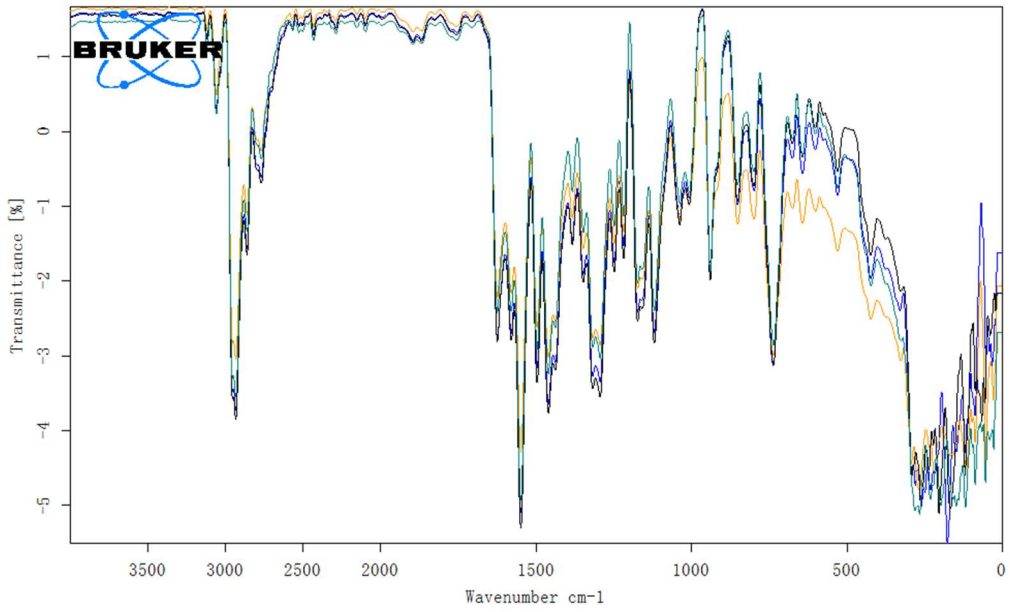


Fig. S112. IR spectrum of complexes **12a-12d**

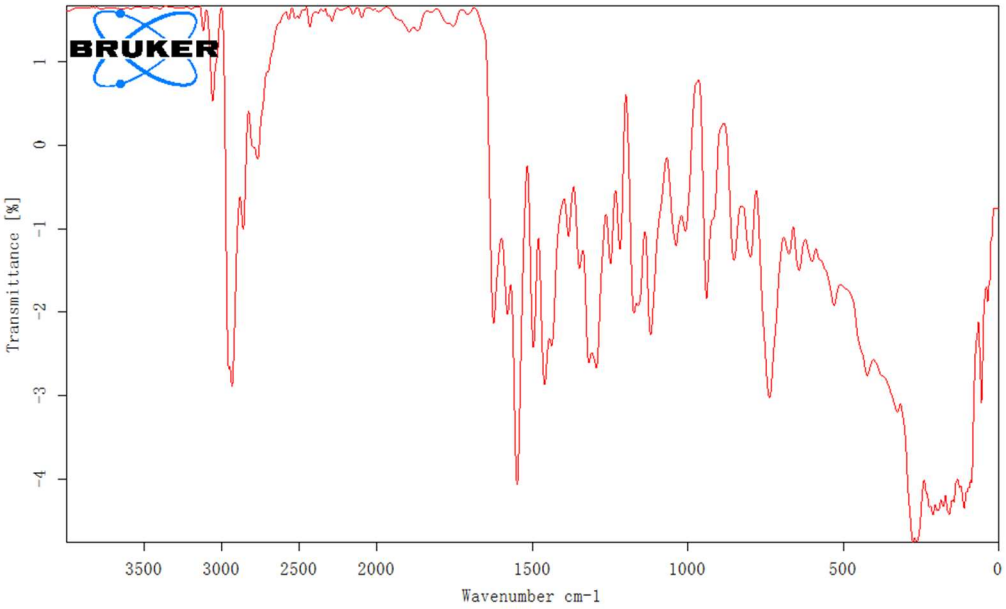


Fig. S113. IR spectrum of complex **13**

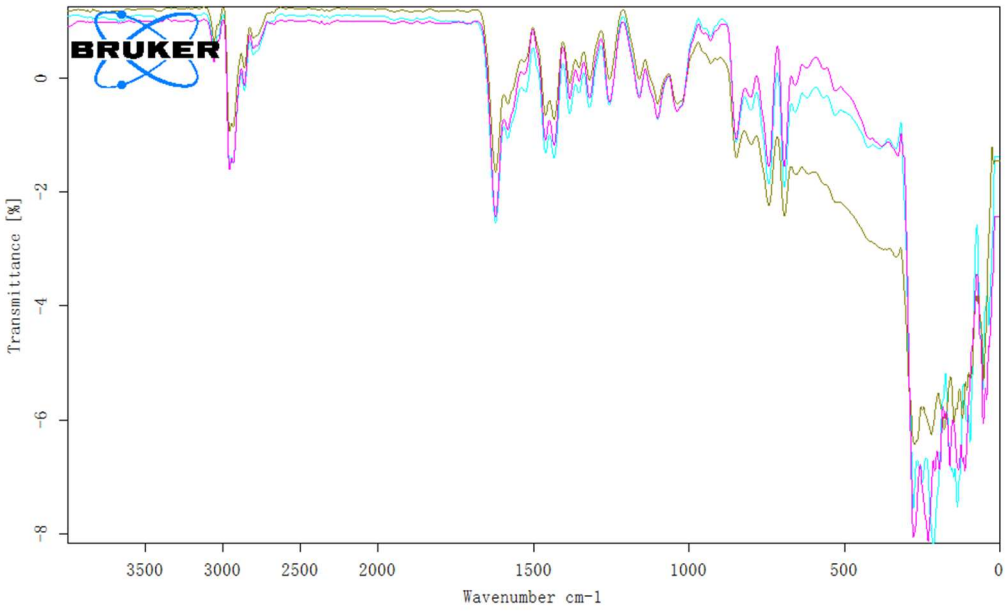


Fig. S114. IR spectrum of complexes **14a-14c**

10. References

1. (*a*) J. B. Reed, B. S. Hopkins and L. F. Audrieth, *Inorg. Synth.,* 1939, **1**, 28–33; (*b*) M. D. Taylor and C. P. Carter, *J. Inorg. Nucl. Chem.,* 1962, **24**, 387–391; (*c*) N. L. Edlema, A. C. Wang, J. A. Belot, A. W. Metz, J. R. Babcock, A. M. Kawaoka, J. Ni, M. V. Metz, C. J. Flaschenriem, C. L. Stern, L. M. Liable-Sands, A. L. Rheingold, P. R. Markworth, R. P. H. Chang, M. P. Chudzik, C. R. Kannewurf and T. J. Marks, *Inorg. Chem.,* 2002, **41**, 5005–5023.
2. (*a*) G. E. Hartwell and T. L. Brown, *J. Am. Chem. Soc.*, 1966, **88**, 4625–4629; (*b*) H. L. Lewi and T. L. Brown, *J. Am. Chem. Soc.*, 1970, **92**, 4664–4670; (*c*) C. Tessier-Youngs and O. T. Beachley, Jr., *Inorg. Synth.*, 1986, **24**, 95–97; (*d*) G. D. Vaughn, K. A. Krein and J. A. Gladysz, *Organometallics*, 1986, **5**, 936–942.
3. (*a*) M. F. Lappert and R. Pearce, *J. Chem. Soc. Chem. Comm.*, 1973, **126**; (*b*) K. C. Hultzsch, P. Voth, K. Beckerle, T. P. Spaniol and J. Okuda, *Organometallics*, 2000, **19**, 228–243; (*c*) W. J. Evans, J. C. Brady and J. W. Ziller, *J. Am. Chem. Soc.*, 2001, **123**, 7711–7712; (*d*) H. Schumann, D. M. M. Freckmann and S. Dechert, *Z. Anorg. Allorg. Chem.,* 2002, **628**, 2422–2426; (*e*) S. Arndt, T. P. Spaniol and J. Okuda, *Angew. Chem., Int. Ed.*, 2003, **42**, 5075–5079; (*f*) F. Estler, G. Eickerling, E. Herdtweck and R. Anwander, *Organometallics*, 2003, **22**, 1212–1222; (*g*) S. M. Chen, Y. Q. Zhang, J. Xiong, B. W. Wang and S. Gao, *Inorg. Chem.*, 2020, **59**, 5835–5844.
4. *SMART* Software Users Guide, Version 4.21; Bruker AXS, Inc.: Madison, WI, 1997.
5. Bruker (2015). *SAINT* (Version 8.37A). Bruker AXS Inc., Madison, Wisconsin, USA.
6. Bruker (2016). *SADABS*-2016/2. Bruker AXS Inc., Madison, Wisconsin, USA.
7. Sheldrick GM. *Acta Cryst,* 2015, A71: 3−8.
8. Dolomanov OV, Bourhis LJ, Gildea RJ, Howard JAK, Puschmann H. *J Appl Cryst,* 2009, 42: 339−341.
9. L. Guo, X. Zhu, G. Zhang, Y. Wei, L. Ning, S. Zhou, Z. Feng, S. Wang, X. Mu, J. Chen and Y. Jiang, *Inorg. Chem.*, 2015, **54**, 5725−5731.

10. W. Wu, T. Rajeshkumar, D. Hong, S. Zhu, Z. Huang, F. Chai, W. Wang, Q. Yuan, Y. Wei, Z. Xie, L. Maron, S. Wang, *Inorg. Chem.,* 2024, **63**, 18365−18378.
11. (*a*) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648−5652; (*b*) K. Burke, J. P. Perdew and W. Yang in *Electronic Density Functional Theory: Recent Progress and New Directions*, Eds: J. F. Dobson, G. Vignale and M. P. Das, Plenum. New York, 1998.
12. (*a*) A. Moritz, X. Cao and M. Dolg, *Theor. Chem. Acc.* 2007, **118**, 845; (*b*) A. Hollwarth, M. Bohme, S. Dapprich, A.W. Ehlers, A. Gobbi, V. Jonas, K.F. Kohler, R. Stegmann, A. Veldkamp, G. Frenking. *J. Chem. Phys.* 1993, **208**, 237.
13. (*a*) P. C. Hariharan and J. A. Pople, *Theoret. Chim. Acta.*, 1973, **28**, 213−222; (*b*) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257−2261.
14. Gaussian 16. Revision D0. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, E. Heyd, J. J. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, J. C. Burant, S. Iyengar, J. Tomasi, M. Cossi, N. Rega, M. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian Inc., 2016, Wallingford CT.