

Ytterbium(II) phosphinidene complexes

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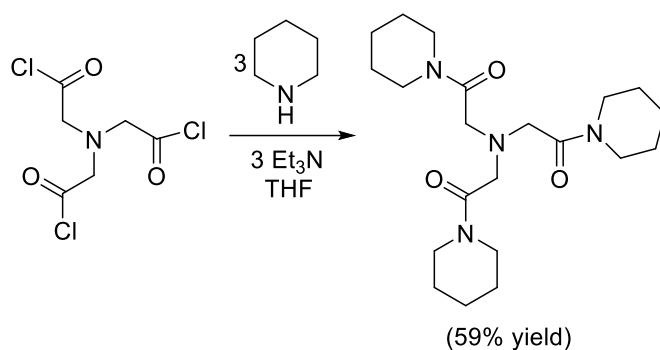
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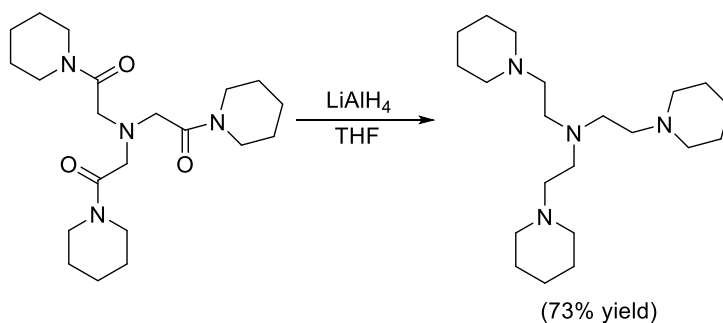
General. All manipulations were performed under an atmosphere of argon using Schlenk techniques or in a nitrogen-filled glovebox. THF, toluene, benzene, hexane, C₆D₆, *d*₈-Toluene and *d*₈-THF were dried over Na/K alloy, transferred under vacuum, and stored in the glovebox. YbI₂(THF)₂,¹ 2,2,2-nitrilotriacetyl chloride,² KCH₂SiMe₃,³ DippPH₂,⁴ and 1,3,4,5-tetramethylimidazolin-2-ylidene⁵ were synthesized following the literature procedures. 1-isocyanoadamantane(AdNC) was purchased from Bide Pharmatech Ltd and used without further purification. ¹H, ¹³C{¹H}, ³¹P, and ³¹P{¹H} NMR spectra of organic compounds and complexes **1–4**, **6** and **7** were recorded on a Bruker AV III 400 spectrometer. ¹H, ³¹P, ³¹P{¹H} solid-state NMR spectra of complex **5** were recorded on a JEOL ECZ-400R/M1 400 MHz spectrometer. Chemical shifts δ were reported in ppm with references to the residual resonance of the deuterated solvents or SiMe₄ for proton and carbon chemical shifts, and to external H₃PO₄ (85%) for phosphorus chemical shifts. ¹⁷¹Yb{¹H} NMR spectra of complexes **2** and **6** were recorded on a Bruker AV III 400 spectrometer and a Bruker AV III 500HD spectrometer, respectively, and the chemical shifts δ were reported in ppm with reference to external [Yb(Cp*)₂(THF)₂].⁶ The assignment of ¹H and ¹³C{¹H} resonances was assisted with gCOSY, gHSQC and gHMBC spectra. Elemental analyses were performed on an Elementar UNICUBE CHN analyzer. Samples were prepared using tin boats in a argon-filled glove box. Calibration was done using standard reference material: acetanilide (C₈H₉NO: C, 71.09%; N, 10.36%; H, 6.71%) were used for C/H/N. UV/vis/NIR spectra were recorded on a Agilent Cary 5000 UV-Vis-NIR Spectrophotometer.

2,2,2-nitrilotrisacetyl piperidine:



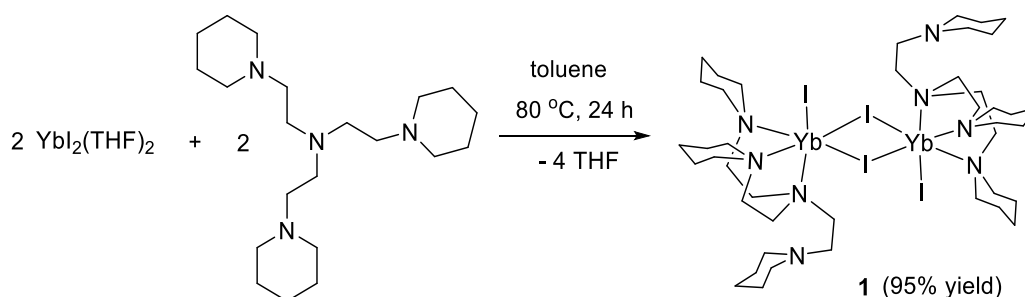
To a THF solution (30 mL) of piperidine (6.11 g, 71.8 mmol) and Et₃N (7.27 g, 71.8 mmol) was added a THF solution (150 mL) of 2,2,2-nitrilotriacetyl chloride (5.90 g, 23.9 mmol) at 0 °C. The reaction solution was allowed to warm to room temperature and stirred for 12 h. The precipitate was moved by filtration, and the volatiles of the solution were removed under vacuum. The resulting oil was dissolved in DCM (20 mL), washed with saturated aqueous NH₄Cl (10 mL × 3) and H₂O (10 mL × 3). The organic layer was dried over anhydrous sodium sulfate. The volatiles were removed under vacuum to give 2,2,2-nitrilotrisacetylpiperidine as a white solid (5.50 g, 59% yield). ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) 3.73 (s, 6H, NCH₂C(O)N), 3.46 (m, 6H, NCH₂CH₂CH₂), 3.19 (m, 6H, NCH₂CH₂CH₂), 1.20 (m, 18H, NCH₂CH₂CH₂ and NCH₂CH₂CH₂). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm) 168.2 (NCH₂C(O)N), 56.9 (NCH₂C(O)N), 46.2 (NCH₂CH₂CH₂), 42.7 (NCH₂CH₂CH₂), 26.7 (NCH₂CH₂CH₂), 25.9 (NCH₂CH₂CH₂), 24.8 (NCH₂CH₂CH₂).

(Pip)₃tren:



Tris(2-(piperidin-1-yl)ethyl)amine ((Pip)₃tren)⁷ was synthesized via a modified route by using 2,2,2-nitrilotrisacetylpiperidine as a starting material: A THF solution (50 mL) of 2,2,2-nitrilotrisacetylpiperidine (9.40 g, 23.9 mmol) was added to LiAlH₄ (9.09 g, 239 mmol) in 250 mL of THF at 0 °C. The reaction mixture was allowed to warm to room temperature and refluxed for 12 hours. Water (12 mL) was added dropwise to the mixture at 0 °C, and then 20% NaOH solution (124 mL) was added. The precipitate was moved by filtration, and the volatiles of the solution were removed under vacuum. The resulting oil was dissolved in DCM (20 mL) and washed with H₂O (10 mL × 3). The organic layer was dried over anhydrous sodium sulfate. The volatiles were removed under vacuum to give (Pip)₃tren as a yellow oil (6.10 g, 73% yield). ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) 2.75 (dd, ³J_{H-H} = 8.3 Hz, ³J_{H-H} = 6.0 Hz, 6H, NCH₂CH₂N), 2.51 (dd, ³J_{H-H} = 8.3 Hz, ³J_{H-H} = 6.0 Hz, 6H, NCH₂CH₂N), 2.37 (m, 6H, NCH₂CH₂CH₂), 1.54 (p, ³J_{H-H} = 5.6 Hz, 12H, NCH₂CH₂CH₂), 1.34 (m, 6H, NCH₂CH₂CH₂). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm) 58.5 (NCH₂CH₂N), 55.5 (NCH₂CH₂CH₂), 53.7 (NCH₂CH₂N), 26.7 (NCH₂CH₂CH₂), 25.1 (NCH₂CH₂CH₂).

[(Pip)₃trenYb(μ-I)]₂ (1):



A toluene solution (2 mL) of (Pip)₃tren (386 mg, 1.14 mmol) was added to YbI₂(THF)₂ (600 mg, 1.04 mmol) in 8 mL of toluene at room temperature. The reaction mixture was stirred at

80 °C for 24 h, and then the volatiles were removed under vacuum. The residue was washed with hexane (5 mL × 3) and dried under vacuum to give complex **1** as a yellow solid (780 mg, 91% yield). ¹H NMR (400 MHz, CD₂Cl₂, 25 °C): δ (ppm) 3.07 (br, 12H, NCH₂CH₂N), 2.72 (br, 24H, NCH₂CH₂CH₂), 2.60 (br, 12H, NCH₂CH₂N), 1.71 (br, 24H, NCH₂CH₂CH₂), 1.48 (br, 12H, NCH₂CH₂CH₂). ¹³C{¹H} NMR (100 MHz, CD₂Cl₂, 25 °C): δ (ppm) 55.1 (NCH₂CH₂CH₂), 52.7 (overlapped with the residue solvent resonance of the deuterated solvent, NCH₂CH₂N), 47.1 (NCH₂CH₂N), 23.8 (NCH₂CH₂CH₂), 22.9 (NCH₂CH₂CH₂). The poor solubility made it difficult to record ¹⁷¹Yb NMR spectrum of this complex. Anal. Calcd for C₄₂H₈₄I₄N₈Yb₂ · toluene: C, 35.73; H, 5.63; N, 6.80. Found: C, 35.24; H, 5.69; N, 7.12.

(Pip)₃trenYb(CH₂SiMe₃)₂ (2): A benzene solution (1 mL) of KCH₂SiMe₃ (97.4 mg, 0.78 mmol) was added to a suspension of complex **1** (300 mg, 0.39 mmol) in 2 mL of benzene at room temperature, resulting in a dark brown solution with gray precipitates. The reaction mixture was stirred for 5 minutes at room temperature, and then the solvent was removed under vacuum. The residue was stirred in 1 mL of hexane, and the volatiles were removed again under vacuum. This operation was repeated for three times to remove benzene completely, and then the residue was extracted with hexane (9 mL). The resulting solution was concentrated to about 3 mL and stood at -35 °C overnight. Complex **2** was isolated as a red solid (142 mg, 53% yield). ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) 2.46 (m, 12H, NCH₂CH₂CH₂), 2.28 (t, ³J_{H-H} = 5.4 Hz, 6H, NCH₂CH₂N), 2.09 (t, ³J_{H-H} = 5.4 Hz, 6H, NCH₂CH₂N), 1.50 (m, 12H, NCH₂CH₂CH₂), 1.32 (m, 6H, NCH₂CH₂CH₂), 0.52 (s, 18H, YbCH₂SiMe₃), -1.03 (s, 4H, YbCH₂SiMe₃). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm) 53.7 (NCH₂CH₂CH₂), 52.2 (NCH₂CH₂N), 49.0 (NCH₂CH₂N), 23.9 (NCH₂CH₂CH₂), 23.4

(NCH₂CH₂CH₂), 22.4 (YbCH₂SiMe₃), 5.8 (YbCH₂SiMe₃). ¹⁷¹Yb{¹H} NMR (71 MHz, C₆D₆, 25 °C): δ (ppm) 1204.7 (YbCH₂SiMe₃). Anal. Calcd for C₂₉H₆₄N₄Si₂Yb: C, 49.90; H, 9.24; N, 8.03. Found: C, 49.54; H, 9.18; N, 7.97.

[Yb₄(μ₄-PDipp)(μ₂-CH₂SiMe₃)₂{μ₂-P(H)Dipp}₄(THF)₄] (3a) and [Yb₄(μ₄-PDipp)₂(μ₂-CH₂SiMe₃)₂{μ₂-P(H)Dipp}₂(THF)₅] (3b): To a hexane solution (2 mL) of **2** (100 mg, 0.14 mmol) was added a THF/hexane mixture (1:20) (0.5 mL) of DippPH₂ (35.2 mg, 0.18 mmol) at room temperature and stood for 15 minutes. After standing at -35 °C for 12 h, the resulting dark red crystalline solid was collected, washed with hexane (1 mL × 3), and dried under vacuum to afford complex **3a** (32.0 mg, 41% yield). The mother liquor was stored at -35 °C for two days to provide a red crystalline solid, which was collected, washed with cold hexane (1 mL), and dried under vacuum to give complex **3b** (23 mg, 15% yield).

3a, ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) 7.36 (m, 2H, *m*-ArH of DippP), 7.28 (m, 1H, *p*-ArH of DippP), 7.13 (m, 4H, *m*-ArH of DippPH), 7.07 (m, 4H, *m*-ArH of DippPH), 7.02 (m, 2H, *p*-ArH of DippPH), 6.96 (m, 2H, *p*-ArH of DippPH), 4.84 (m, ³J_{C-H} = 6.8 Hz, 2H, CHMe₂ of DippP), 3.94 (m, ³J_{C-H} = 6.7 Hz, 4H, CHMe₂ of DippPH), 3.54 (m, 16H, CH₂CH₂OCH₂CH₂), 3.41 (m, ³J_{C-H} = 7.1 Hz, 6H, CHMe₂ of DippPH, DippPH and DippPH), 2.95 (1H, DippPH), 2.79 (1H, DippPH), 1.80 (d, ³J_{C-H} = 6.8 Hz, 12H, CHMe₂ of DippP), 1.49 (d, ³J_{C-H} = 6.7 Hz, 24H, CHMe₂ of DippPH), 1.25 (d, ³J_{C-H} = 7.1 Hz, 32H, CHMe₂ of DippPH and hexane-*H*), 1.08 (m, 16H, CH₂CH₂OCH₂CH₂), 0.89 (t, ³J_{C-H} = 6.9 Hz, 6H, hexane-*H*), 0.59 (s, 18H, YbCH₂SiMe₃), 0.51 (s, 4H, YbCH₂SiMe₃). ³¹P{¹H} NMR (162 MHz, C₆D₆, 25 °C): δ (ppm) 0.3 (m, DippP), -117.6 (m, ¹J_{Yb-PH} = 535 Hz, ²J_{PH-P} = 48.6 Hz, ²J_{PH-PH} = 17.4 Hz, DippPH), -130.1 (m, ¹J_{Yb-PH} = 502 Hz, ²J_{PH-P} = 64.8 Hz, ²J_{PH-PH} = 17.4 Hz, DippPH). ³¹P NMR (162 MHz, C₆D₆,

25 °C): δ (ppm) 0.3 (m, DippP), -117.6 (m, $^1J_{P-H} = 261.9$ Hz, DippPH), -130.1 (m, $^1J_{P-H} = 202.8$ Hz, DippPH). Poor solubility and instability made it difficult to record $^{13}C\{^1H\}$ and ^{171}Yb NMR spectra of this complex. Anal. Calcd for $C_{84}H_{143}O_4P_5Si_2Yb_4 \cdot \text{hexane}$: C, 48.99; H, 7.17. Found: C, 48.88; H, 7.08.

3b, 1H NMR (400 MHz, d_8 -Toluene, -30 °C): δ (ppm) 7.28 (d, 4H, $^3J_{H-H} = 7.8$ Hz, *m*-ArH of DippP), 7.17 (t, 2H, $^3J_{H-H} = 7.8$ Hz, *p*-ArH of DippP), 4.36 (m, 4H, CHMe₂ of DippP), 3.71 (m, 4H, CHMe₂ of DippP), 3.59 (d, 2H, $^1J_{P-H} = 224.0$ Hz, DippPH), 3.45 (m, 20H, CH₂CH₂OCH₂CH₂), 1.72 (d, 24H, $^3J_{H-H} = 6.7$ Hz, CHMe₂ of DippP), 1.24 (d, 24H, $^3J_{H-H} = 6.7$ Hz, CHMe₂ of DippP), 1.17 (m, 20H, CH₂CH₂OCH₂CH₂), 0.29 (s, 18H, YbCH₂SiMe₃), -0.73 (s, 4H, YbCH₂SiMe₃). $^{31}P\{^1H\}$ NMR (162 MHz, d_8 -Toluene, -30 °C): δ (ppm) -1.2 (m, DippP), -115.0 (m, DippPH). ^{31}P NMR (162 MHz, d_8 -Toluene, -30 °C): δ (ppm) -1.2 (m, DippP), -115.1 (m, $^1J_{P-H} = 224.0$ Hz, DippPH). Low solubility and instability made it difficult to record $^{13}C\{^1H\}$ and ^{171}Yb NMR spectra of this complex. Anal. Calcd for $C_{76}H_{132}O_5P_4Si_2Yb_4 \cdot \text{hexane}$: C, 47.25; H, 7.06. Found: C, 48.06; H, 6.87.

[Yb₅(μ_3 -PDipp)₂(μ_4 -PDipp)₂{ μ_2 -P(H)Dipp}₂(THF)₅] (4): Complex **3a** (50.0 mg, 0.02 mmol) was dissolved in 1 mL of THF/hexane mixture (1:10) solution. After standing at room temperature for 48 h, a purple crystalline solid was isolated, washed with 0.5 mL of hexane, and dried under vacuum to afford complex **4** (25.0 mg, 58% yield). 1H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) 7.19-7.09 (m, overlapped with the residue solvent resonance of the deuterated solvent, 10H, ArH of Dipp), 7.06 (d, 4H, $^3J_{H-H} = 7.6$ Hz, *m*-ArH of DippP), 7.01 (t, 2H, $^3J_{H-H} = 7.5$ Hz, *p*-ArH of DippP), 6.90 (t, 2H, $^3J_{H-H} = 7.5$ Hz, *p*-ArH of DippP), 4.82 (m, 4H, CHMe₂ of DippP), 4.48 (m, 4H, $^3J_{H-H} = 6.9$ Hz, CHMe₂ of DippP), 4.15 (m, 4H, $^3J_{H-H} = 6.8$ Hz,

CHMe₂ of DippPH), 3.21 (d, 2H, ¹J_{P-H} = 218.1 Hz, DippPH), 1.64 (m, 24H, CHMe₂ of DippP), 1.44 (d, 24H, ³J_{H-H} = 6.9 Hz, CHMe₂ of DippP), 1.38 (d, 24H, ³J_{H-H} = 6.8 Hz, CHMe₂ of DippPH). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm) 155.5 (t, ¹J_{P-C} = 23.9 Hz, *i*-ArC of DippP), 151.6 (t, ¹J_{P-C} = 12.5 Hz, *i*-ArC of DippP), 150.7 (*o*-ArC of DippP), 150.3 (t, ²J_{P-C} = 2.9 Hz, *o*-ArC of DippPH), 149.8 (t, ²J_{P-C} = 4.9 Hz, *o*-ArC of DippP), 140.9 (t, ¹J_{P-C} = 9.95 Hz, *i*-ArC of DippPH), 124.5 (*p*-ArC of DippPH), 122.8 (*m*-ArC of DippP), 122.3 (*m*-ArC of DippPH), 122.1 (*p*-ArC of DippP), 121.5 (*m*-ArC of DippP), 120.8 (*p*-ArC of DippP), 35.5 (CHMe₂ of DippP), 34.6 (t, ³J_{P-C} = 5.5 Hz, CHMe₂ of DippP), 33.8 (t, ³J_{P-C} = 5.6 Hz, CHMe₂ of DippPH), 25.0 (CHMe₂ of DippP), 24.4 (CHMe₂ of DippP), 24.2 (CHMe₂ of DippPH). ³¹P{¹H} NMR (162 MHz, C₆D₆, 25 °C): δ (ppm) 7.2 (m, ¹J_{Yb-P} = 533 Hz, DippP), -20.1 (m, ¹J_{Yb-P} = 703.9 Hz, DippP), -121.7 (m, ¹J_{Yb-PH} = 488.4 Hz, DippPH). ³¹P{¹H} NMR (162 MHz, C₆D₆, 25 °C): δ (ppm) 7.2 (m, ¹J_{Yb-P} = 533 Hz, DippP), -20.1 (m, ¹J_{Yb-P} = 703.9 Hz, DippP), -121.06 (m, ¹J_{Yb-PH} = 488.4 Hz, DippPH). ³¹P NMR (162 MHz, C₆D₆, 25 °C): δ (ppm) 7.2 (m, ¹J_{Yb-P} = 533 Hz, DippP), -20.1 (m, ¹J_{Yb-P} = 703.9 Hz, DippP), -121.7 (m, ¹J_{Yb-PH} = 488.4 Hz, ¹J_{P-H} = 218.1 Hz, DippPH). The poor solubility made it difficult to record ¹⁷¹Yb NMR spectra of this complex. Anal. Calcd for C₉₂H₁₄₄O₅P₆Yb₅: C, 46.40; H, 6.10. Found: C, 46.77; H, 5.97.

[Yb₆P(μ₃-PDipp)₄(μ₄-PDipp)₂(IMe₄)₄] (5): A benzene solution (2 mL) of 1,3,4,5-tetramethylimidazolin-2-ylidene (IMe₄) (13.2 mg, 0.11 mmol) was added to **4** (50.0 mg, 0.021 mmol) in 2 mL of benzene at room temperature. After standing at 60 °C for 24 h, the resulting violet crystalline solid was collected, washed with toluene (1 mL × 3), and dried under vacuum to afford complex **5** (21.0 mg, 42% yield). ³¹P solid-state NMR (162 MHz, 25 °C): δ (ppm) 12.4 (s, DippP), 6.5 (s, DippP) -20.8 (s, DippP). ³¹P{¹H} solid-state NMR (162 MHz, 25 °C): δ

(ppm) 12.3(s, DippP), 6.5 (s, DippP), -20.6 (s, DippP). Anal. Calcd for C₁₀₀H₁₅₀N₈P₆Yb₆ · 2 benzene: C, 47.29; H, 5.74; N, 3.94. Found: C, 47.43; H, 5.69; N, 3.76.

Reaction of Complex 4 with 1 equiv. of AdNC: A benzene solution (1 mL) of AdNC (4.8 mg, 0.03 mmol) was added to complex 4 (71.4 mg, 0.03 mmol) in 1 mL of benzene at room temperature. The reaction mixture was stood for 20 minutes at room temperature. The volatiles of the reaction solution were removed under vacuum, the residue was dissolved in hexane (1 mL). The hexane solution was stored at -35 °C for 12 h, the resulting purple crystalline solid was collected, washed with cold hexane (1 mL), and dried under vacuum to afford complex 6 (58.4 mg, 82% yield). ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) 7.21-6.89 (m, overlapped with C₆D₆, ArH of DippP), 4.57 (m, 4H, CHMe₂ of DippP), 4.40 (m, 2H, CHMe₂ of DippP), 4.32 (m, 2H, CHMe₂ of DippP), 4.11 (m, 4H, CHMe₂ of DippP), 3.50 (d, 2H, ¹J_{P-H} = 232.1 Hz, DippPH), 3.24 (m, 12H, CH₂CH₂OCH₂CH₂), 3.19 (d, 2H, ¹J_{P-H} = 220.9 Hz, DippPH), 1.98 (m, 3H, NCCH₂CHCH₂), 1.83 (m, 6H, NCCH₂CHCH₂), 1.64-1.43 (m, 60H, CHMe₂ of DippP and NCCH₂CHCH₂), 1.40 (d, 12H, ³J_{H-H} = 6.8 Hz, CHMe₂ of DippP), 1.31 (m, 3H, NCCH₂CHCH₂), 1.06 (m, 12H, CH₂CH₂OCH₂CH₂). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm) 154.7 (d, ¹J_{P-C} = 39.6 Hz, *i*-ArC of DippP), 152.5 (d, ²J_{P-C} = 4.7 Hz, *o*-ArC of DippP), 151.2 (*o*-ArC of DippP), 150.0 (d, ¹J_{P-C} = 12.0 Hz, *i*-ArC of DippP), 149.8 (*o*-ArC of DippP), 149.6 (d, ²J_{P-C} = 6.7 Hz, *o*-ArC of DippP), 146.5 (d, ¹J_{P-C} = 113.4 Hz, PC(=NAd)), 140.6 (d, ¹J_{P-C} = 16.6 Hz, *i*-ArC of DippP), 139.0 (d, ¹J_{P-C} = 17.2 Hz, *i*-ArC of DippP), 126.1 (*p*-ArC of DippP), 124.6 (*p*-ArC of DippP), 123.2 (*m*-ArC of DippP), 122.7 (*m*-ArC of DippP), 122.6 (*m*-ArC of DippP), 122.4 (*m*-ArC of DippP), 121.7 (*p*-ArC of DippP), 121.0 (*p*-ArC of DippP), 69.1 (CH₂CH₂OCH₂CH₂), 59.4 (NCCH₂CHCH₂), 42.7 (NCCH₂CHCH₂), 36.8

(NCCH₂CHCH₂), 35.5 (CHMe₂ of DippP), 34.6 (m, CHMe₂ of DippP), 34.4 (d, ³J_{P-C} = 9.2 Hz, CHMe₂ of DippP), 33.7 (d, ³J_{P-C} = 9.9 Hz, CHMe₂ of DippP), 30.5 (NCCH₂CHCH₂), 26.5 (CHMe₂ of DippP), 25.1 (CH₂CH₂OCH₂CH₂), 24.9 (CHMe₂ of DippP), 24.3 (CHMe₂ of DippP), 24.2 (CHMe₂ of DippP), 23.7 (CHMe₂ of DippP), 22.5 (CHMe₂ of DippP). ³¹P{¹H} NMR (162 MHz, C₆D₆, 25 °C): δ (ppm) 3.9 (m, DippP), -29.7 (m, DippP), -115.1 (m, ¹J_{Yb-P} = 543.7 Hz, DippPH), -125.4 (m, ¹J_{Yb-P} = 495.6 Hz, DippPH). ³¹P NMR (162 MHz, C₆D₆, 25 °C): δ (ppm) 3.9 (m, ¹J_{Yb-P} = 544.3 Hz), -29.7 (m, DippP), -115.1 (m, ¹J_{Yb-P} = 543.7 Hz, ¹J_{P-H} = 232.1 Hz, DippPH), -125.4 (m, ¹J_{Yb-P} = 495.6 Hz, ¹J_{P-H} = 220.9 Hz, DippPH). ¹⁷¹Yb{¹H} NMR (87 MHz, C₆D₆, 25 °C): δ (ppm) 1286.9 (qd, ¹J_{PH-Yb} = 269.7 Hz, ¹J_{P-Yb} = 579.4 Hz, Yb(μ₄-Pdipp)₂(μ₂-Pdipp)(μ₂-PHdipp) and Yb(μ₄-Pdipp)₂(μ₃-Pdipp)(μ₂-PHdipp)), 1241.4 (m, Yb(μ₄-Pdipp)(μ₃-Pdipp)(μ₂-Pdipp) and Yb(μ₄-Pdipp)(μ₃-Pdipp)), 981.8 (p, ¹J_{P-Yb} = 529.8 Hz, Yb(μ₄-Pdipp)₂(μ₂-PHdipp)₂). Anal. Calcd for C₉₅H₁₄₃NO₃P₆Yb₅: C, 47.58; H, 6.01; N, 0.58. Found: C, 47.84; H, 5.75; N, 0.73.

Reaction of Complex 4 with 10 equiv. of AdNC: A benzene solution (1 mL) of AdNC (48.4 mg, 0.3 mmol) was added to complex 4 (71.4 mg, 0.03mmol) in 1 mL of benzene at room temperature. The reaction mixture was stirred for 24 h at room temperature, and then the solvent was removed under vacuum. The residue was washed with hexane (1 mL × 3) and dried under vacuum to give complex 7 as a dark green solid (46 mg, 41% yield). This complex is paramagnetic. ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) 40.07, 34.04, 33.26, 30.68, 22.19, 21.08, 19.99, 16.38, 14.75, 10.50, 2.49, -3.23, -3.98, -4.69, -6.79, -7.61, -9.30, -9.42, -10.57, -11.39, -12.02, -15.57, -16.89, -16.92, -21.01, -21.46, -25.62, -38.15, -38.76, -69.37. Anal. Calcd for C₁₁₄H₁₅₈N₆P₄Yb₃ · 0.5 hexane: C, 61.13; H, 7.24; N, 3.66. Found: C, 61.55; H, 7.66;

N, 3.82.

X-ray Crystallography:

Single crystals of **1** suitable for single-crystal X-ray diffraction were grown by slow evaporation of toluene solution at room temperature, those of **2**, **3a**, **3b** and **6** were from hexane solutions at -35 °C, those of **4** were by slow evaporation of hexane solution at room temperature, those of **5** were by slow evaporation of benzene solution at room temperature, those of **7** were from slow evaporation the hexane/toluene mixture at room temperature. The crystals were mounted under a nitrogen atmosphere on a glass fiber at low temperature. Data collections of **1–7** were performed on a XtaLAB Synergy R, DW system, HyPix with Mo K α radiation (λ = 0.71073 Å). The CrysAlisPro package was used to determine the unit cell parameters. Empirical absorption correction was applied using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.⁸ The structure was solved with the ShelXT structure solution program using Intrinsic Phasing and refined with the ShelXL refinement package using Least Squares minimization.⁹ Hydrogen atoms were placed at calculated positions and were included in the structure calculation. Calculations were carried out using the SHELXL-2018 and Olex2 program.^{10,11} Crystallographic data and refinement parameters are listed in Table S1. CCDC 2466216 (for **1**), 2466217 (for **2**), 2466218 (for **3a**), 2525567 (for **3b**), 2466219 (for **4**), 2466220 (for **5**), 2525568 (for **6**), and 2525569 (for **7**) contain the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe [Access Structures](#) service

Table S1 Crystallographic data and refinement parameters.

	0.5(1)·0.5 toluene	2
sum formula	C _{24.5} H ₄₅ I ₂ N ₄ Yb	C ₂₉ H ₆₄ N ₄ Si ₂ Yb
fw	822.48	698.06
color	green	red
crystal system	monoclinic	orthorhombic
space group	<i>P2₁/c</i>	<i>Pca2₁</i>
a, Å	9.0815(3)	17.5071(3)
b, Å	14.3166(4)	15.5743(2)
c, Å	22.1543(7)	25.7310(3)
α, deg	90	90
β, deg	96.580(3)	90
γ, deg	90	90
V, Å ³	2861.46(15)	7015.84(17)
Z	2	8
D _{calcd} , (mg/m ³)	1.912	1.322
F(000)	1584	2912
T(K)	173	173
θ range, deg	1.851, 25.027	1.921, 31.139
no. of refns collected	26943	81582
no. of unique refns	5052	17791
no. of obsd refns (I > 2σ(I))	4307	15136
No. of params	253	662
Final R, Rw (I > 2σ(I))	0.0403, 0.1029	0.0241, 0.0487
Goodness-of-fit on F ²	1.038	1.021
Δρ _{max} , min, eÅ ⁻³	1.79, -0.95	0.84, -0.68

	3a ·hexane	3b ·hexane
sum formula	C ₉₀ H ₁₅₇ O ₄ P ₅ Si ₂ Yb ₄	C ₈₂ H ₁₄₆ O ₅ P ₄ Si ₂ Yb ₄
fw	2206.34	2084.20
color	red	red
crystal system	triclinic	triclinic
space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
a, Å	14.8703(2)	14.5523(2)
b, Å	14.9904(2)	14.8785(2)
c, Å	23.0767(3)	24.8265(3)
α , deg	84.8990(10)	76.6050(10)
β , deg	80.8560(10)	80.0700(10)
γ , deg	79.8900(10)	61.8240(10)
V, Å ³	4989.98(12)	4596.99(11)
Z	2	2
D _{calcd} , (mg/m ³)	1.468	1.506
F(000)	2224	2092
T(K)	173	173
θ range, deg	1.879, 25.027	1.691, 25.027
no. of refns collected	94104	87278
no. of unique refns	17614	16247
no. of obsd refns ($I > 2\sigma(I)$)	15359	13495
No. of params	1005	964
Final R, R _w ($I > 2\sigma(I)$)	0.0338, 0.0815	0.0394, 0.0940
Goodness-of-fit on F ²	1.046	1.029
$\Delta\rho$ max, min, eÅ ⁻³	2.59, -0.97	2.62, -1.86

	4	5·2 benzene
sum formula	C ₉₂ H ₁₄₄ O ₅ P ₆ Yb ₅	C ₁₁₂ H ₁₆₂ N ₈ P ₆ Yb ₆
fw	2381.08	2844.55
color	violet	violet
crystal system	triclinic	triclinic
space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
a, Å	12.6396(2)	14.5134(3)
b, Å	14.9690(2)	15.0289(3)
c, Å	25.9073(4)	15.4131(3)
α , deg	92.7310(10)	84.471(2)
β , deg	104.0350(10)	64.199(2)
γ , deg	93.5450(10)	69.869(2)
V, Å ³	4736.35(12)	2836.17(11)
Z	2	1
D _{calcd} , (mg/m ³)	1.670	1.665
F(000)	2352	1400
T(K)	173	173
θ range, deg	2.020, 31.152	1.885, 30.975
no. of refns collected	108075	64805
no. of unique refns	25301	14982
no. of obsd refns ($I > 2\sigma(I)$)	19805	12046
No. of params	1023	615
Final R, R _w ($I > 2\sigma(I)$)	0.0351, 0.0631	0.0382, 0.0961
Goodness-of-fit on F ²	1.009	1.019
$\Delta\rho$ _{max} , min, eÅ ⁻³	1.03, -0.98	6.47, -1.82

	6a ·0.5 hexane	4(7) ·4 hexane· 9 toluene
sum formula	C ₉₈ H ₁₅₀ NO ₃ P ₆ Yb ₅	C ₅₄₃ H ₇₆₀ N ₂₄ P ₁₆ Yb ₁₂
fw	2441.20	10195.71
color	violet	violet
crystal system	triclinic	triclinic
space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
a, Å	14.3375(2)	20.1515(2)
b, Å	15.11949(2)	24.7399(2)
c, Å	27.4075(4)	28.4472(4)
α , deg	77.8500(10)	92.5630(10)
β , deg	81.6100(10)	92.9270(10)
γ , deg	73.4890(10)	109.6680(10)
V, Å ³	5545.12(14)	13306.8(2)
Z	2	1
D _{calcd} , (mg/m ³)	1.462	1.272
F(000)	2418	5266
T(K)	173	150
θ range, deg	1.767, 30.933	1.733, 25.000
no. of refns collected	125160	251905
no. of unique refns	28852	46819
no. of obsd refns ($I > 2\sigma(I)$)	21082	38580
No. of params	1051	3636
Final R, R _w ($I > 2\sigma(I)$)	0.0332, 0.0663	0.0392, 0.0955
Goodness-of-fit on F ²	1.030	1.101
$\Delta\rho$ max, min, eÅ ⁻³	0.90, -0.85	1.65, -0.80

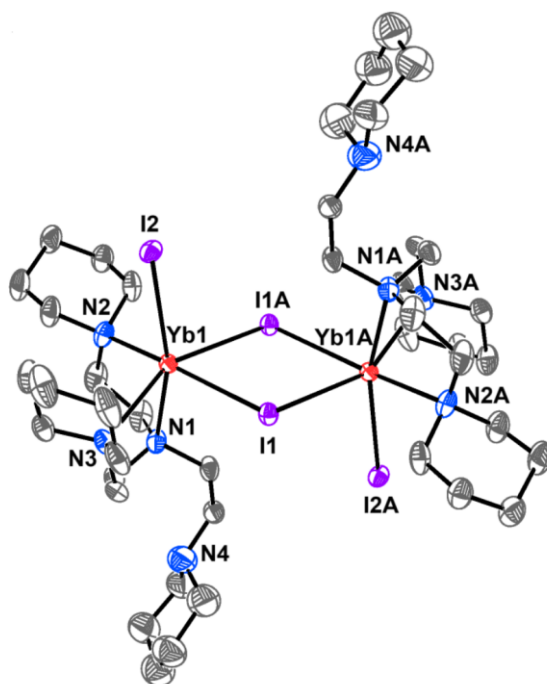


Fig. S1 Molecular structure of complex **1** with ellipsoids at 30% probability level. Hydrogen atoms were omitted for clarity. Selected bond distances [Å] and angles [°]: Yb1–N1 2.544(6), Yb–N2 2.618(7), Yb–N3 2.658(7), Yb–I1 3.1491(6), Yb–I1A 3.2109(6), Yb–I2 3.0712(6), Yb1–I–Yb1(A) 100.048, I1–Yb–I1(A) 79.952.

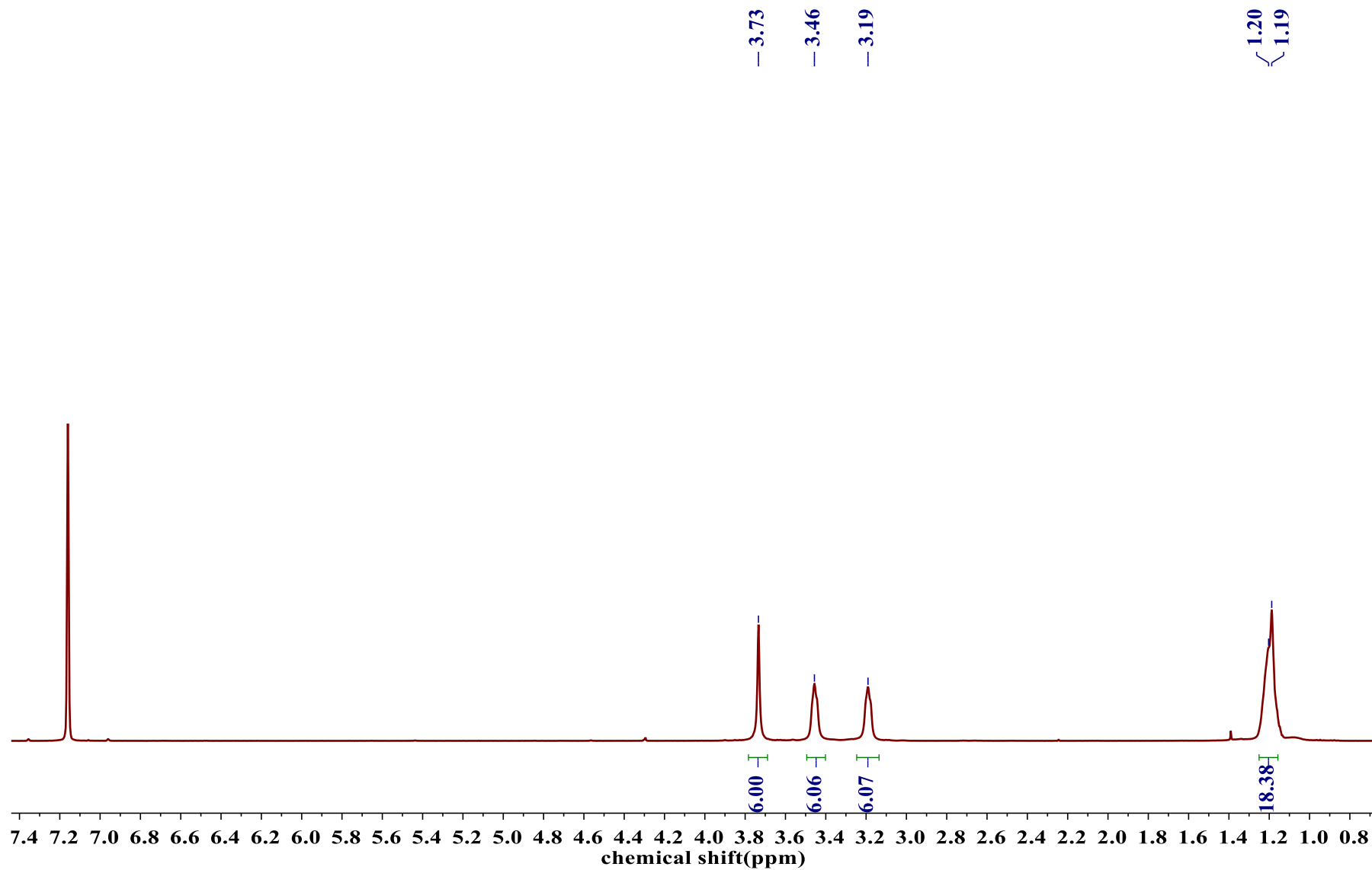


Fig. S2 ^1H NMR spectrum of 2,2,2-nitrilotrisacetyl piperidine (400 MHz, C_6D_6 , 25 $^\circ\text{C}$).

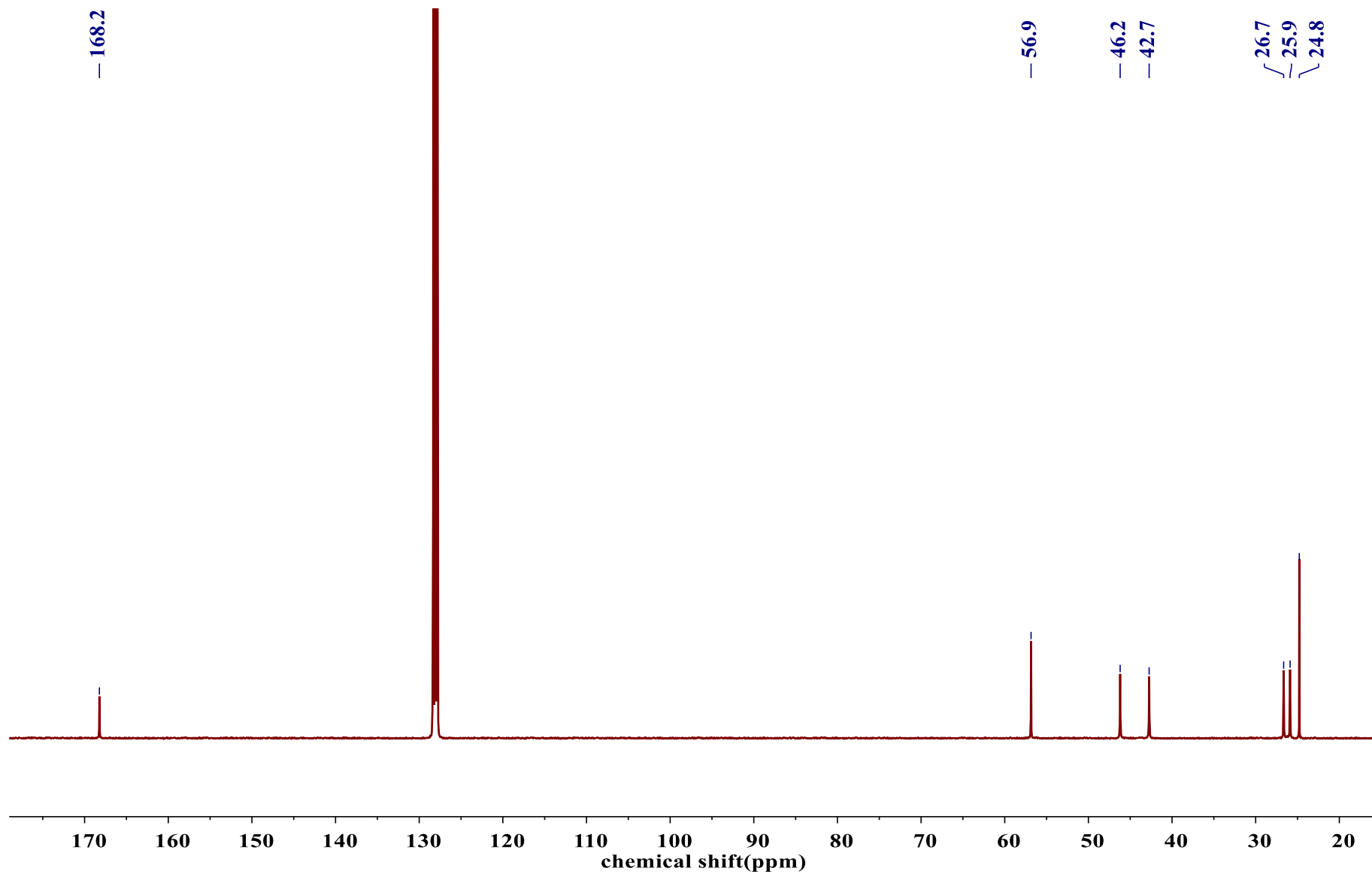


Fig. S3 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 2,2,2-nitrotrisacetyl piperidine (100 MHz, C_6D_6 , 25 °C).

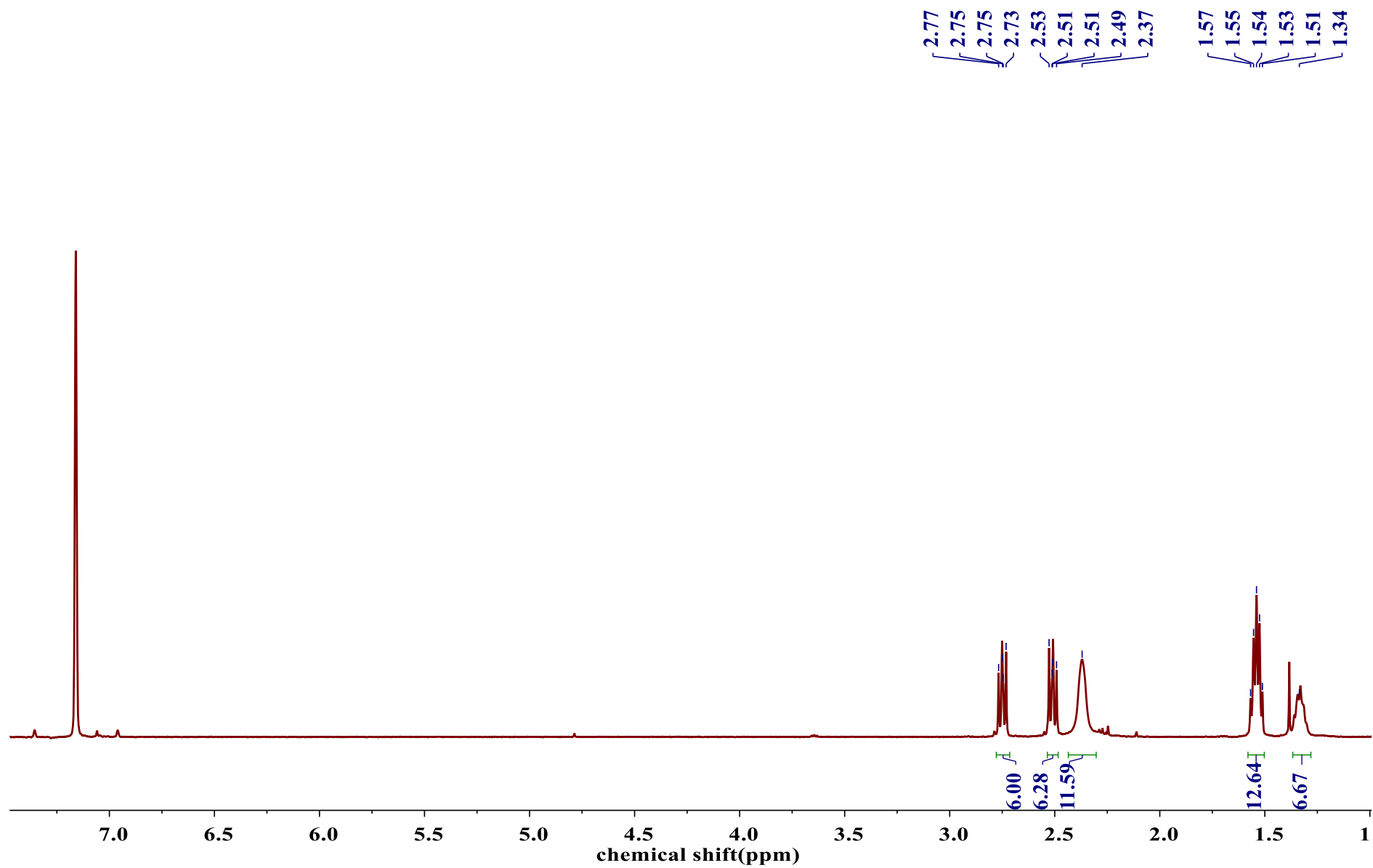


Fig. S4 ^1H NMR spectrum of $(\text{Pip})_3\text{tren}$ (400 MHz, C_6D_6 , 25 $^\circ\text{C}$).

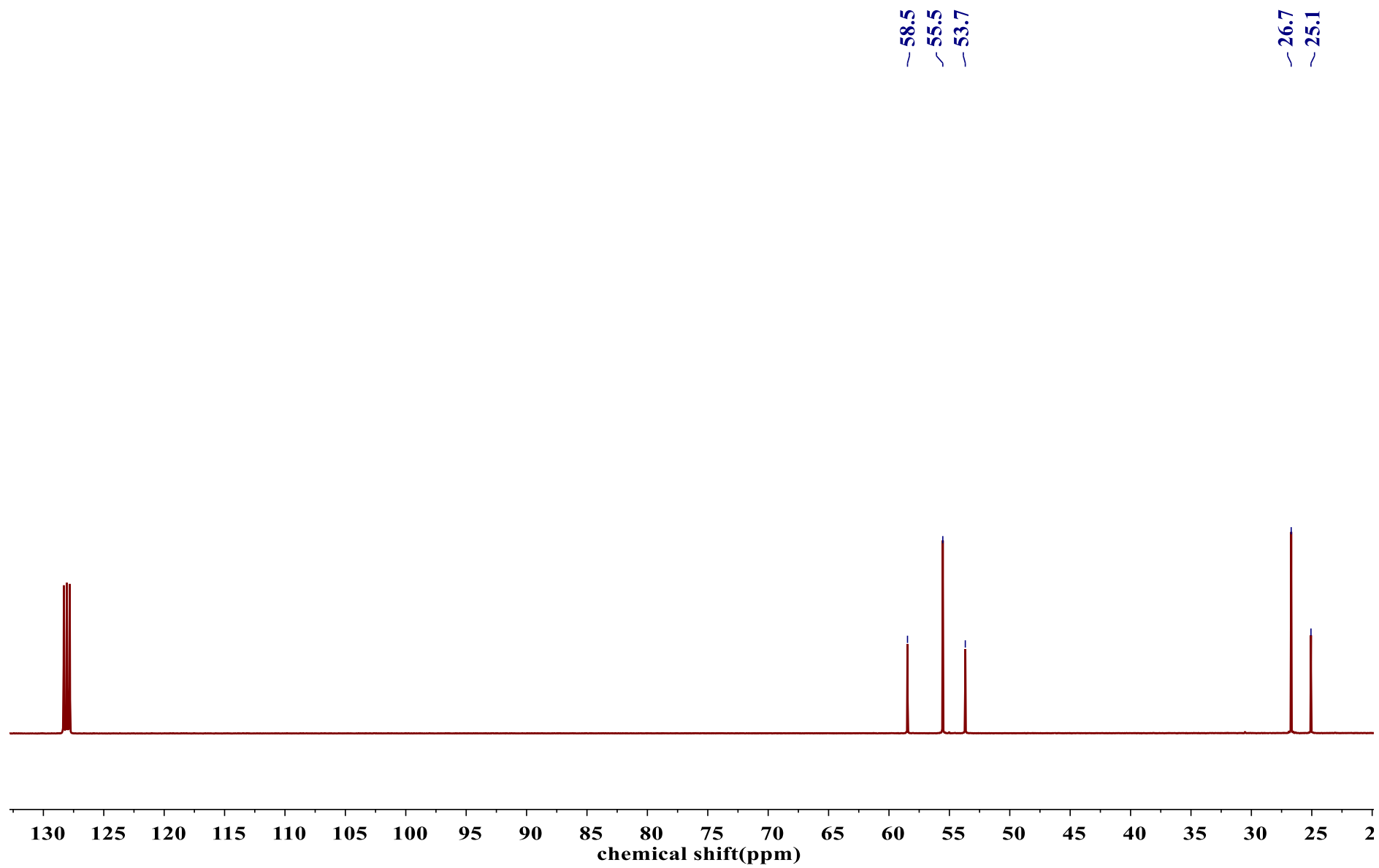


Fig. S5 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $(\text{Pip})_3\text{tren}$ (100 MHz, C_6D_6 , $25\text{ }^\circ\text{C}$).

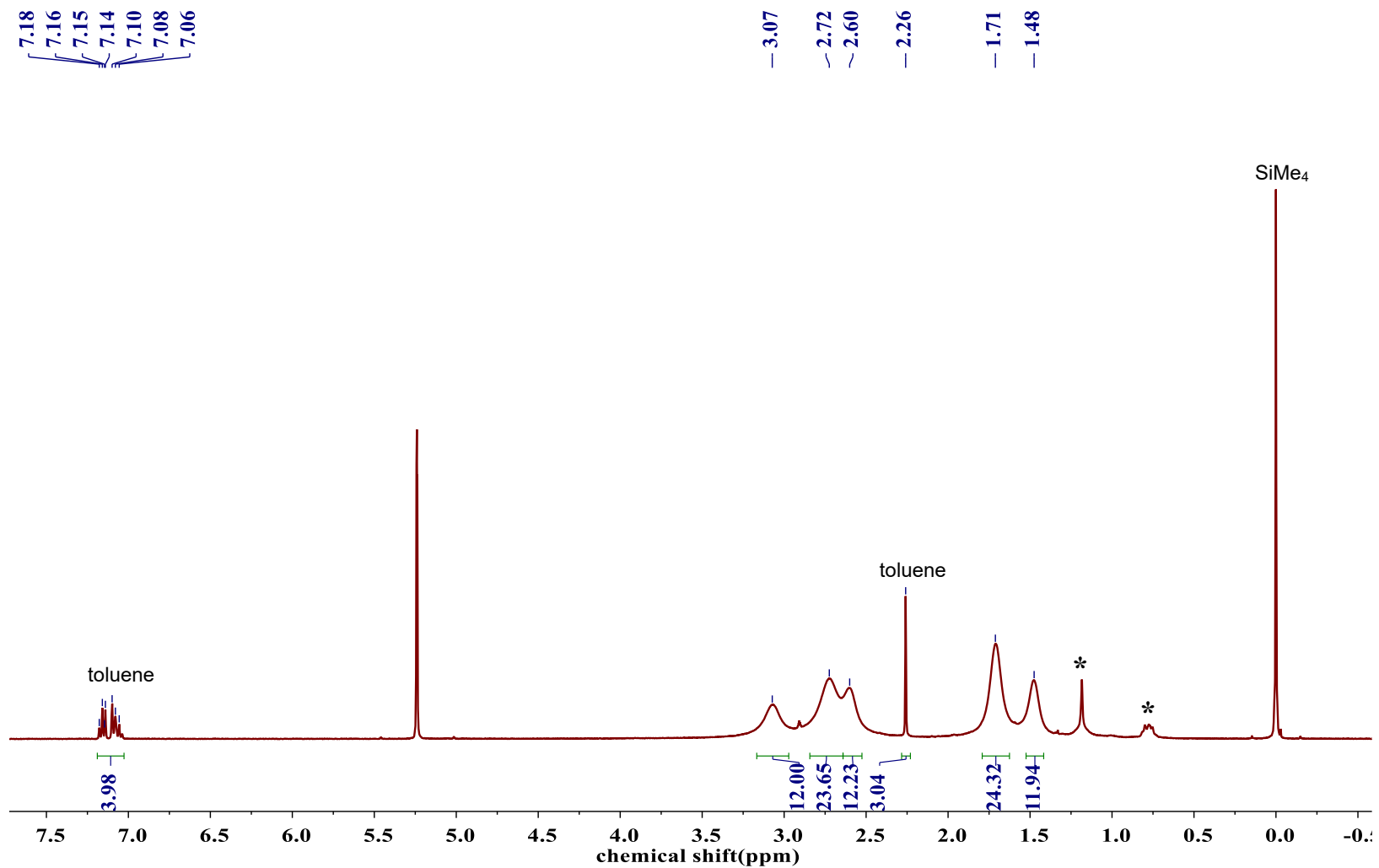


Fig. S6 ¹H NMR spectrum of complex **1** · toluene with SiMe₄ as the internal standard (400 MHz, CD₂Cl₂, 25 °C). Asterisks denote the residue *n*-hexane.

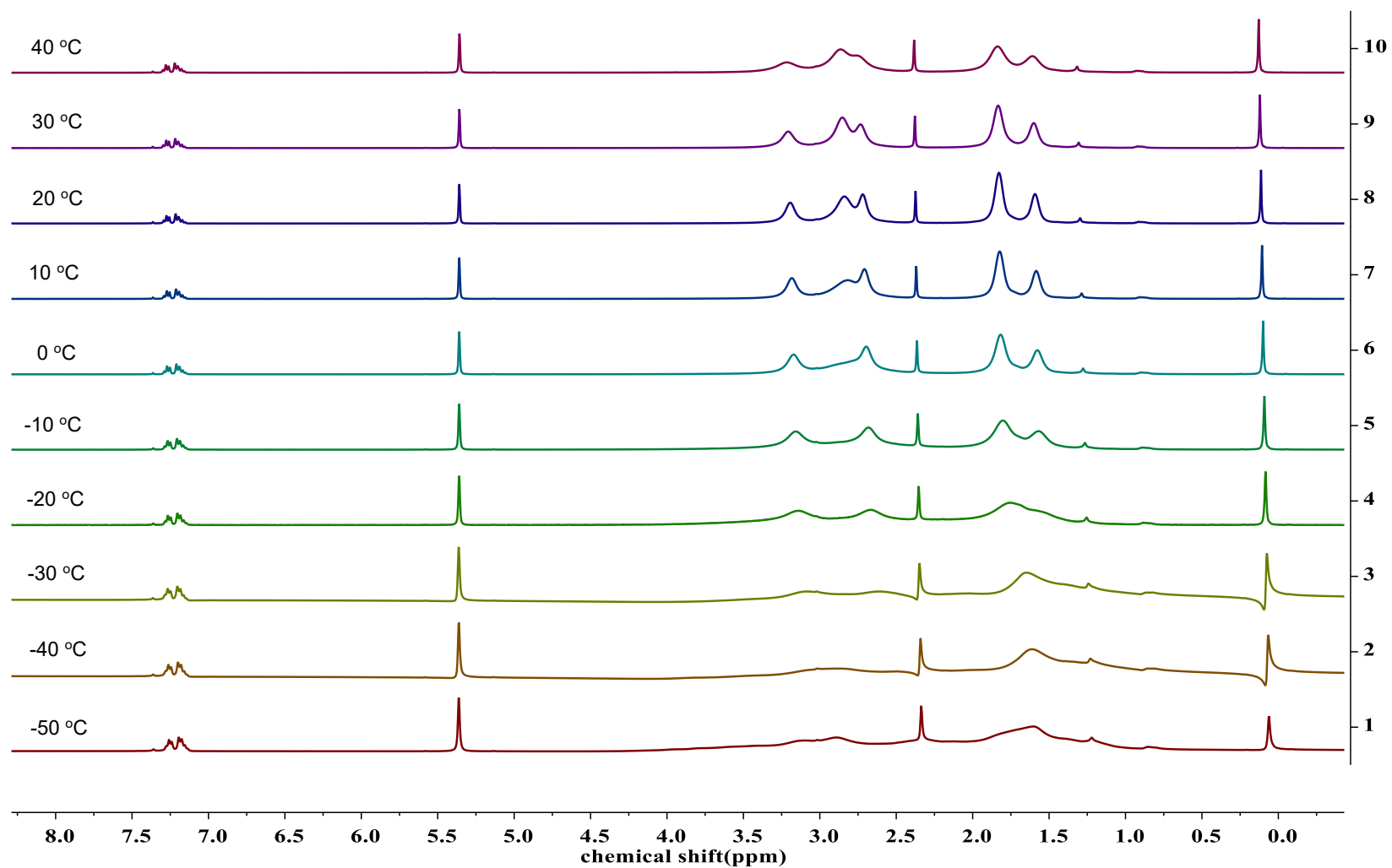


Fig. S7 Variant temperature ¹H NMR spectrum of complex **1** · toluene with SiMe₄ as the internal standard (400 MHz, CD₂Cl₂, -50, -40, -30, -20, -10, 0, 10, 20, 30 and 40 °C).

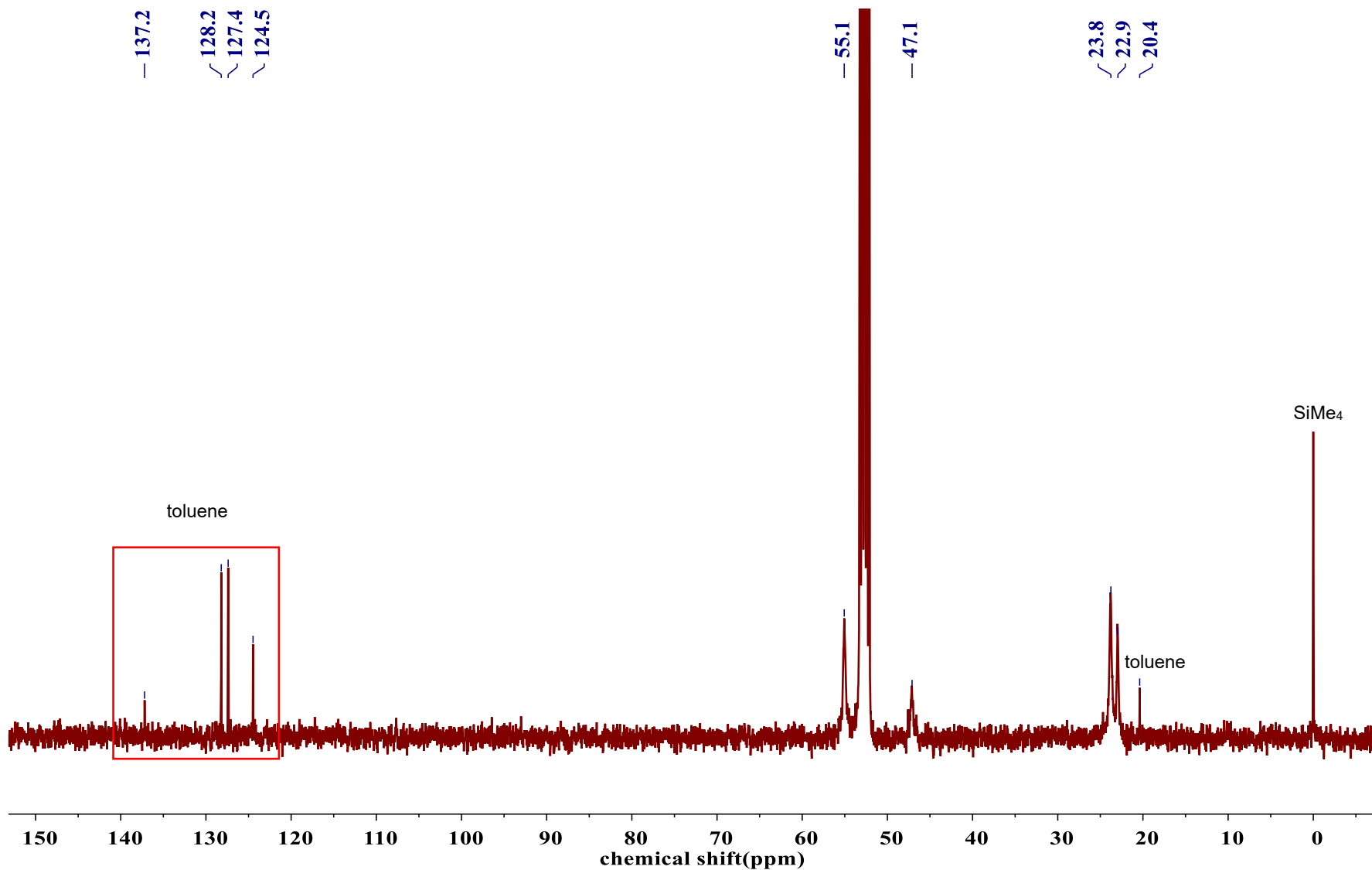


Fig. S8 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex 1 with SiMe₄ as the internal standard (100 MHz, CD₂Cl₂, 25 °C).

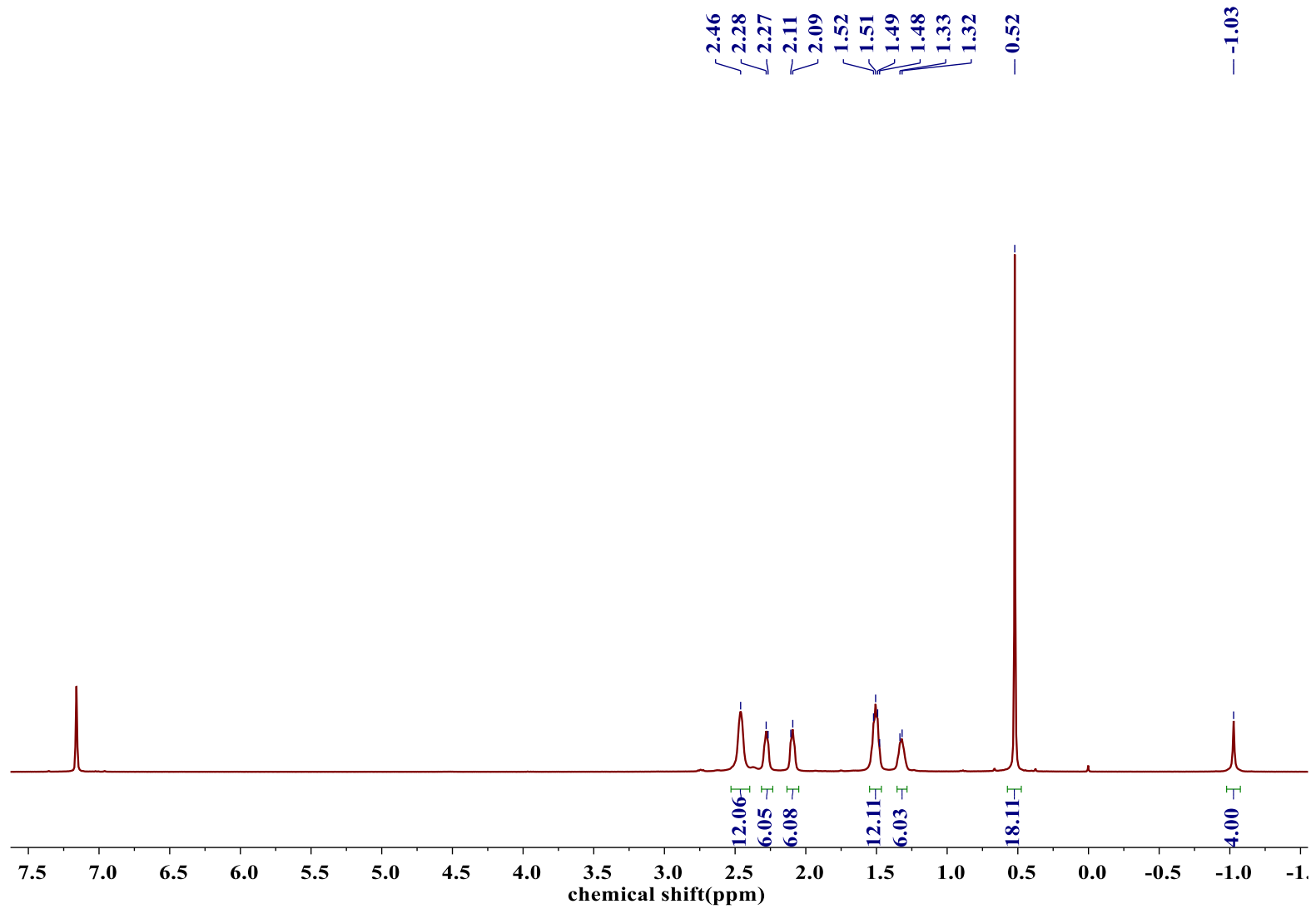


Fig. S9 ^1H NMR spectrum of complex **2** (400 MHz, C_6D_6 , 25 $^\circ\text{C}$).

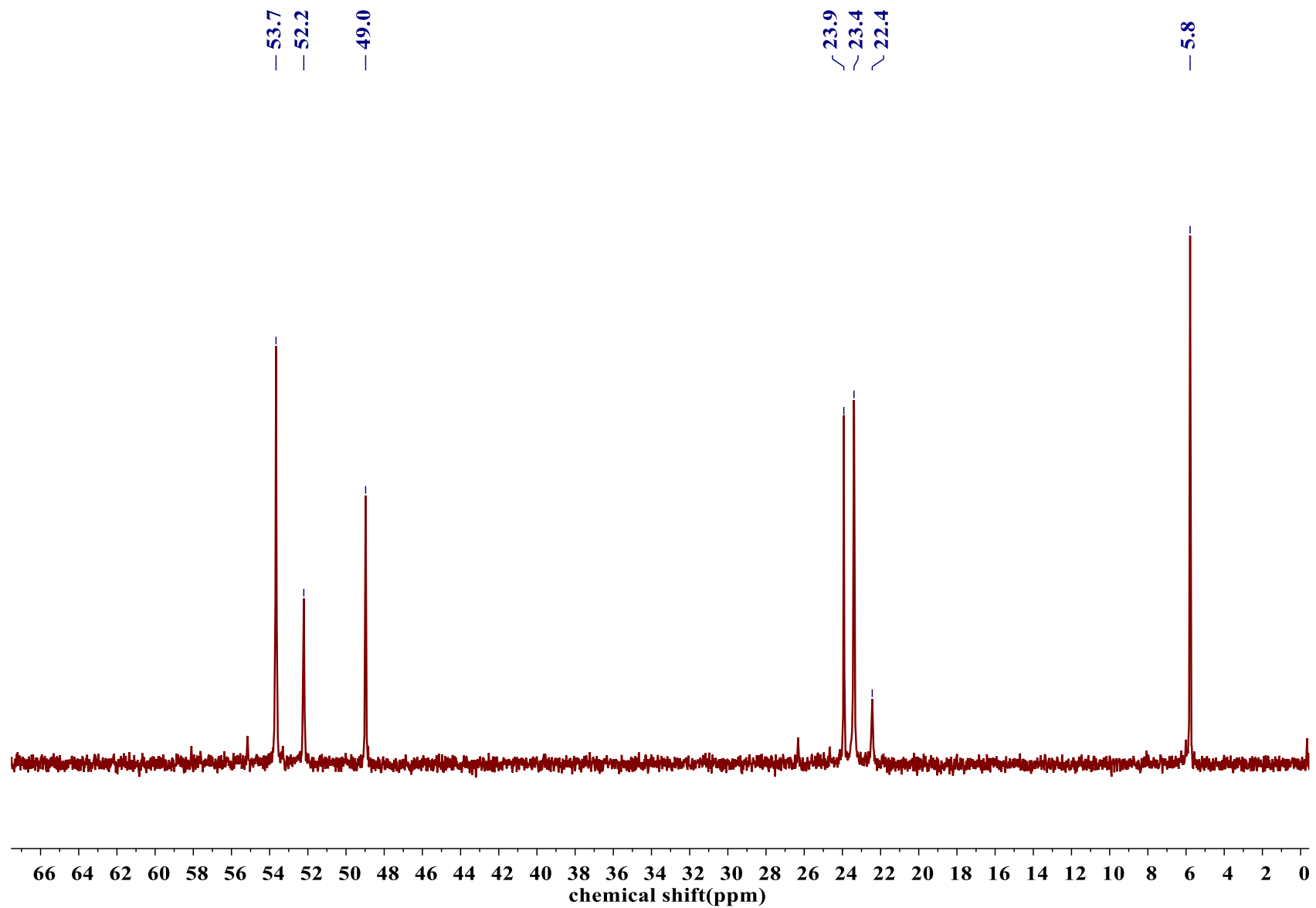


Fig. S10 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex **2** (100 MHz, C_6D_6 , 25 °C).

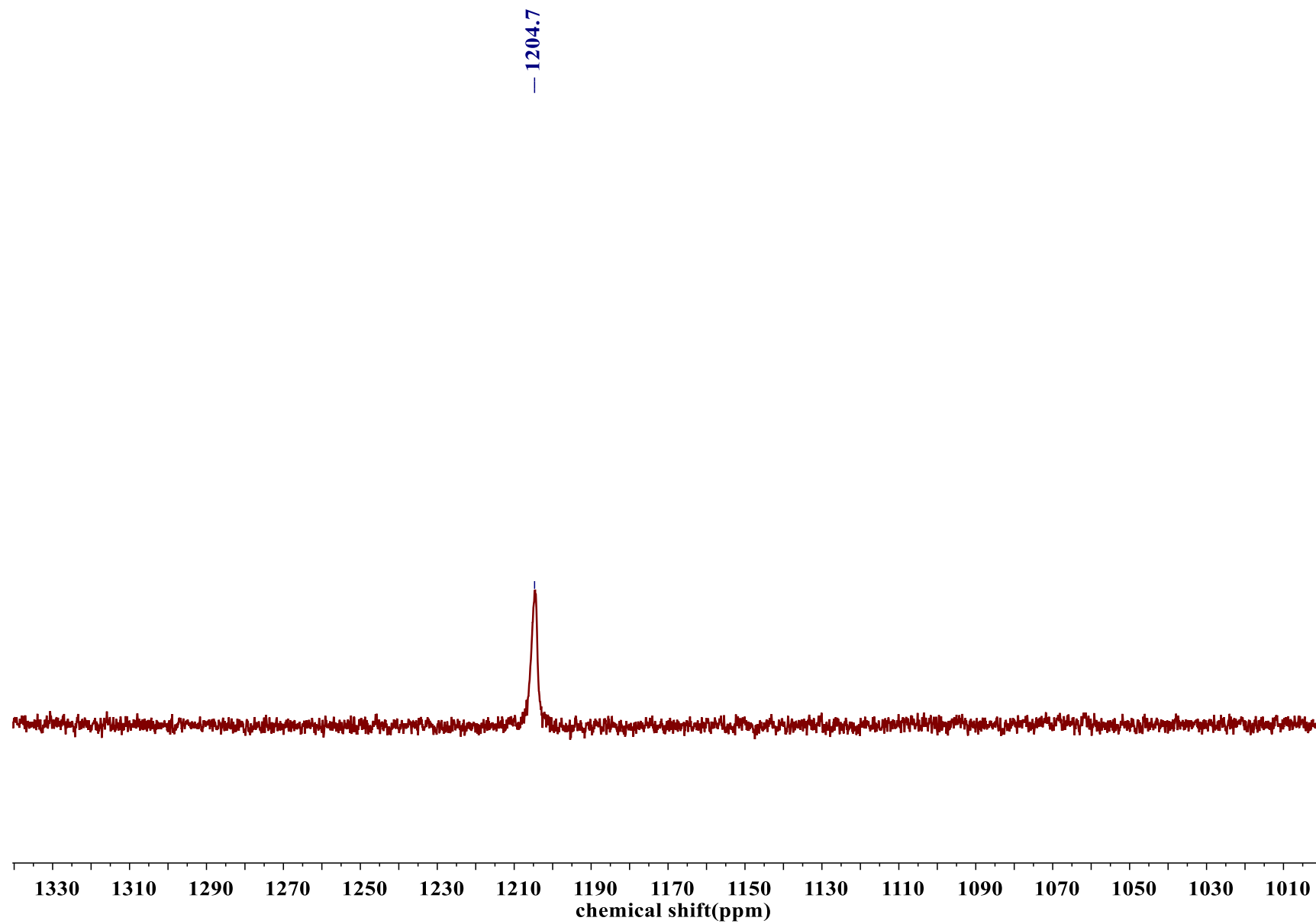


Fig. S11 $^{171}\text{Yb}\{^1\text{H}\}$ NMR spectrum of complex **2** (71 MHz, C_6D_6 , 25 °C).

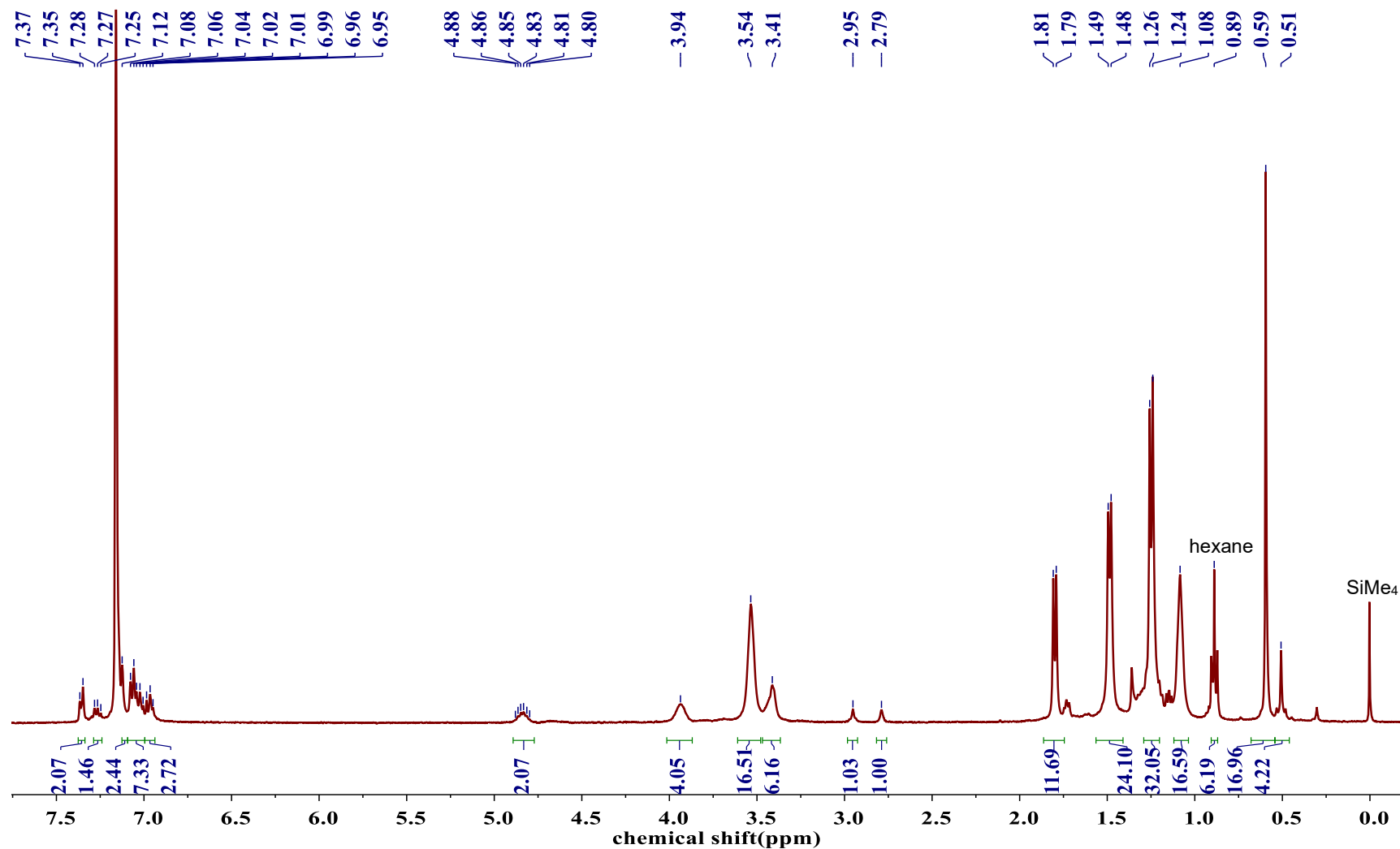


Fig. S12 ¹H NMR spectrum of complex **3a** · hexane (400 MHz, C₆D₆, 25 °C). (A small amount of complex **3** have decomposed, SiMe₄ is one of the decomposition products)

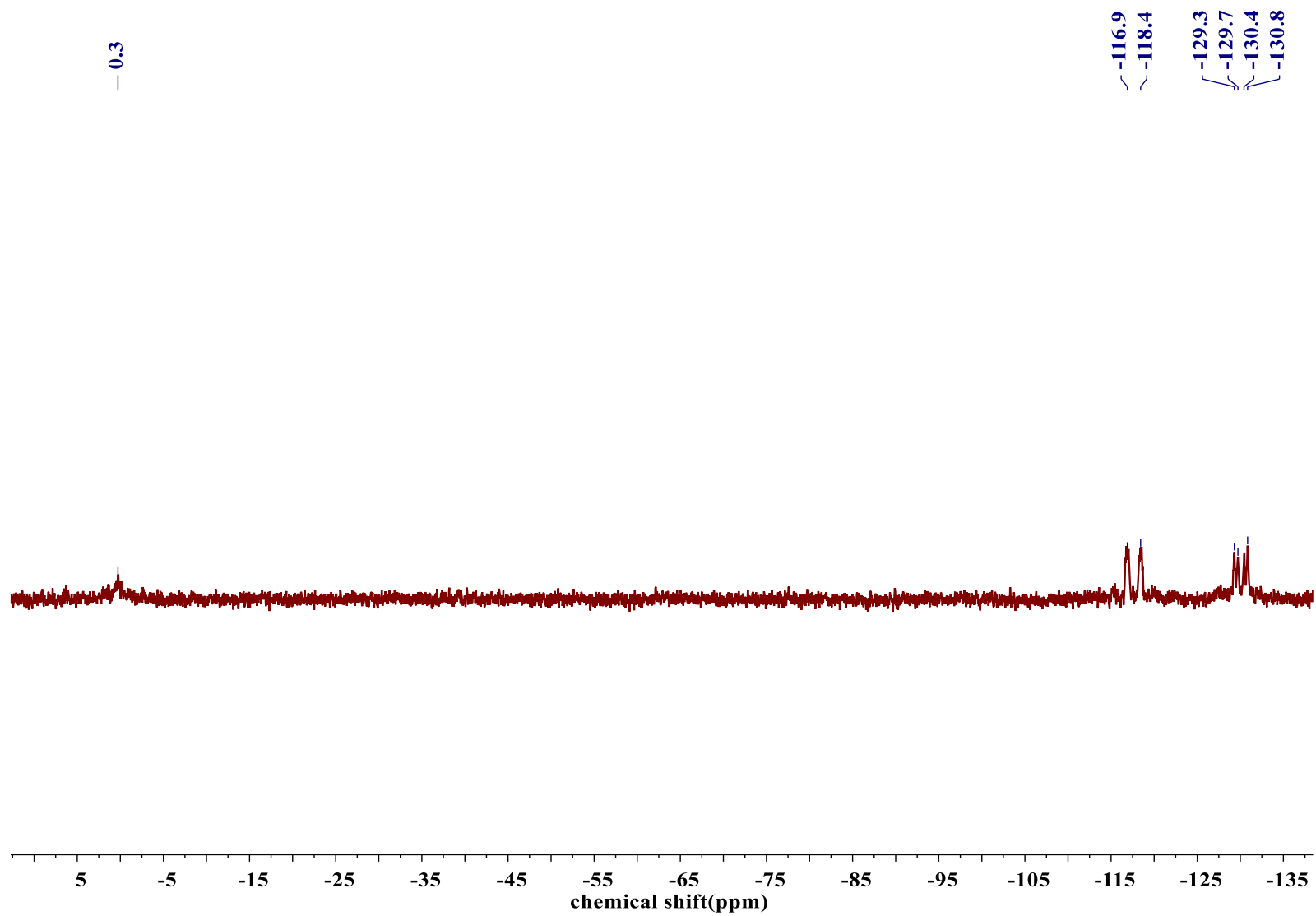


Fig. S13 ^{31}P NMR spectrum of complex 3a (162 MHz, C_6D_6 , 25 °C)

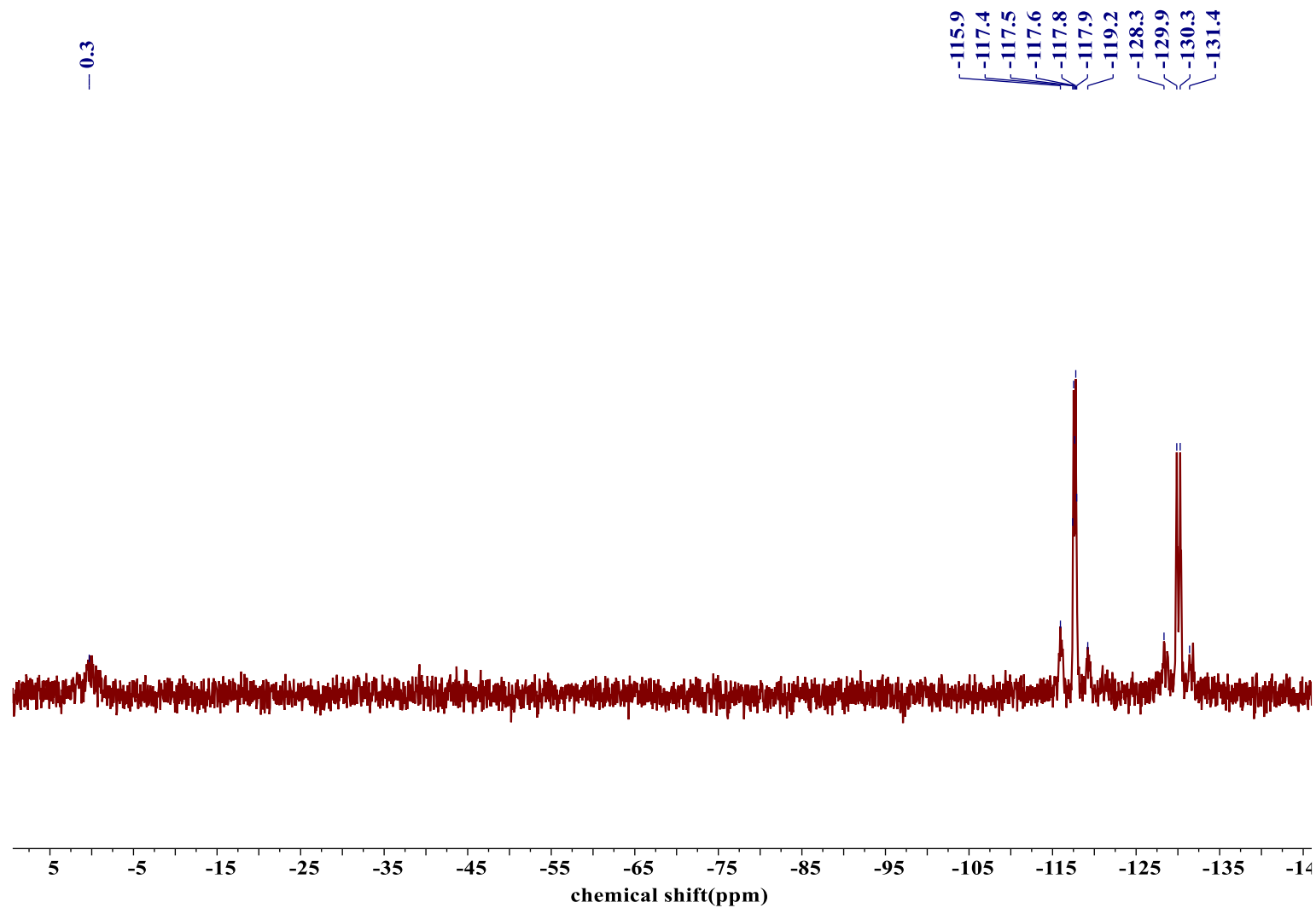


Fig. S14 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **3a** (162 MHz, C_6D_6 , 25 °C)

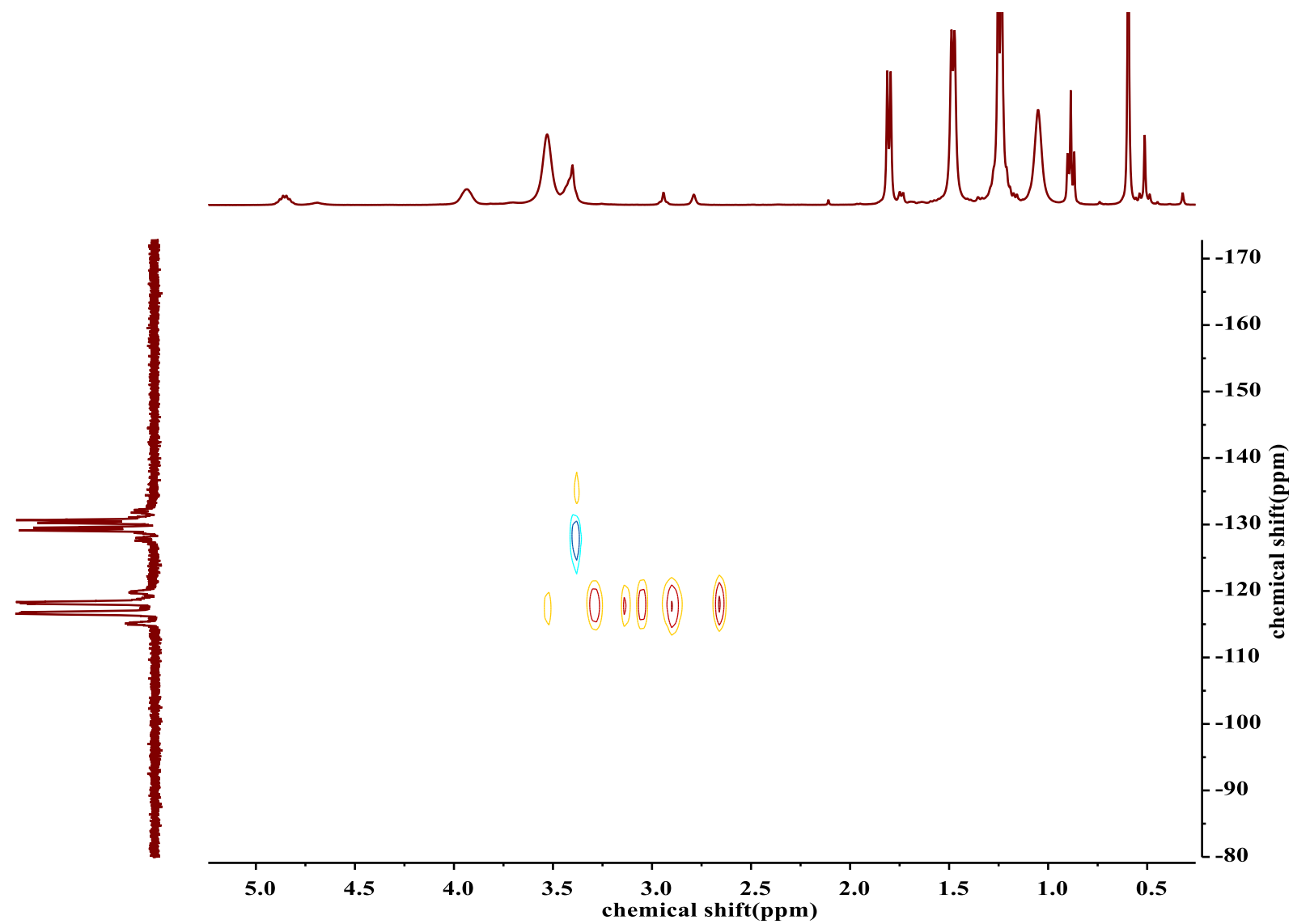


Fig. S15 $^1\text{H}/^{31}\text{P}$ HSQC NMR spectra of complex **3a** (400/162 MHz, C_6D_6 , 25 $^\circ\text{C}$).

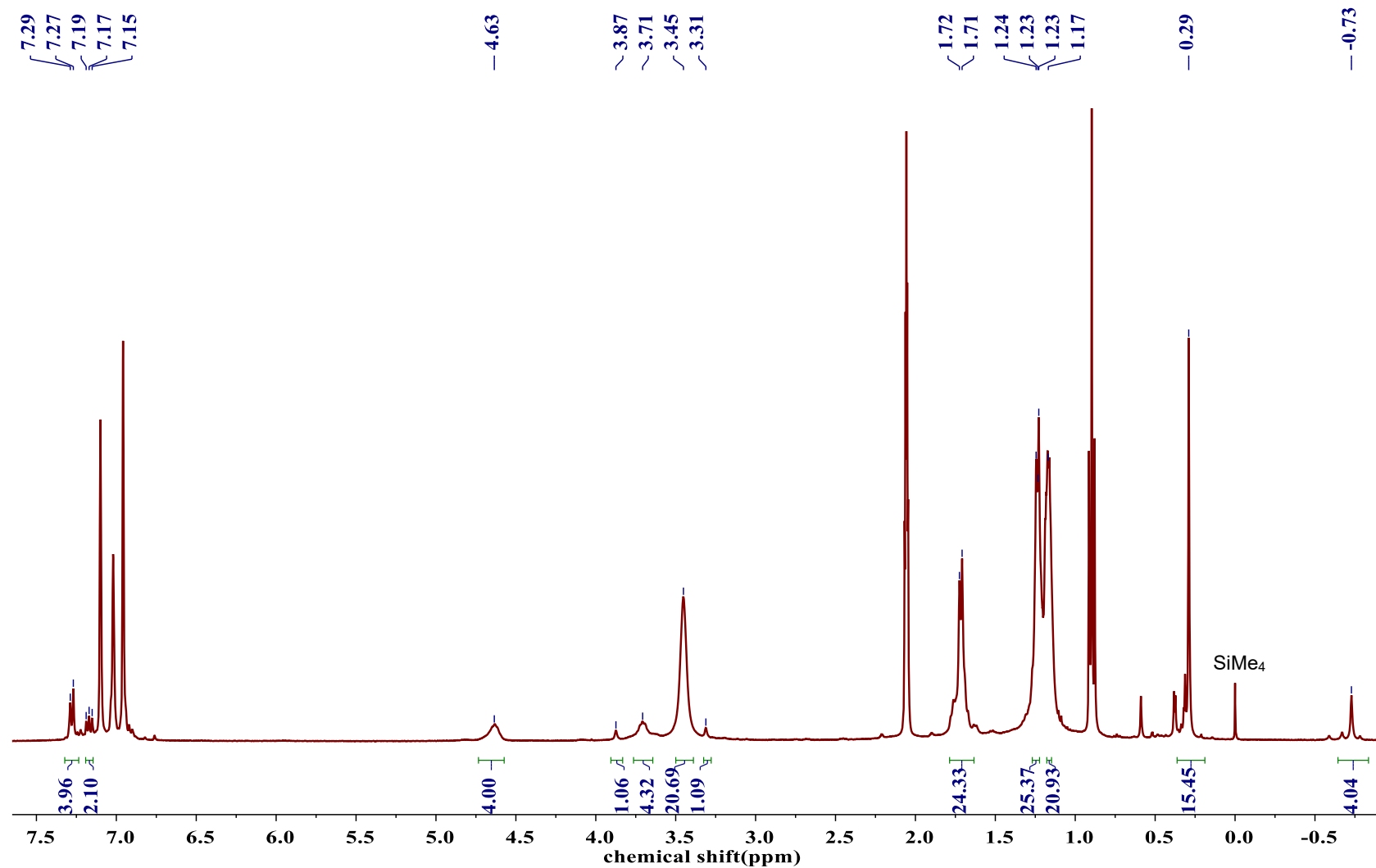


Fig. S16 ¹H NMR spectrum of complex **3b** (400 MHz, *d*₈-toluene, -30 °C). (A small amount of complex **3b** have decomposed, SiMe₄ is one of the decomposition products)

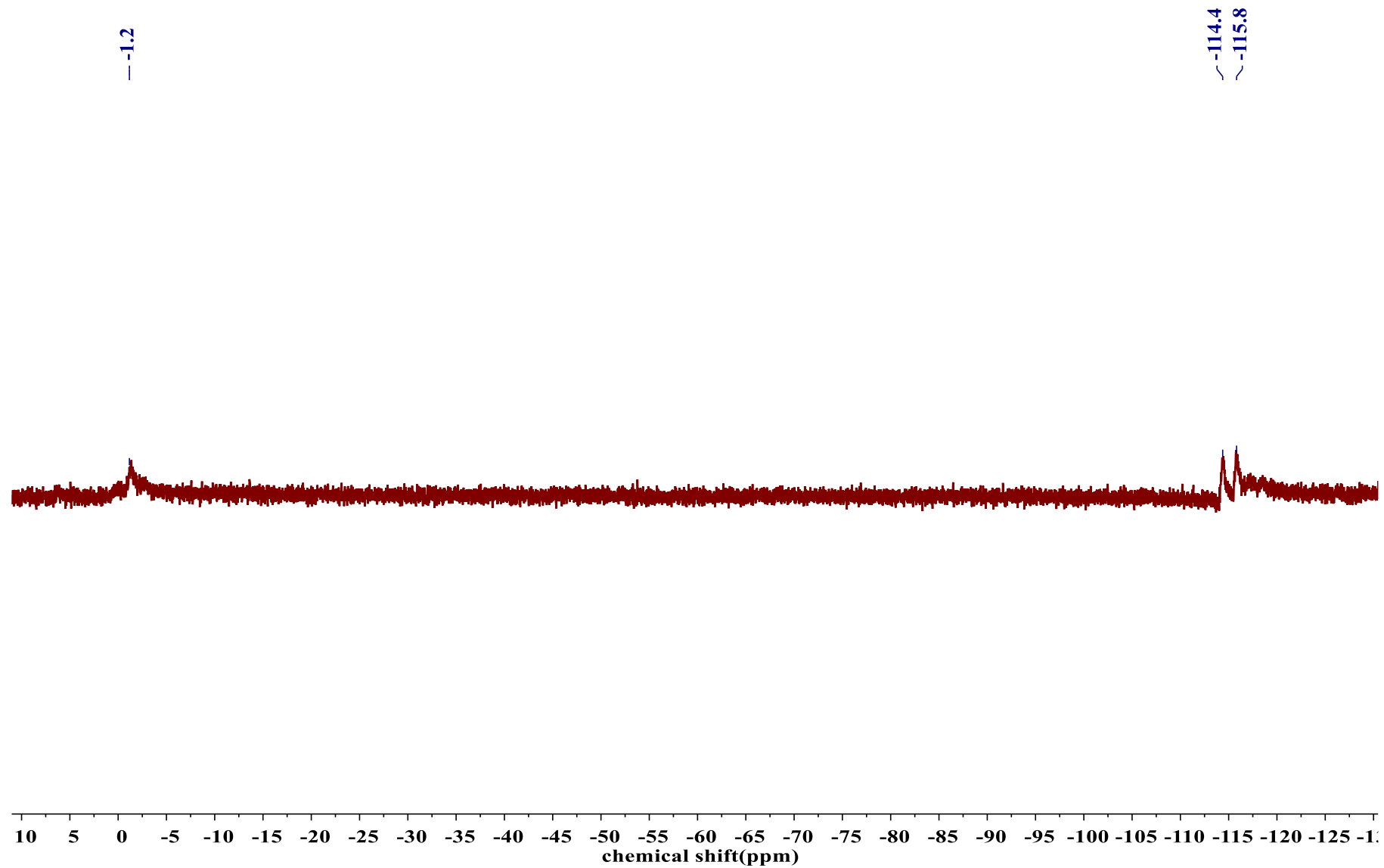


Fig. S17 ^{31}P NMR spectrum of complex **3b** (162 MHz, d_8 -toluene, -30 °C)

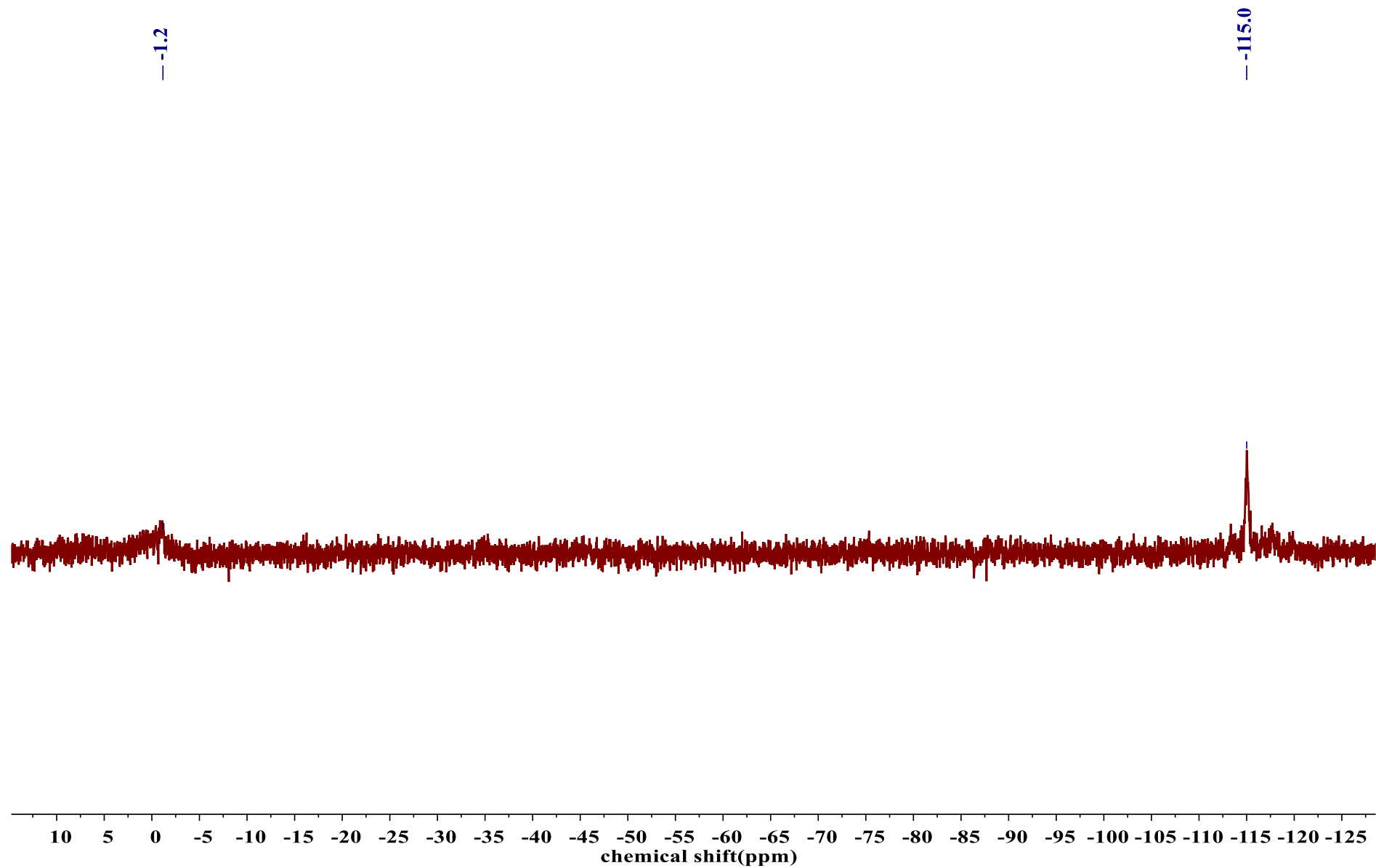


Fig. S18 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **3b** (162 MHz, d_8 -toluene, -30 °C)

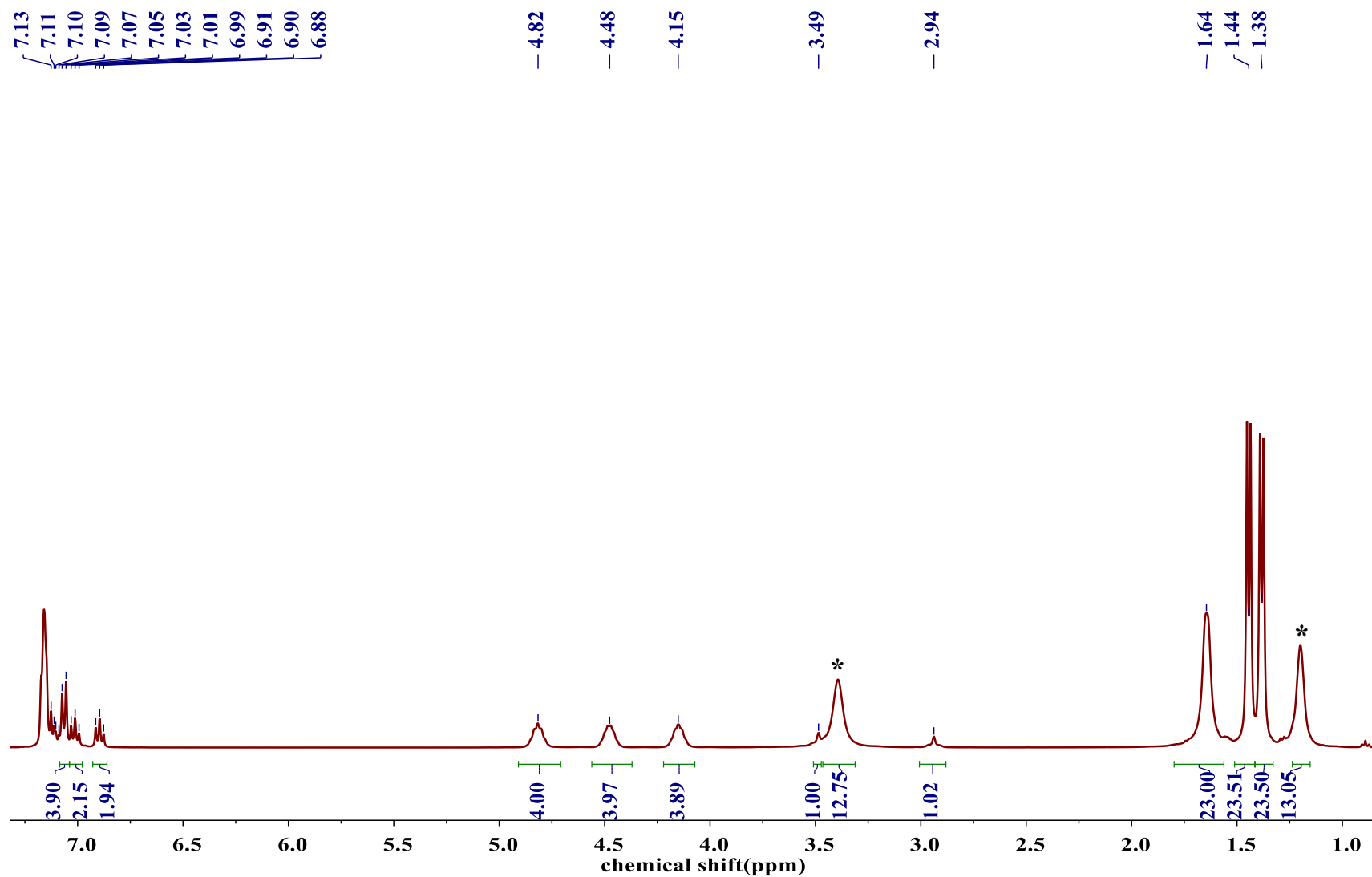


Fig. S19 ^1H NMR spectrum of complex **4** (400 MHz, C_6D_6 with a drop of d_8 -THF, 25 $^\circ\text{C}$). Asterisks denote THF.

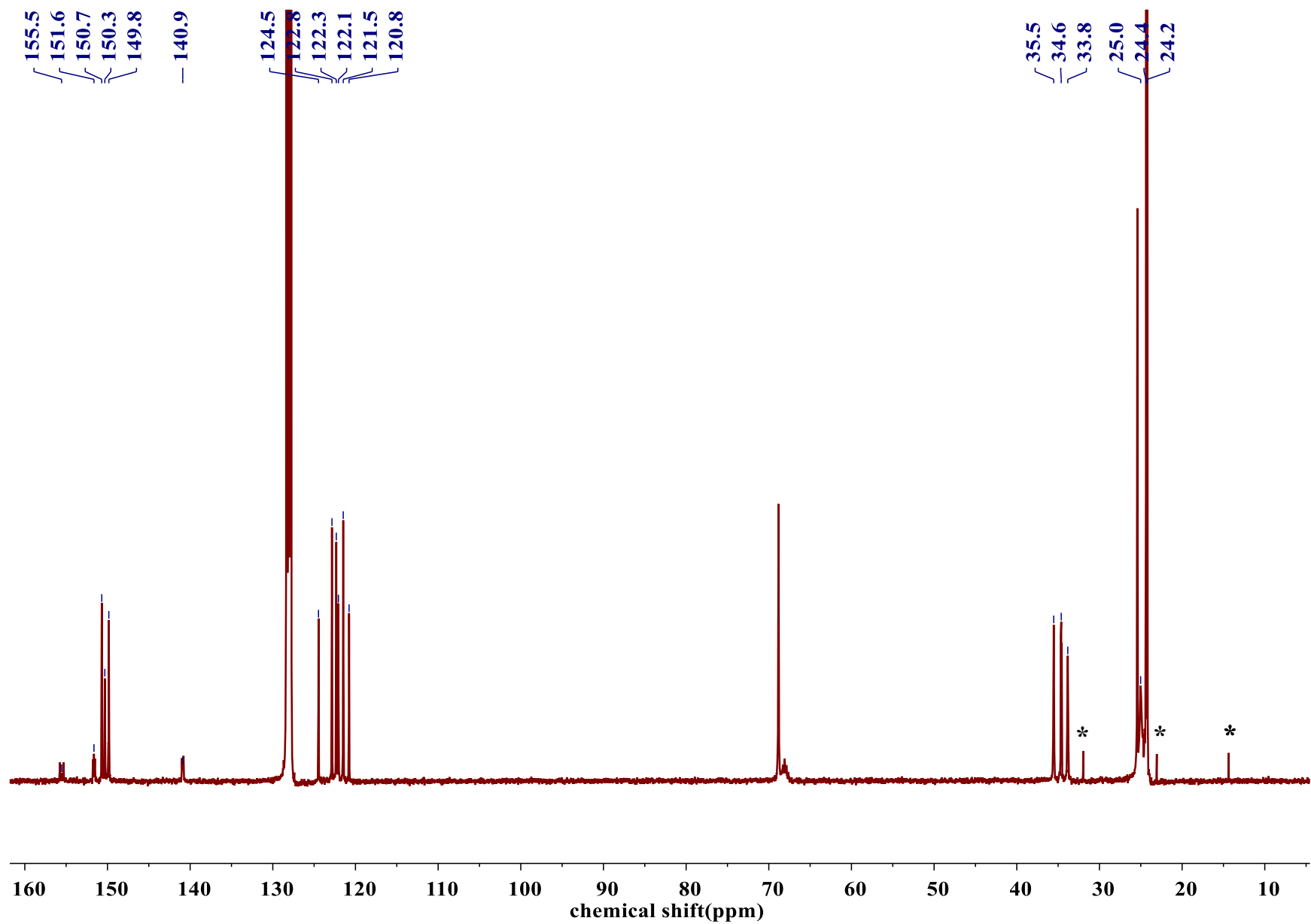


Fig. S20 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex **4** (100 MHz, C_6D_6 with a drop of d_8 -THF, 25 °C). Asterisks denote the residue *n*-hexane.

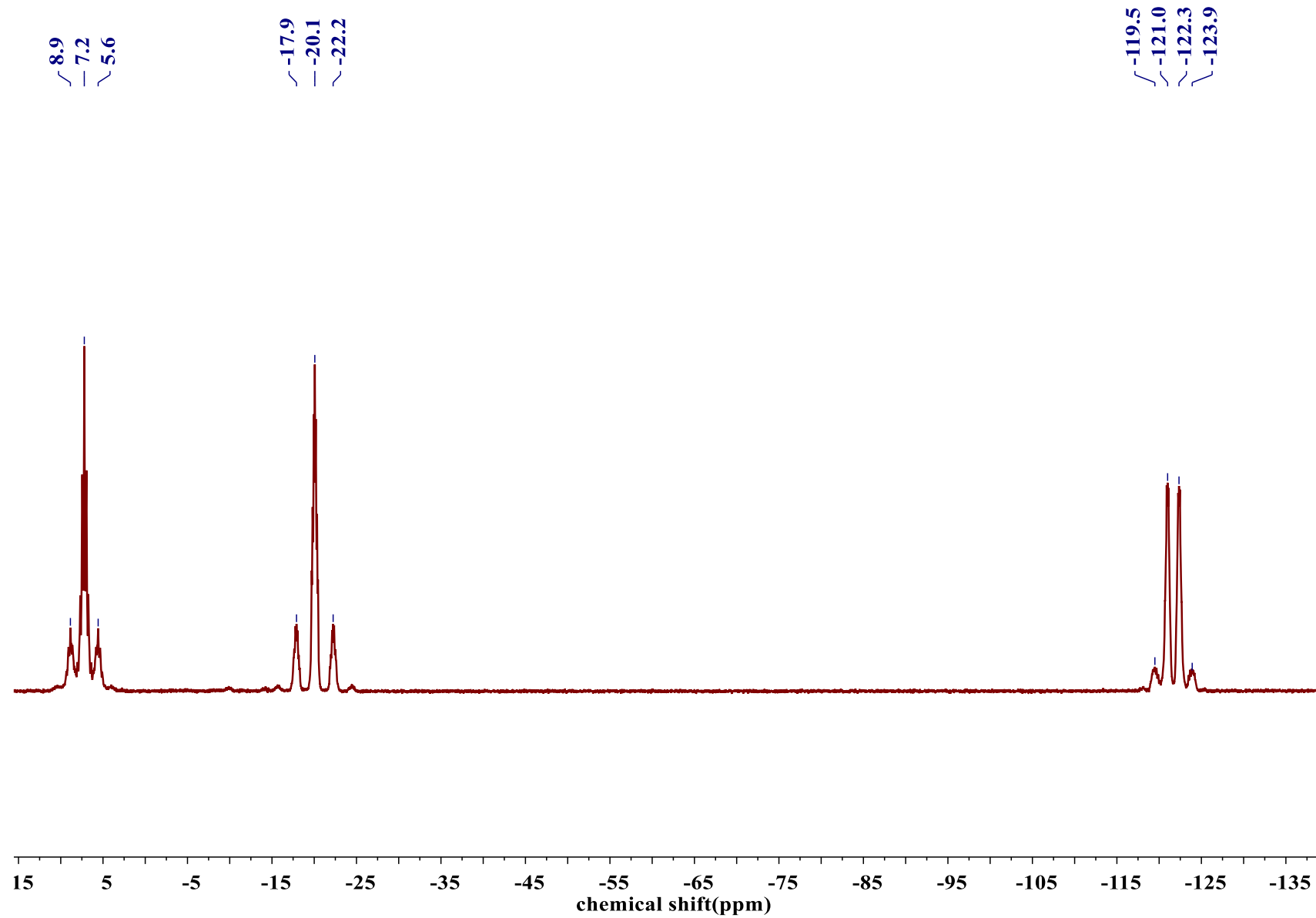


Fig. S21 ^{31}P NMR spectrum of complex **4** (162 MHz, C_6D_6 with a drop of d_8 -THF, 25 °C).

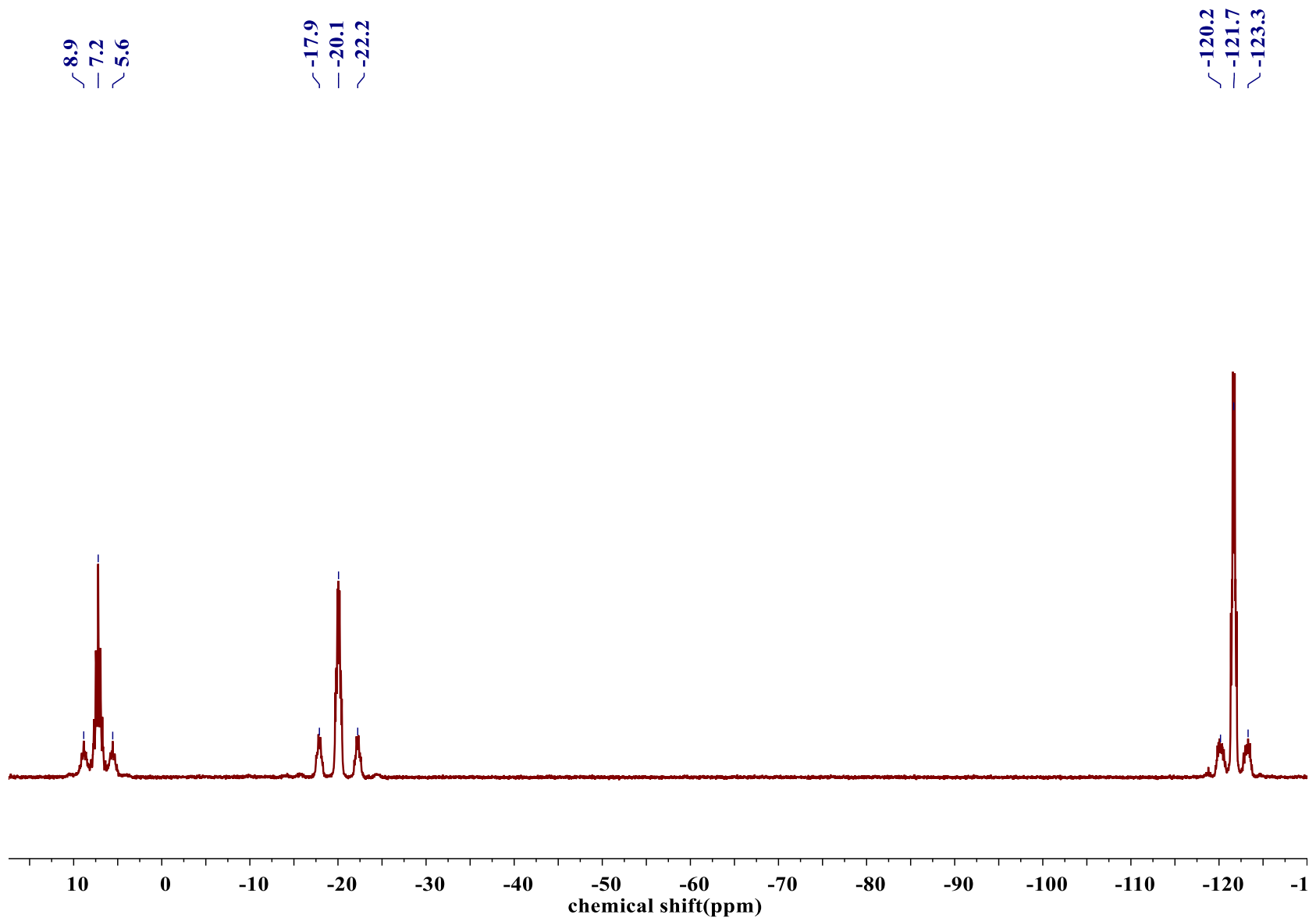


Fig. S22 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **4** (162 MHz, C_6D_6 with a drop of d_8 -THF, 25 °C).

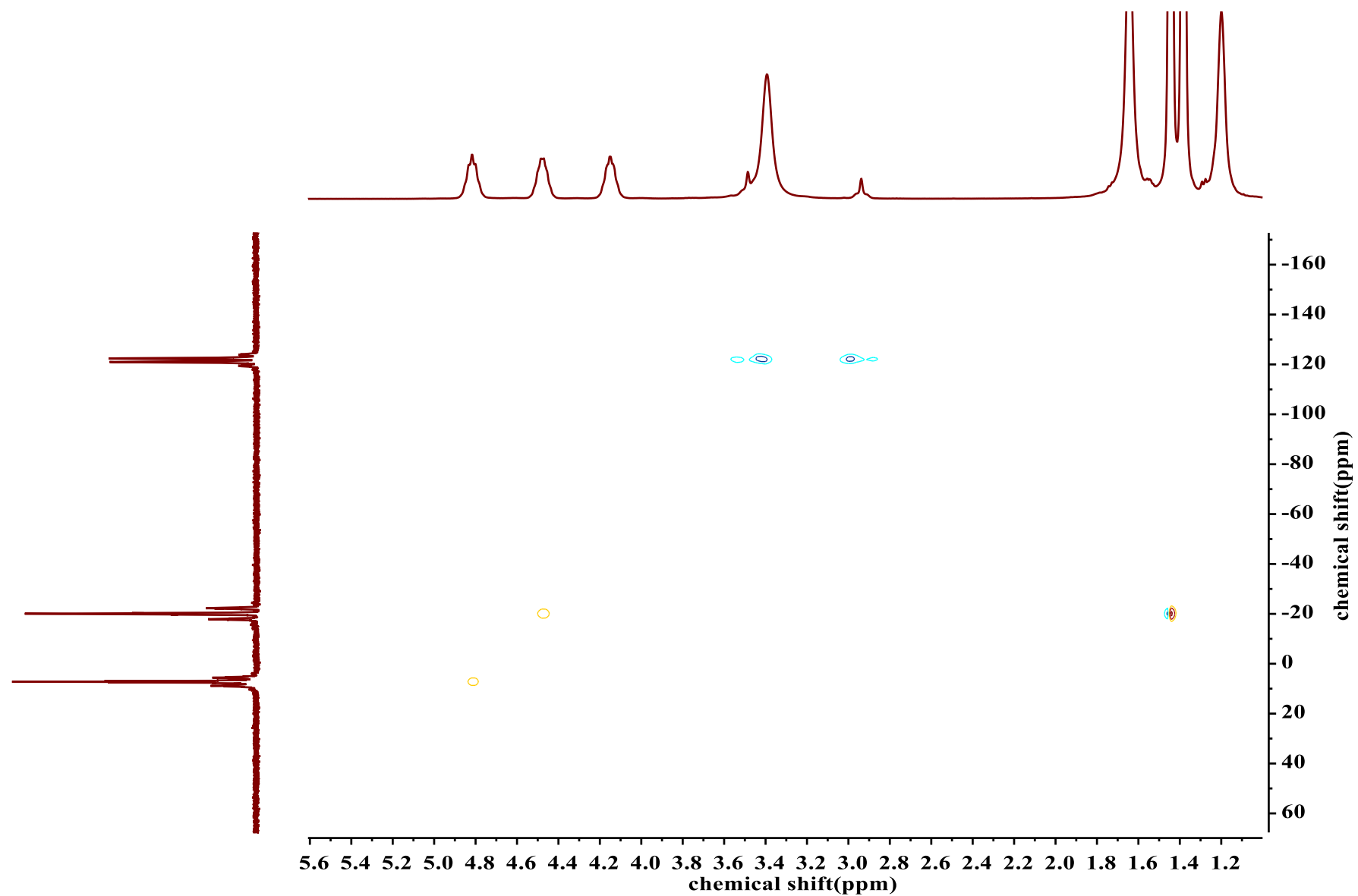


Fig. S23 ^1H ^{31}P HSQC spectra of complex **4** (400/162 MHz, C_6D_6 with a drop of d_8 -THF, 25 $^\circ\text{C}$).

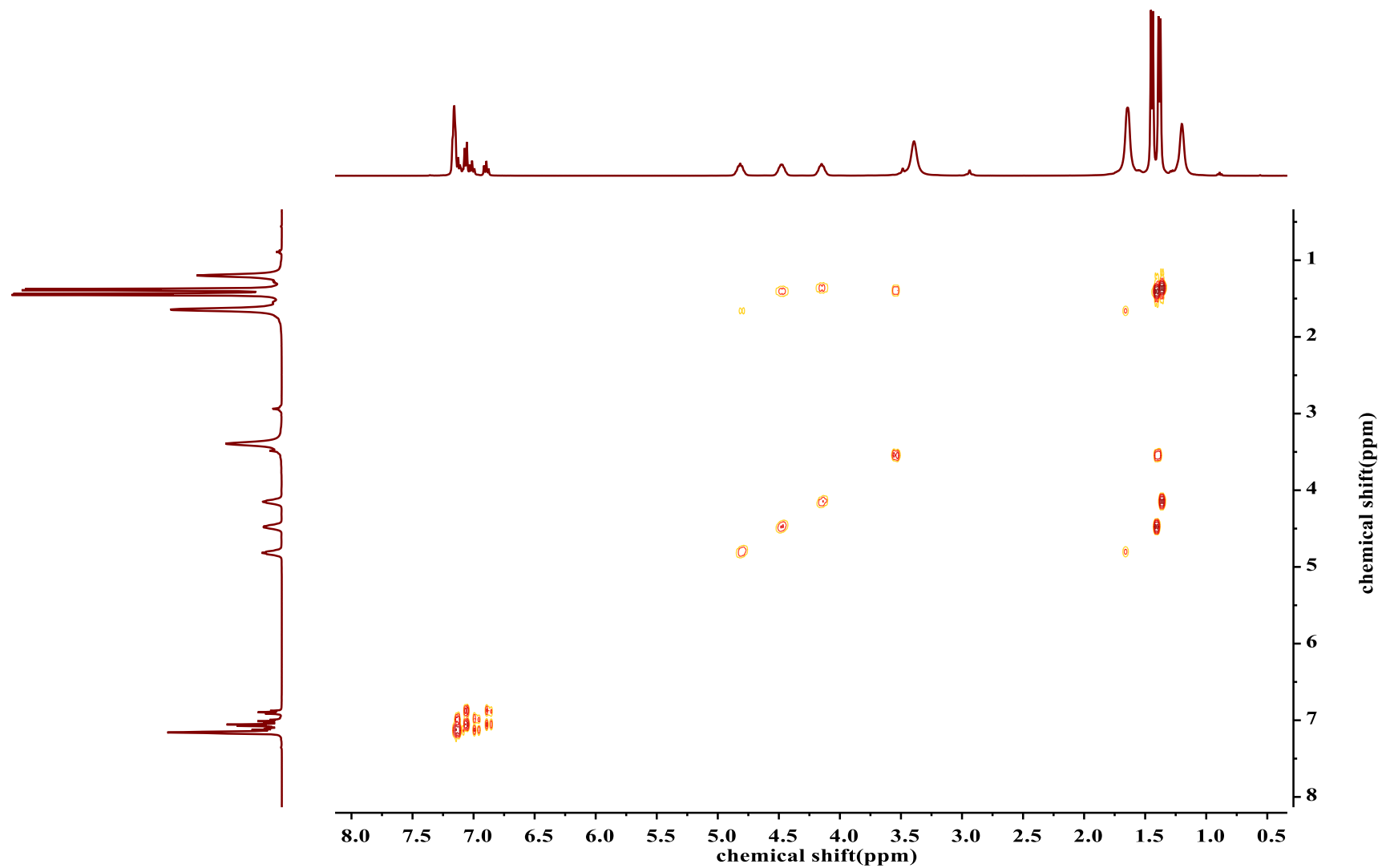


Fig. S24 gCOSY spectra of complex **4** (400 MHz, C₆D₆ with a drop of *d*₈-THF, 25 °C).

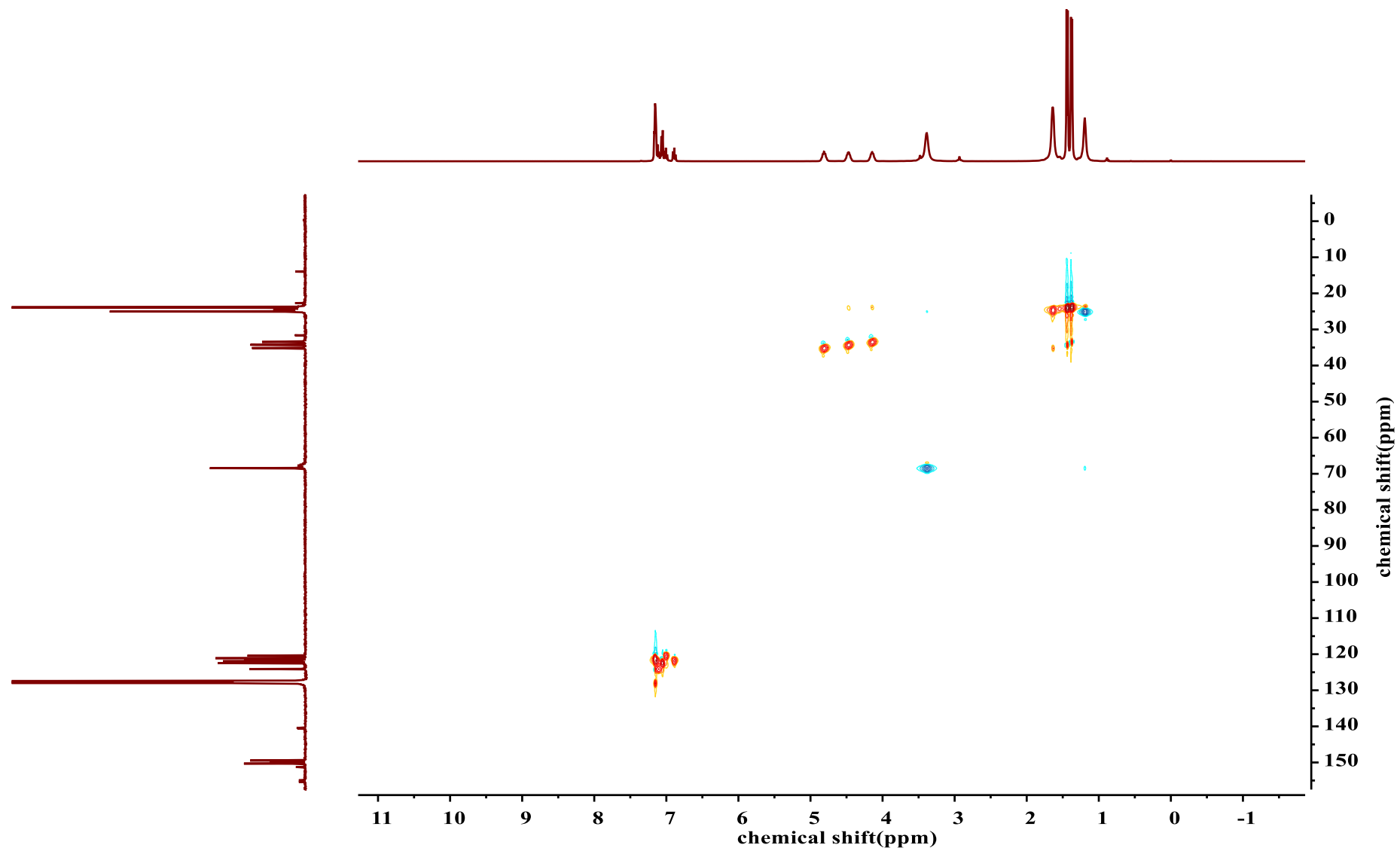


Fig. S25 gHSQC spectra of complex **4** (400 MHz, C_6D_6 with a drop of d_8 -THF, 25 °C).

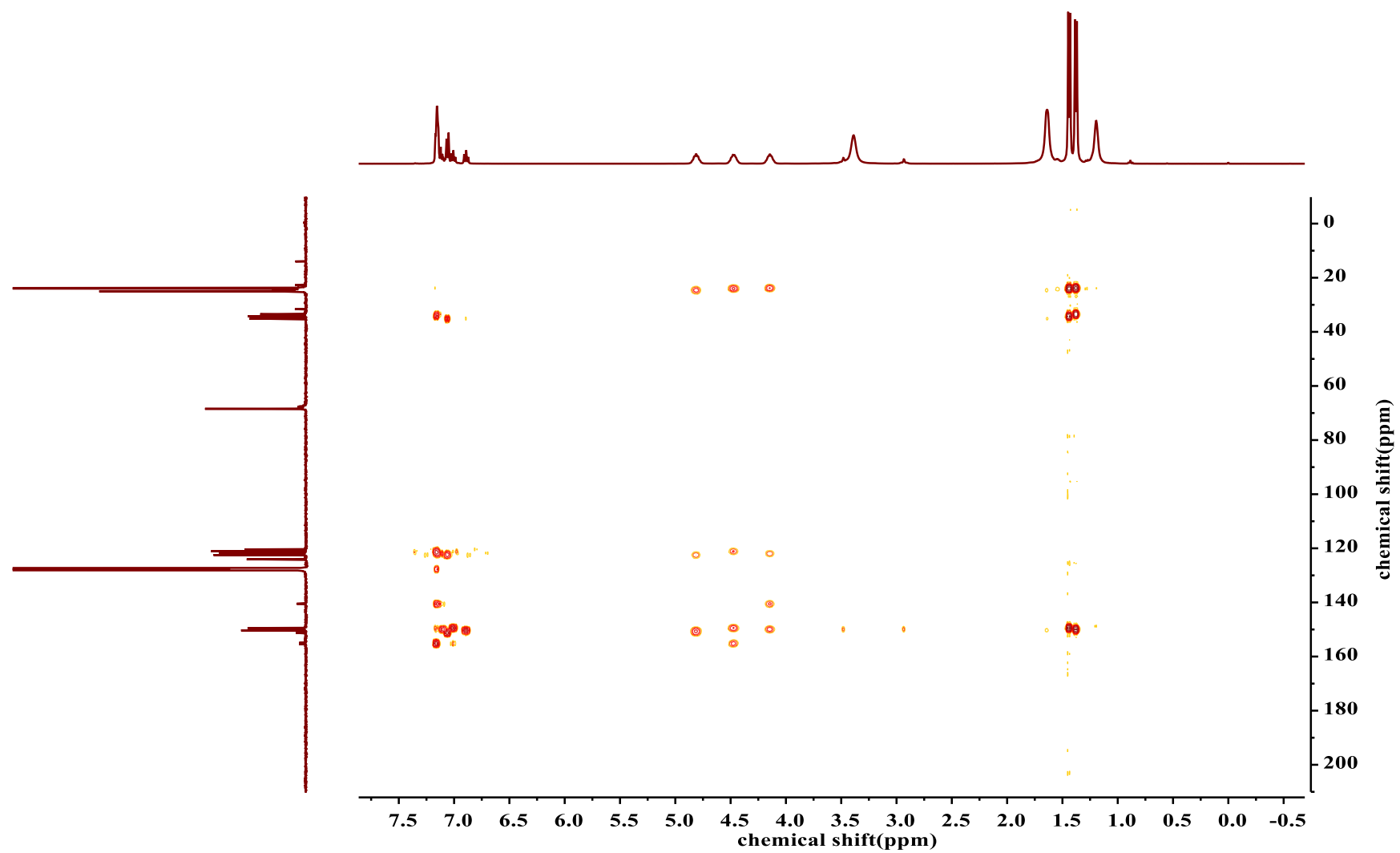


Fig. S26 gHMBC spectra of complex **4** (400 MHz, C₆D₆ with a drop of *d*₈-THF, 25 °C).

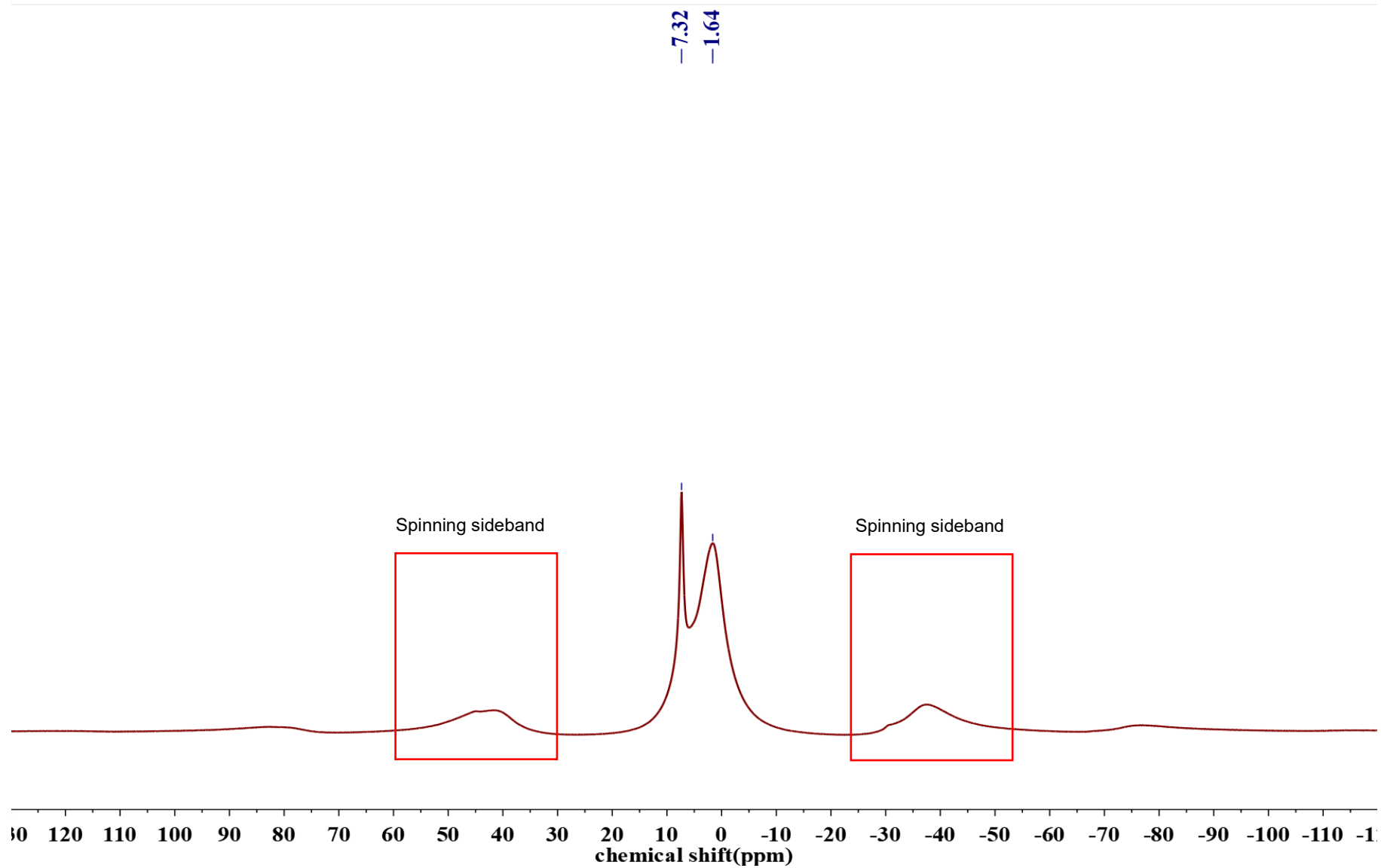


Fig. S27 ^1H solid-state NMR spectrum of complex **5** (400 MHz, 25 °C).

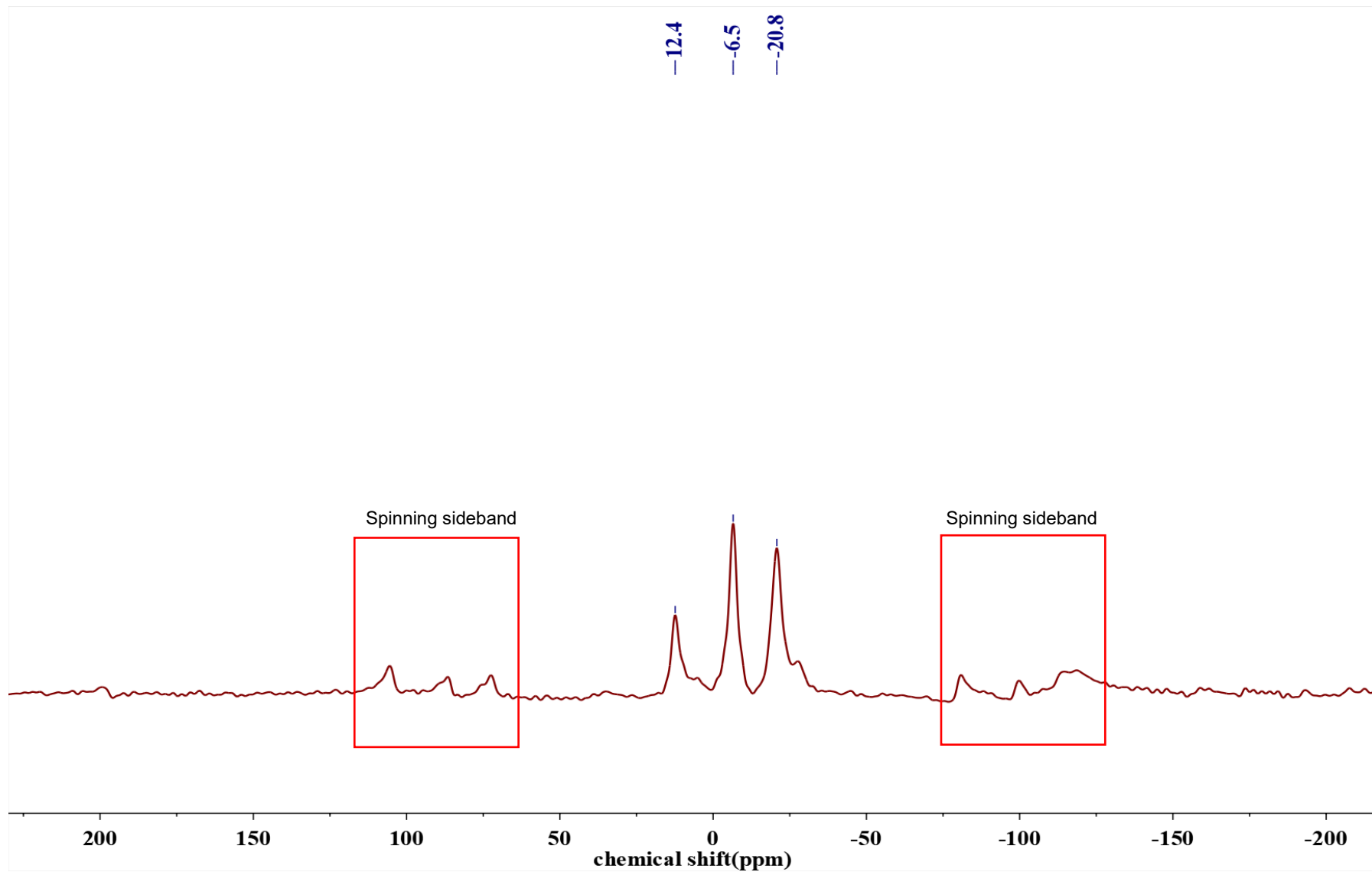


Fig. S28 ^{31}P solid-state NMR spectrum of complex 5 (162 MHz, 25 °C).

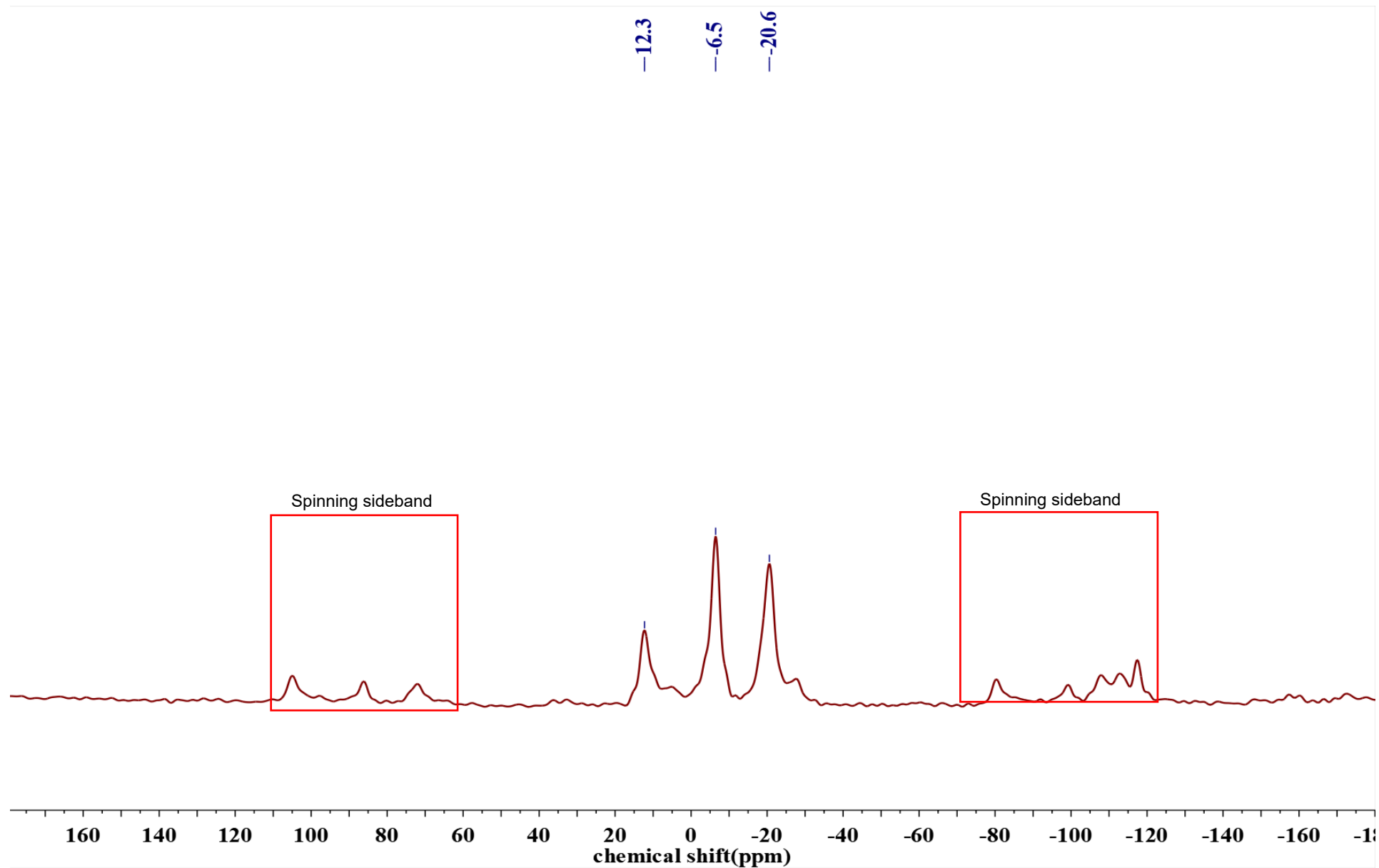


Fig. S29 $^{31}\text{P}\{^1\text{H}\}$ solid-state NMR spectrum of complex **5** (162 MHz, 25 °C).

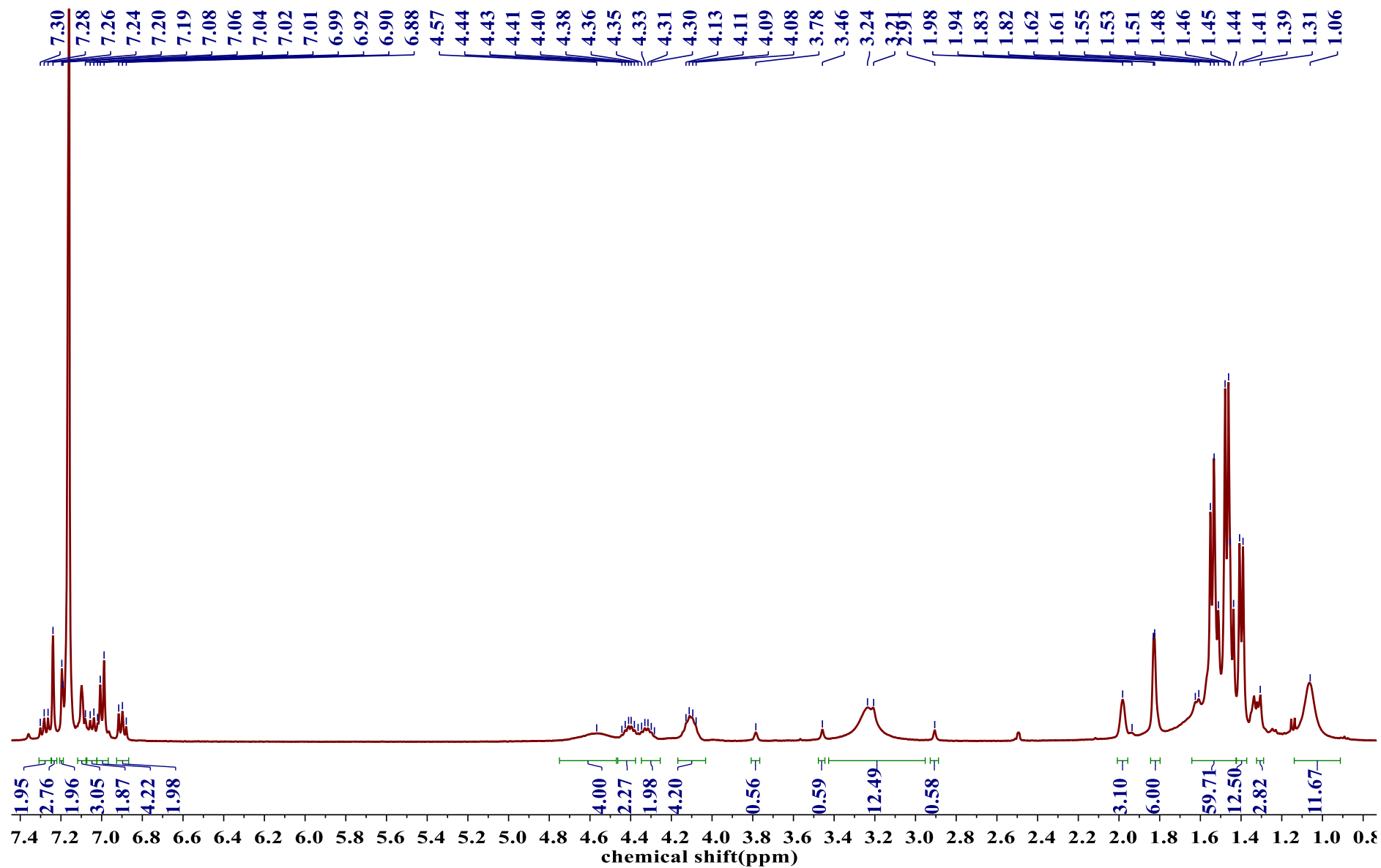


Fig. S30 ¹H NMR spectrum of complex 6 (400 MHz, C₆D₆, 25 °C).

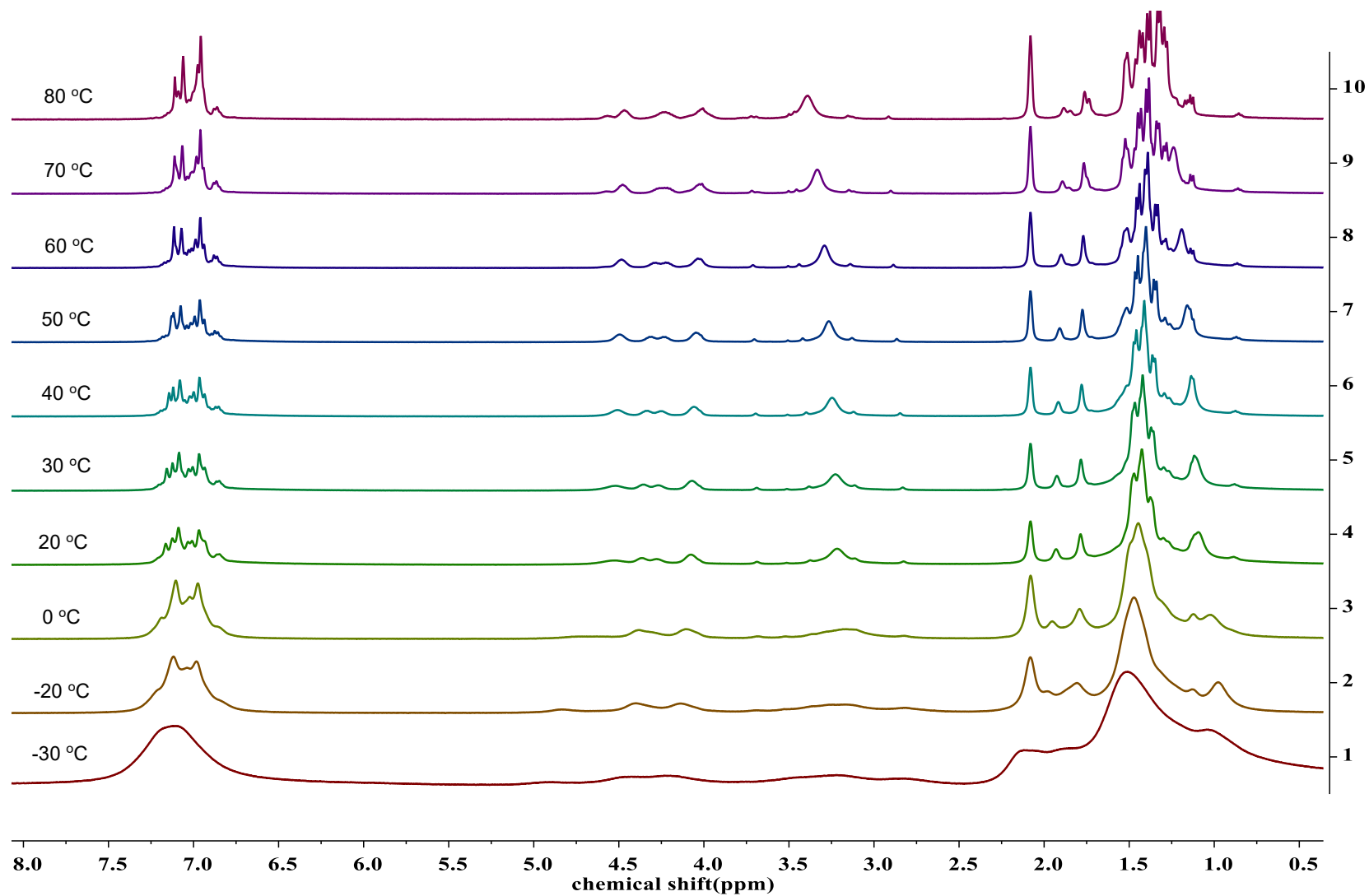


Fig. S31 Variant temperature ¹H NMR spectrum of complex **6** (400 MHz, *d*₈-toluene, -30, -20, -0, 20, 30, 40, 50, 60, 70 and 80 °C).

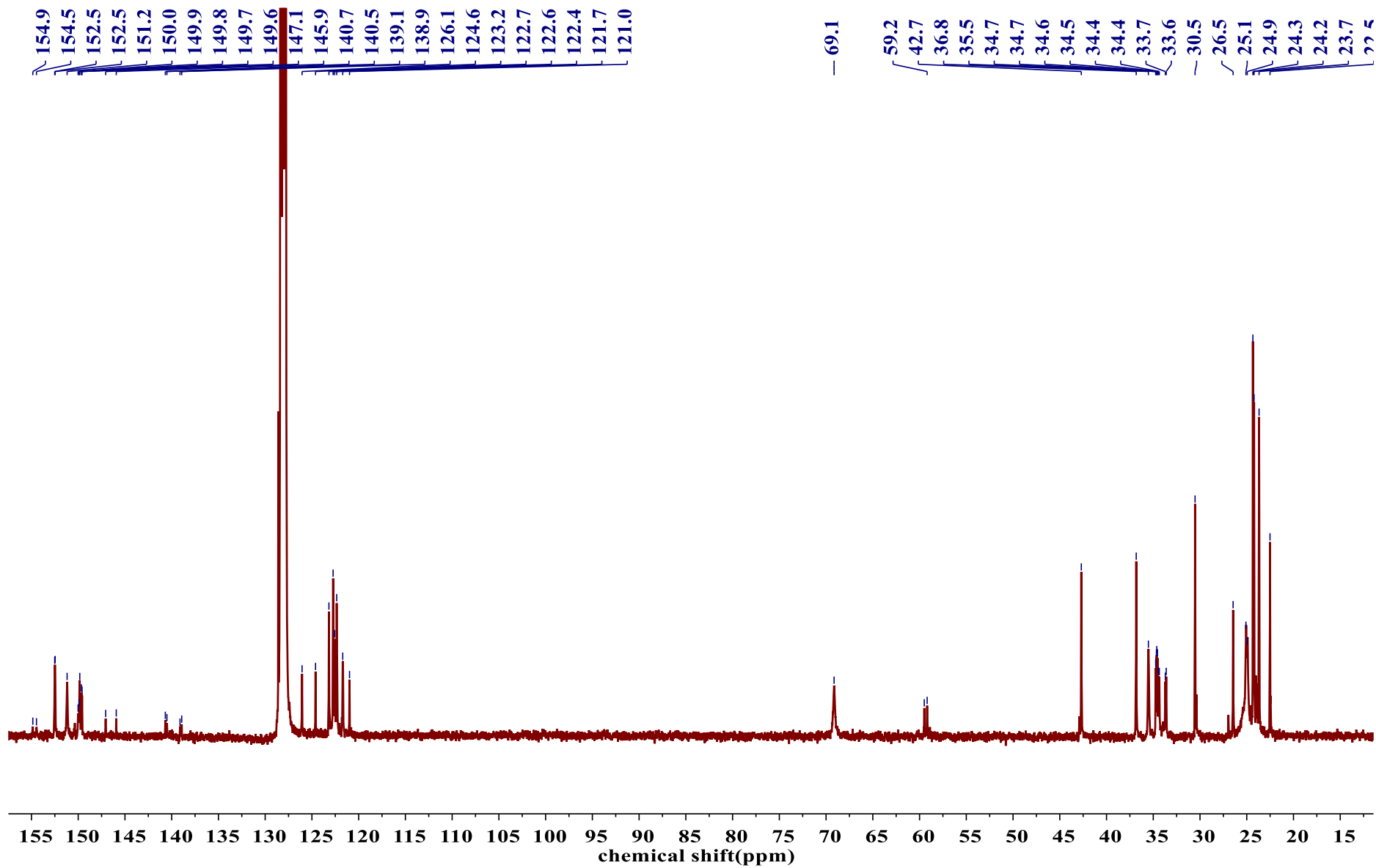


Fig. S32 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex **6** (100 MHz, C_6D_6 , 25 °C).

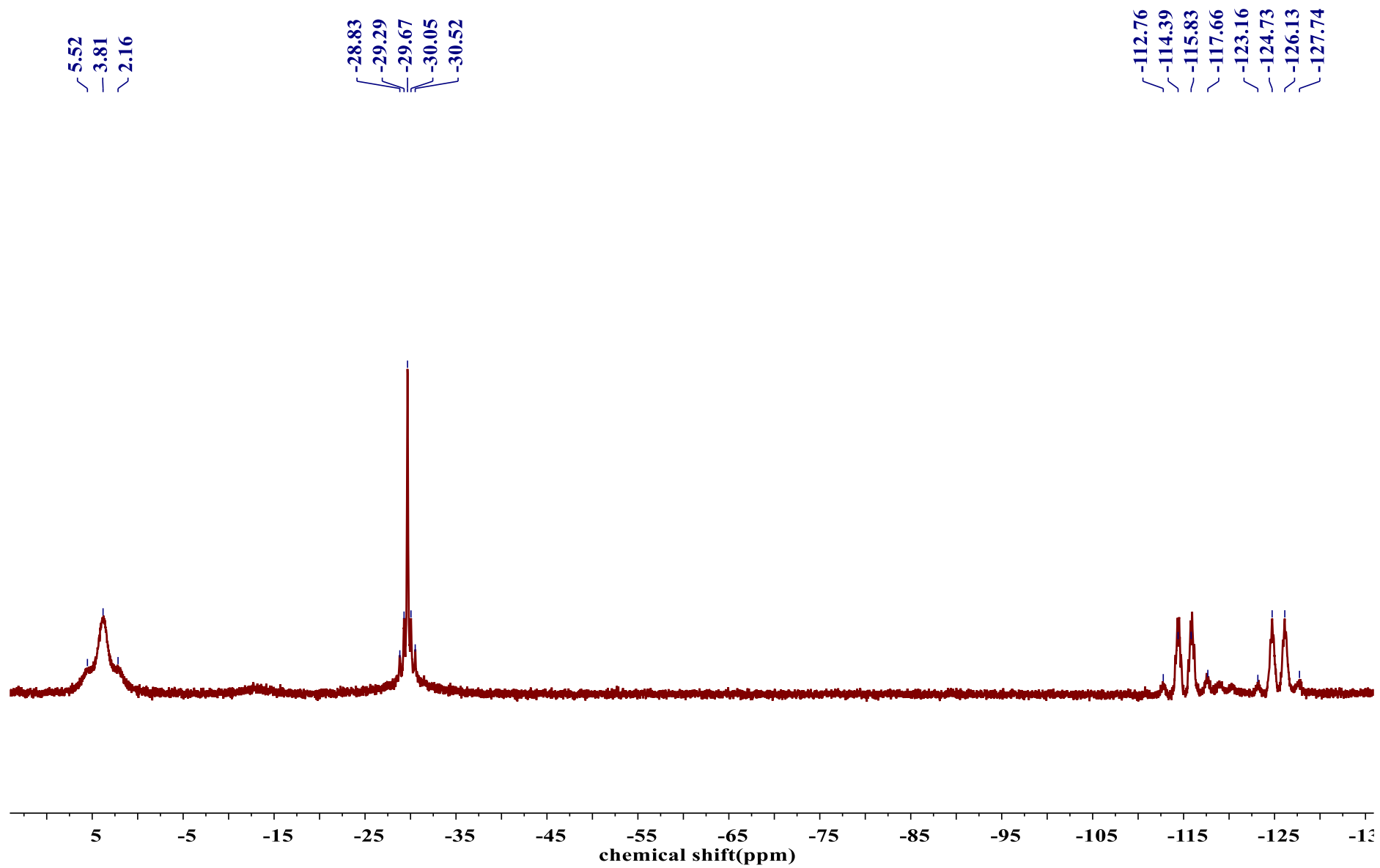


Fig. S33 ^{31}P NMR spectrum of complex **6** (162 MHz, C_6D_6 , 25 °C).

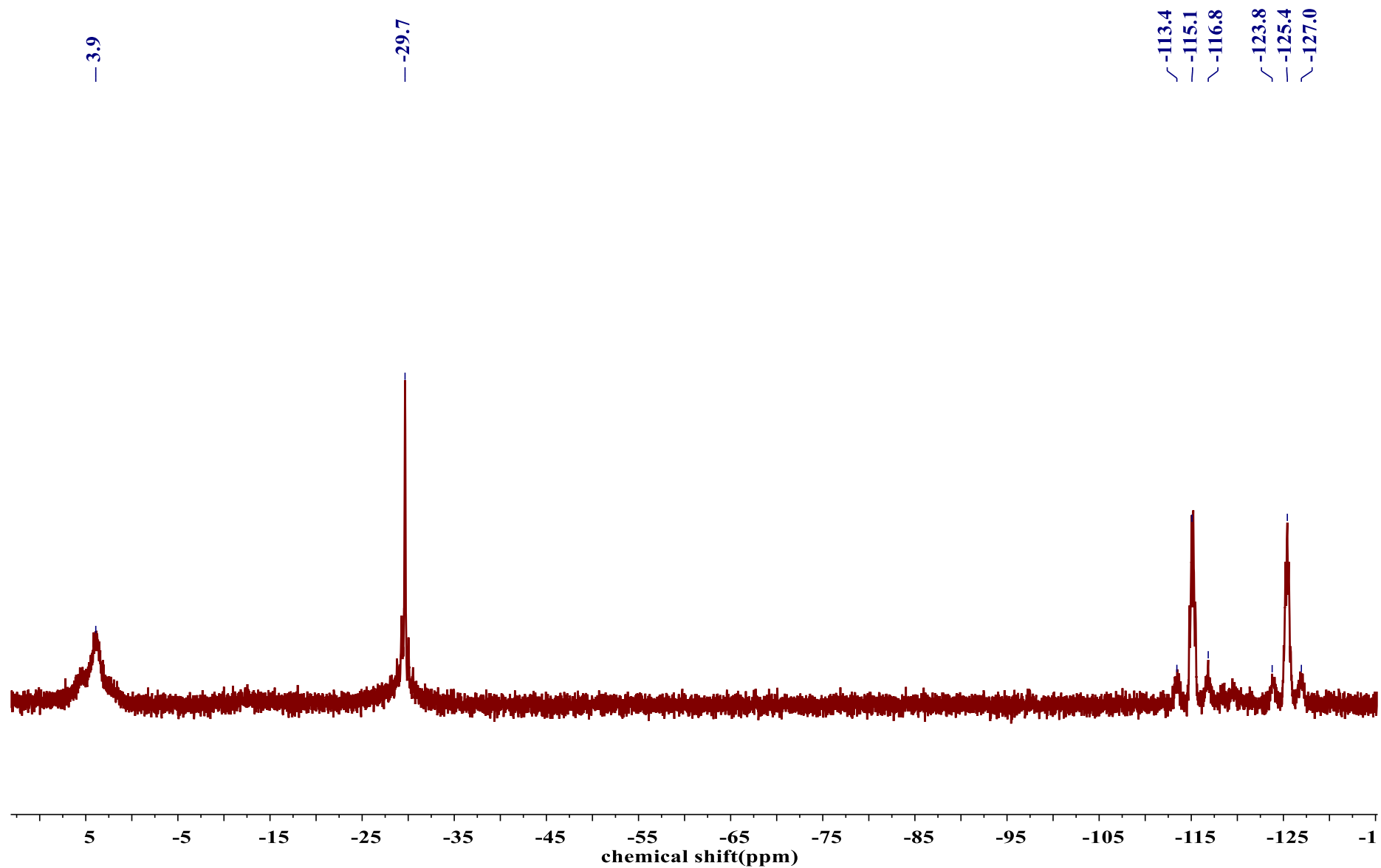


Fig. S34 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **6** (162 MHz, C_6D_6 , 25 °C).

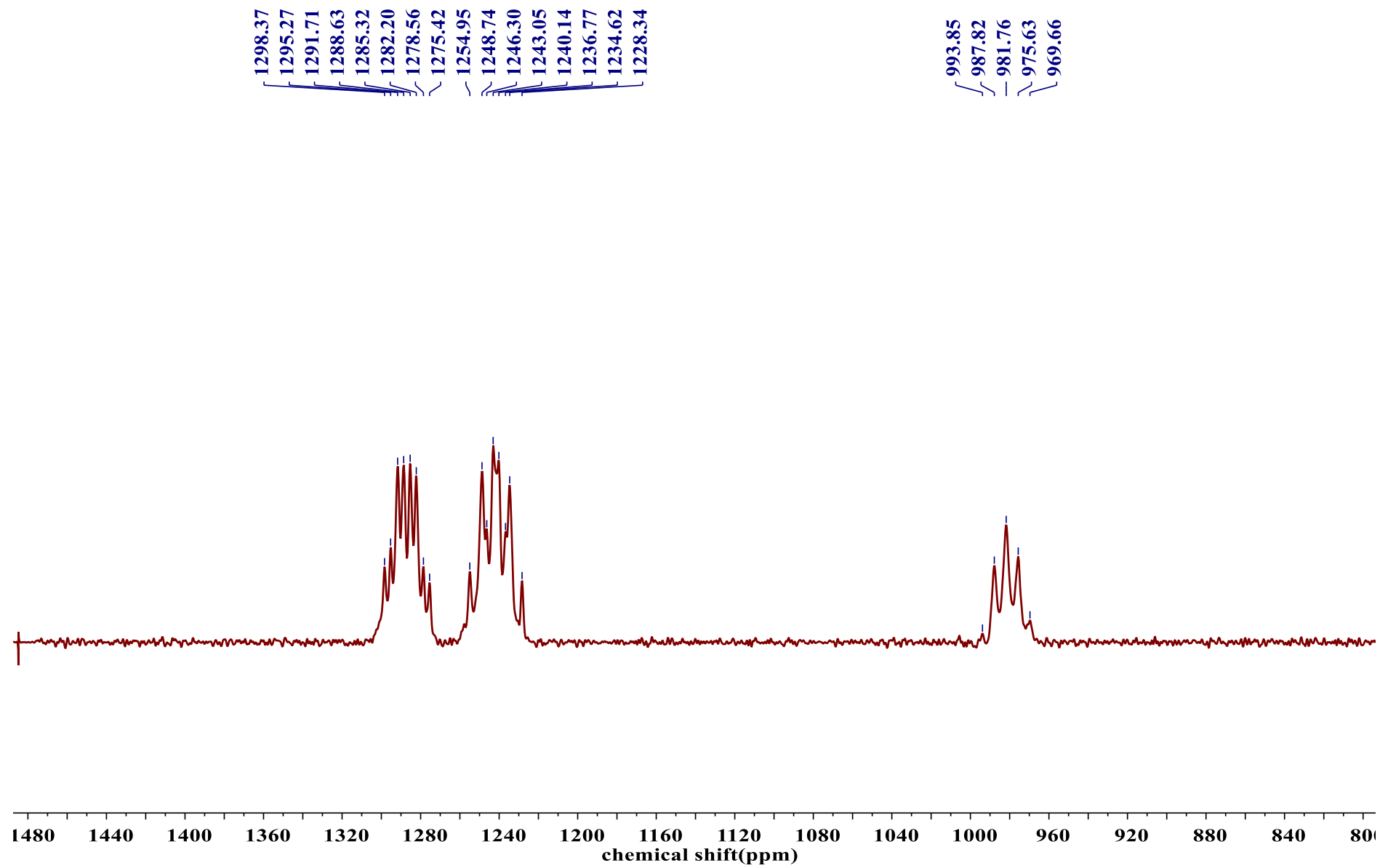


Fig. S35 $^{171}\text{Yb}\{^1\text{H}\}$ NMR spectrum of complex **6** (87 MHz, C_6D_6 , 25 °C).

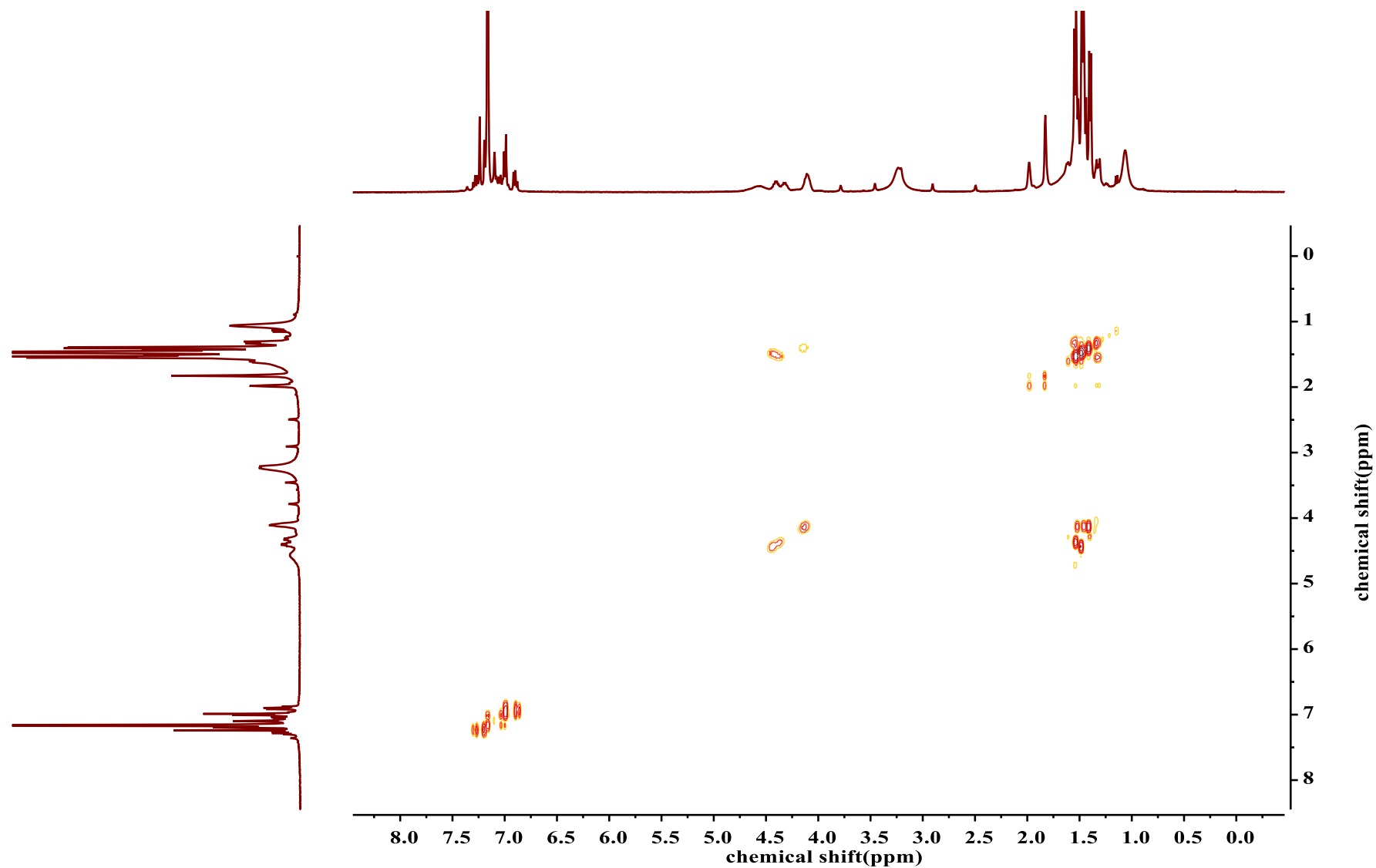


Fig. S36 gCOSY spectra of complex **6** (400 MHz, C₆D₆, 25 °C).

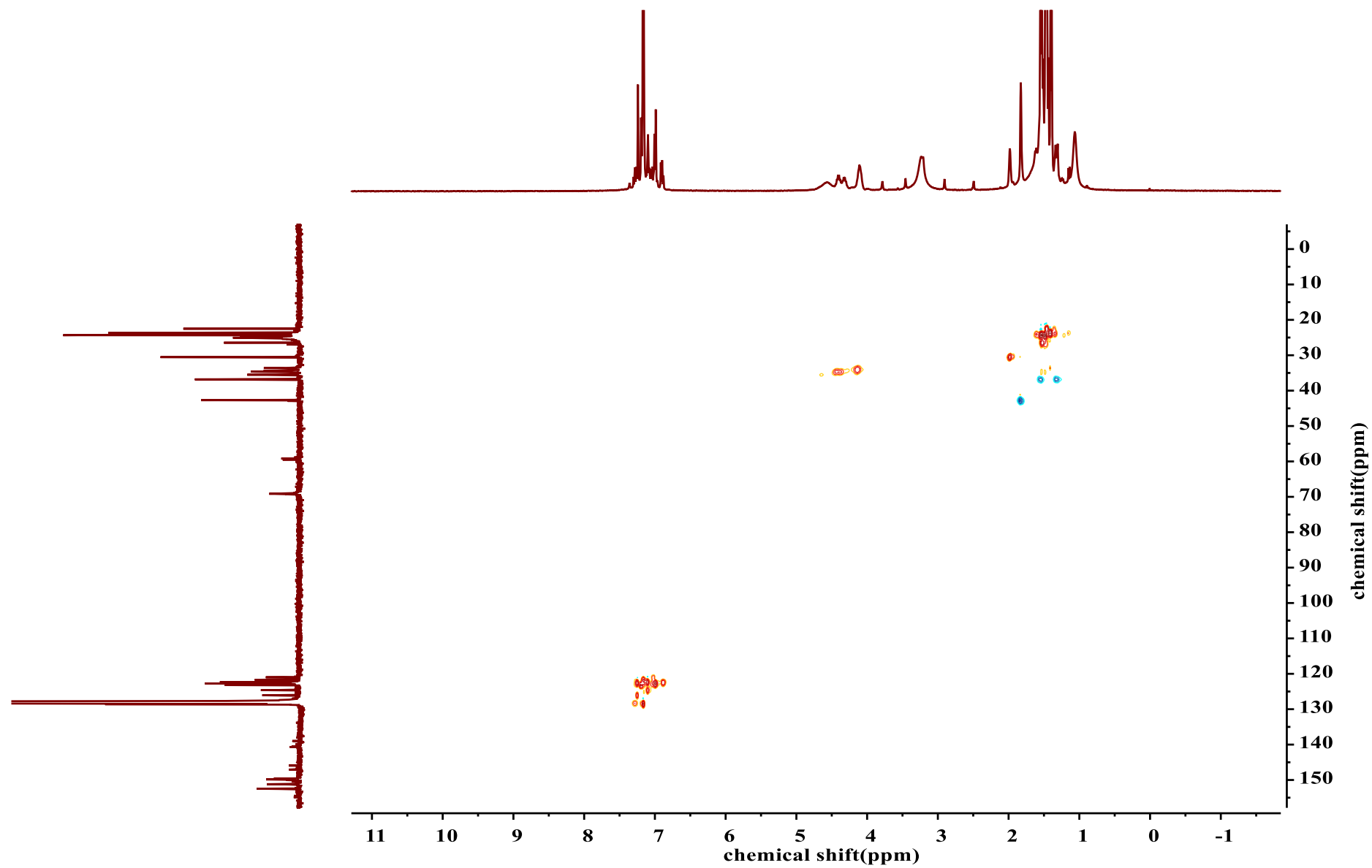


Fig. S37 gHSQC spectra of complex **6** (400 MHz, C_6D_6 , 25 $^\circ\text{C}$).

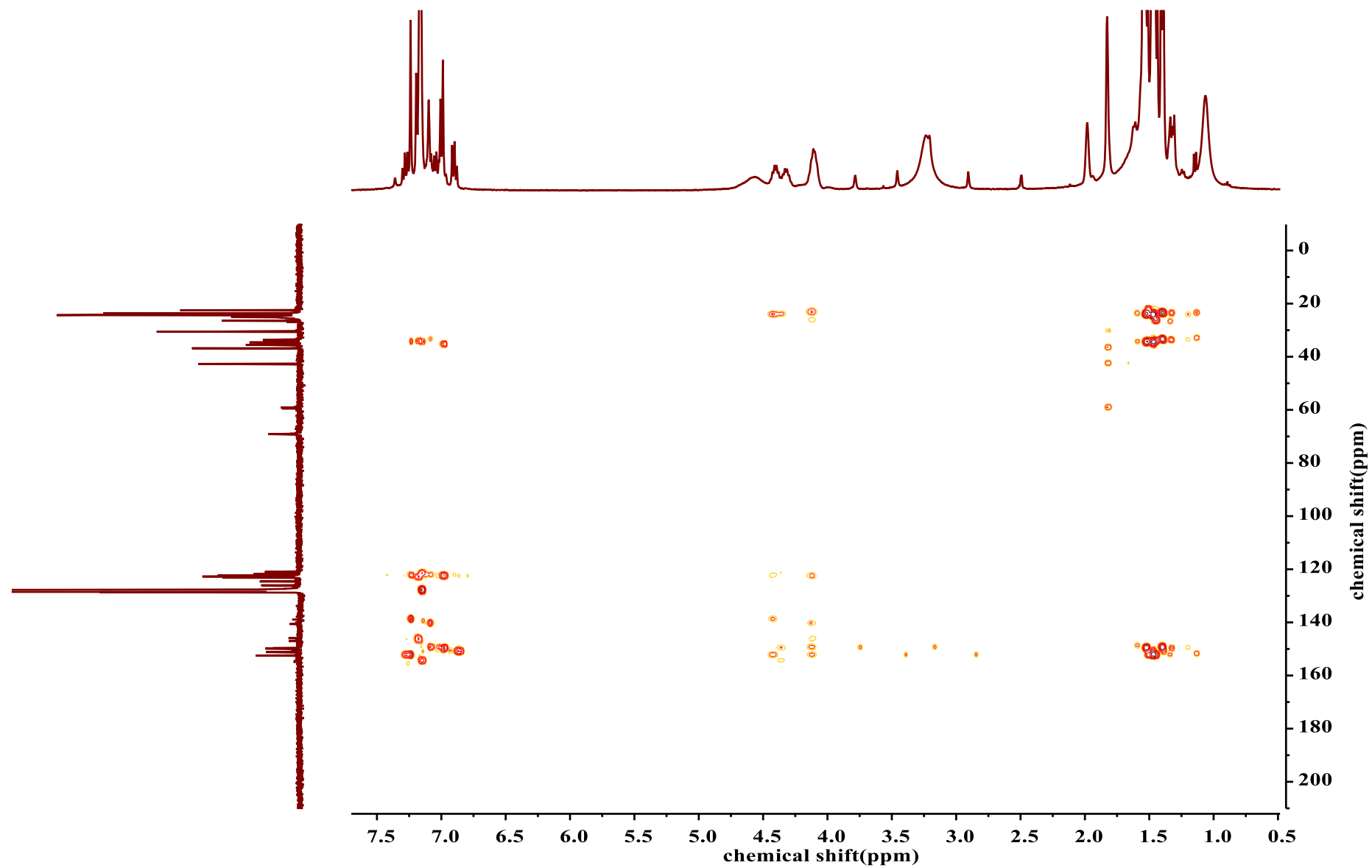


Fig. S38 gHMBC spectra of complex **6** (400 MHz, C_6D_6 , 25 $^\circ\text{C}$).

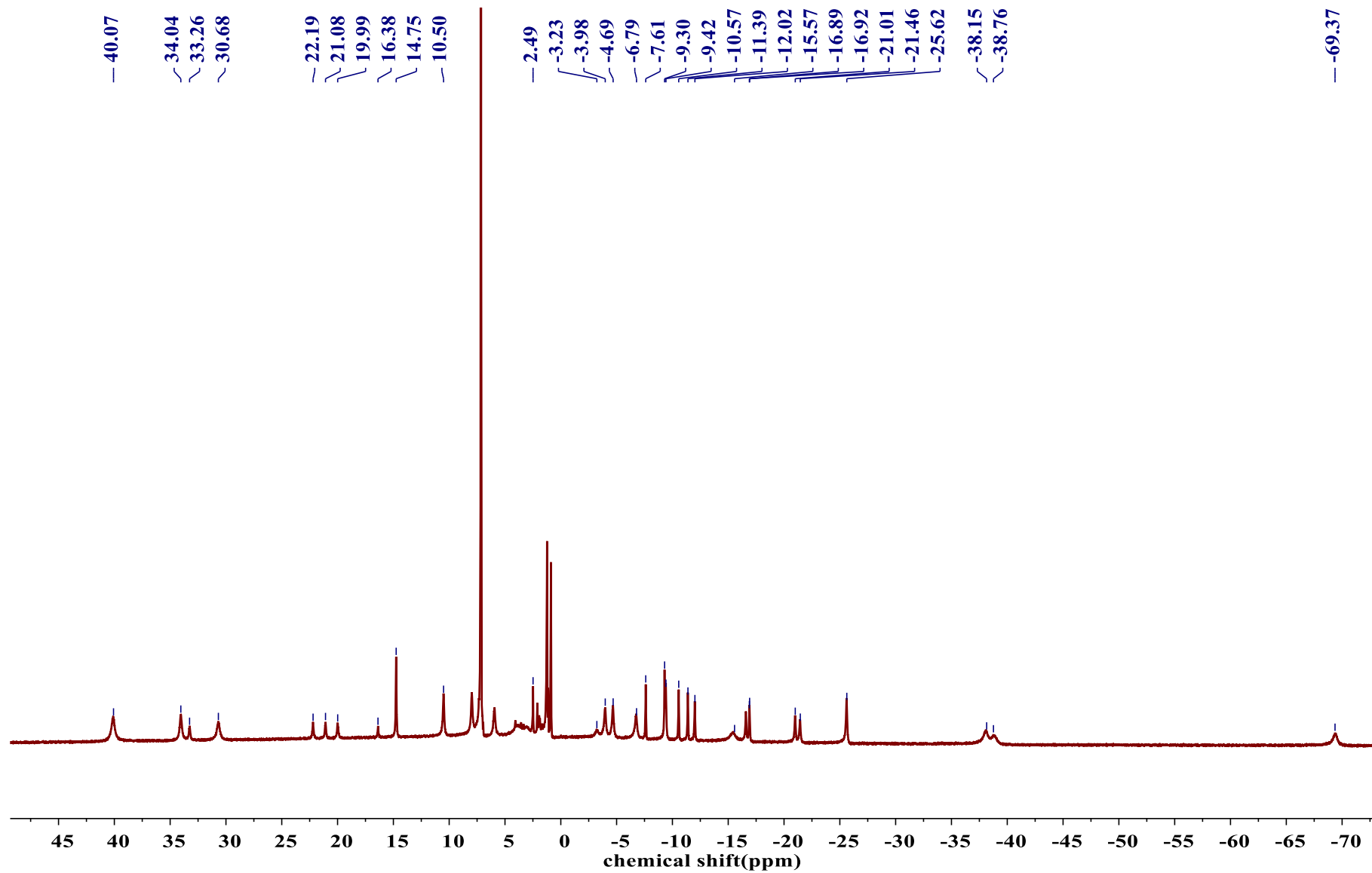


Fig. S39 ^1H NMR spectrum of complex 7 (400 MHz, C_6D_6 , 25 $^\circ\text{C}$).

Formation of AdPh and AdH in the reaction of complex 4 with 10 equiv. of AdNC

d_5 -Phenyladamantane (AdC₆D₅) and adamantane (AdH): To a C₆D₆ solution (1 mL) of complex **4** (71.4 mg, 0.03mmol) was added a C₆D₆ solution (1 mL) of AdNC (48.4 mg, 0.3 mmol) at room temperature. The reaction mixture was stirred for 24 h at room temperature, and then recorded by ¹H NMR spectroscopy (Fig. S40). The volatiles of the reaction solution were removed under vacuum, and the residue was divided into two parts. One was extracted with C₆H₆ and recorded by ²H NMR spectroscopy (Fig. S41), the other part was washed with hexane (1 mL × 3). The hexane wash was passed through silica gel and analyzed by GC-MS, which indicated the formation of d_5 -Phenyladamantane(Ad-C₆D₅) and adamantane AdH (Fig. S42).

Phenyladamantane (AdPh) and AdH: To a benzene solution (1 mL) of complex **4** (71.4 mg, 0.03mmol) was added a benzene solution (1 mL) of AdNC (48.4 mg, 0.3 mmol) at room temperature. The reaction mixture was stirred for 24 h at room temperature, and then the solvent was removed under vacuum. The residue was washed with hexane (1 mL × 3). The hexane wash was passed through silica gel and analyzed by GC-MS, which indicated the formation of phenyladamantane (AdPh) and adamantane (AdH) (Fig. S43).

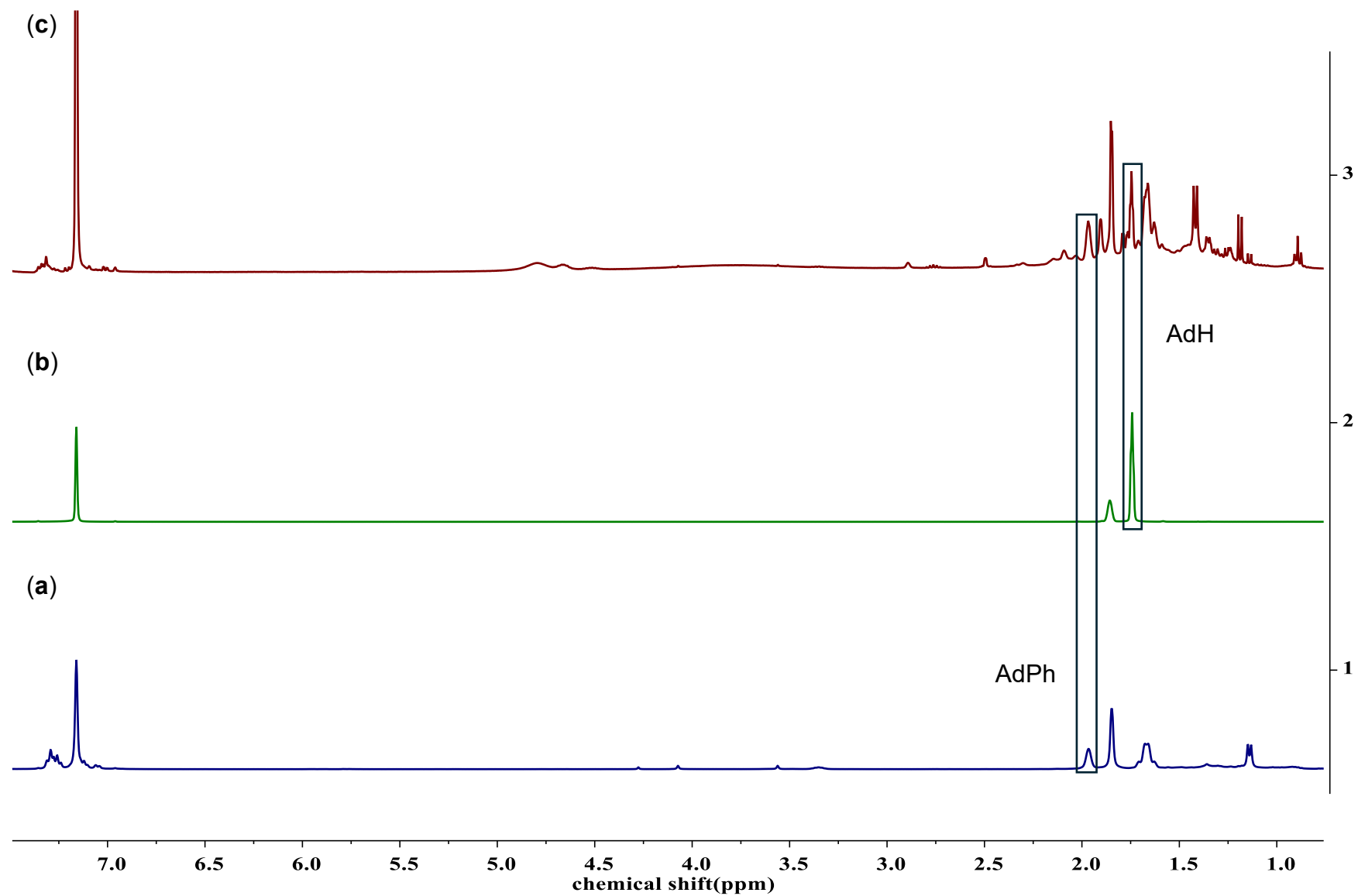


Fig. S40 ¹H NMR spectra of (a) AdPh, (b) AdH, and (c) the reaction of complex **4** with 10 equiv. of AdNC in C₆D₆ after 24 h (400 MHz, C₆D₆, 25 °C).

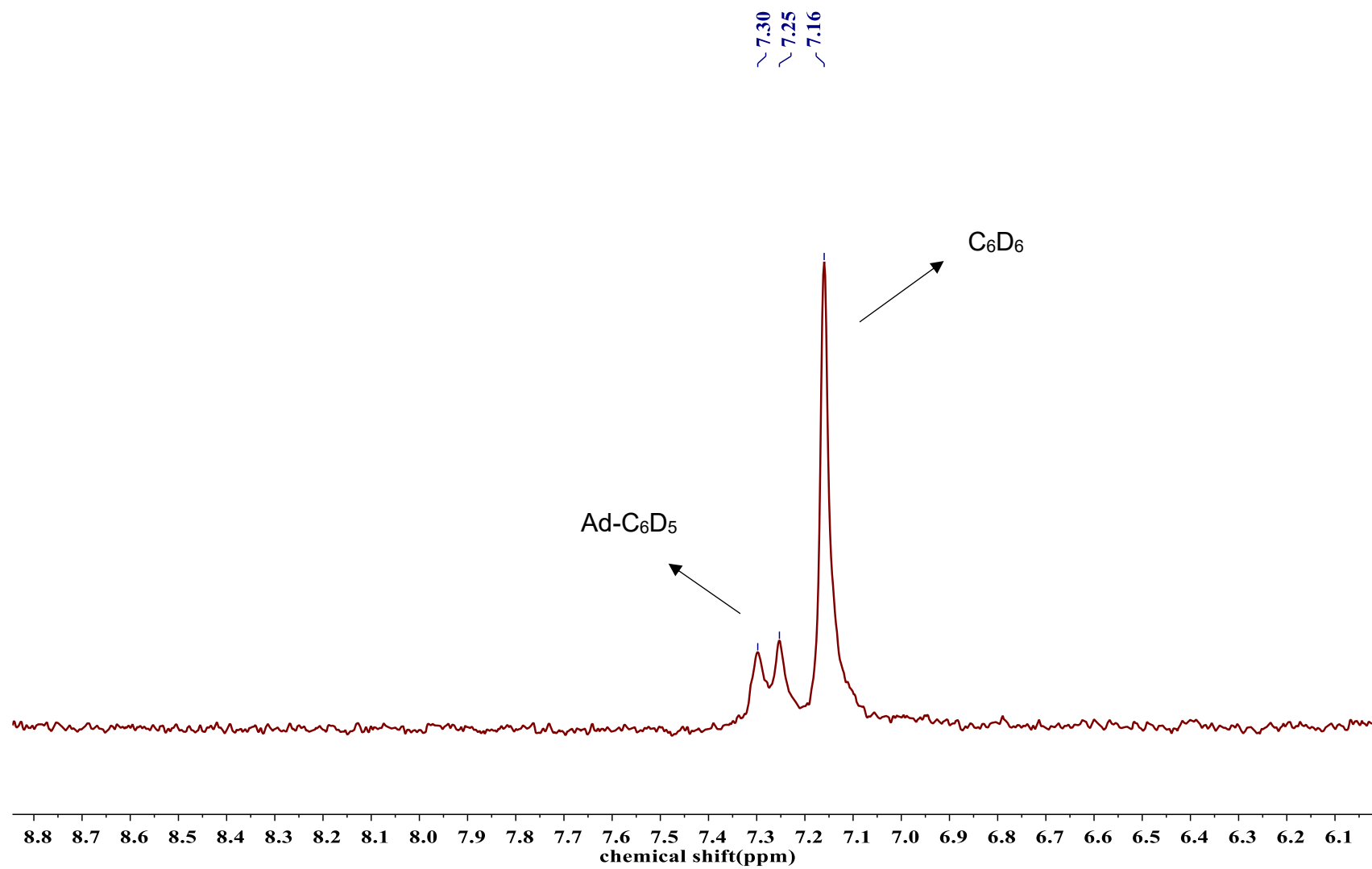


Fig. S41 ^2H NMR spectra of the hexane wash from the reaction of complex **4** with 10 equiv. of AdNC in C_6D_6 (60 MHz, C_6H_6 , 25 °C). C_6D_6 as the reference.

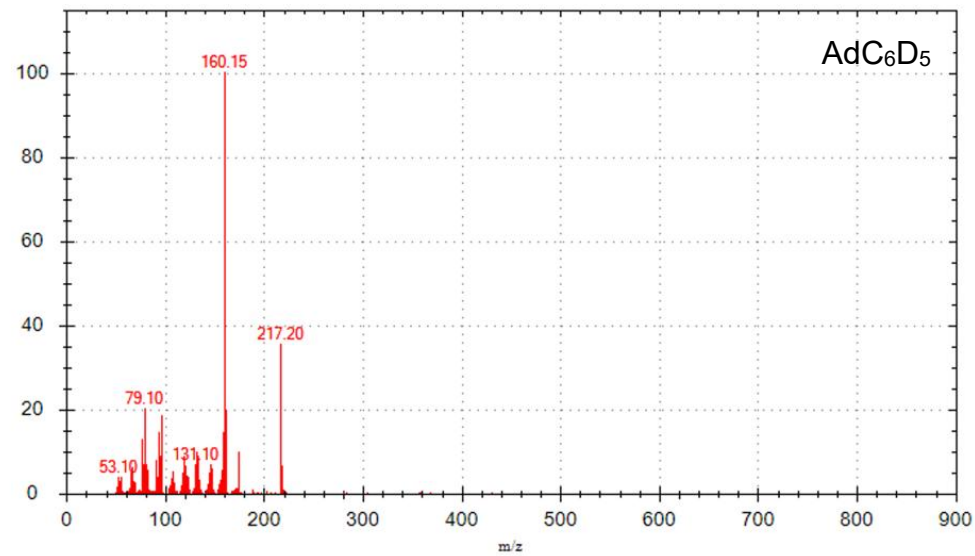
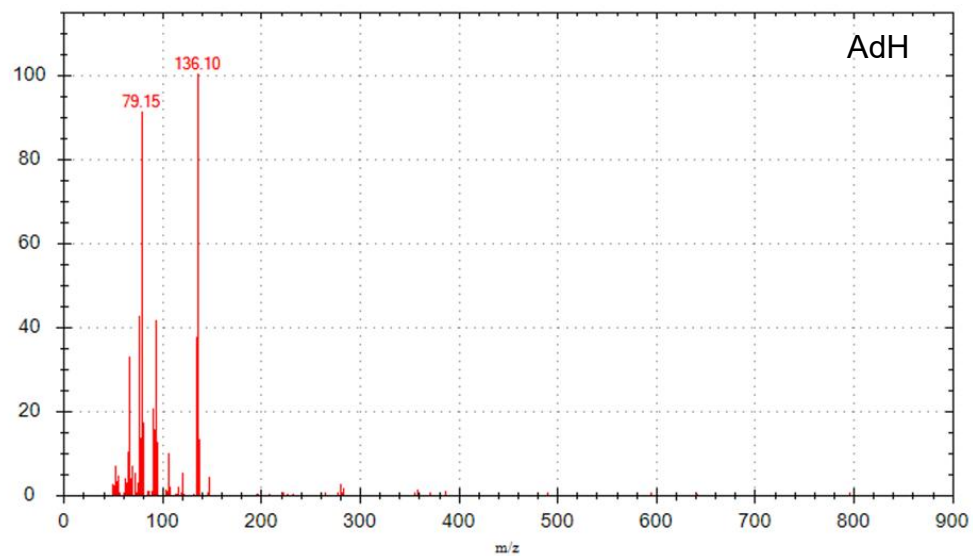
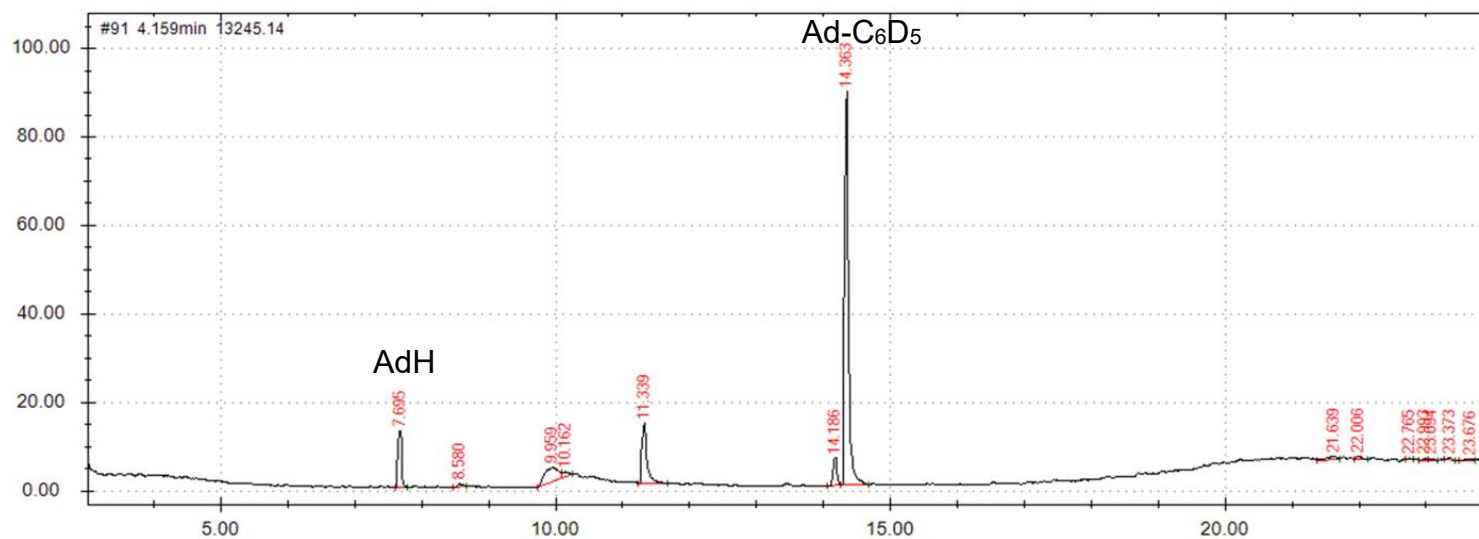


Fig. S42 GC-MS analysis of the hexane wash from the reaction of complex **4** with 10 equiv. of AdNC in C₆D₆.

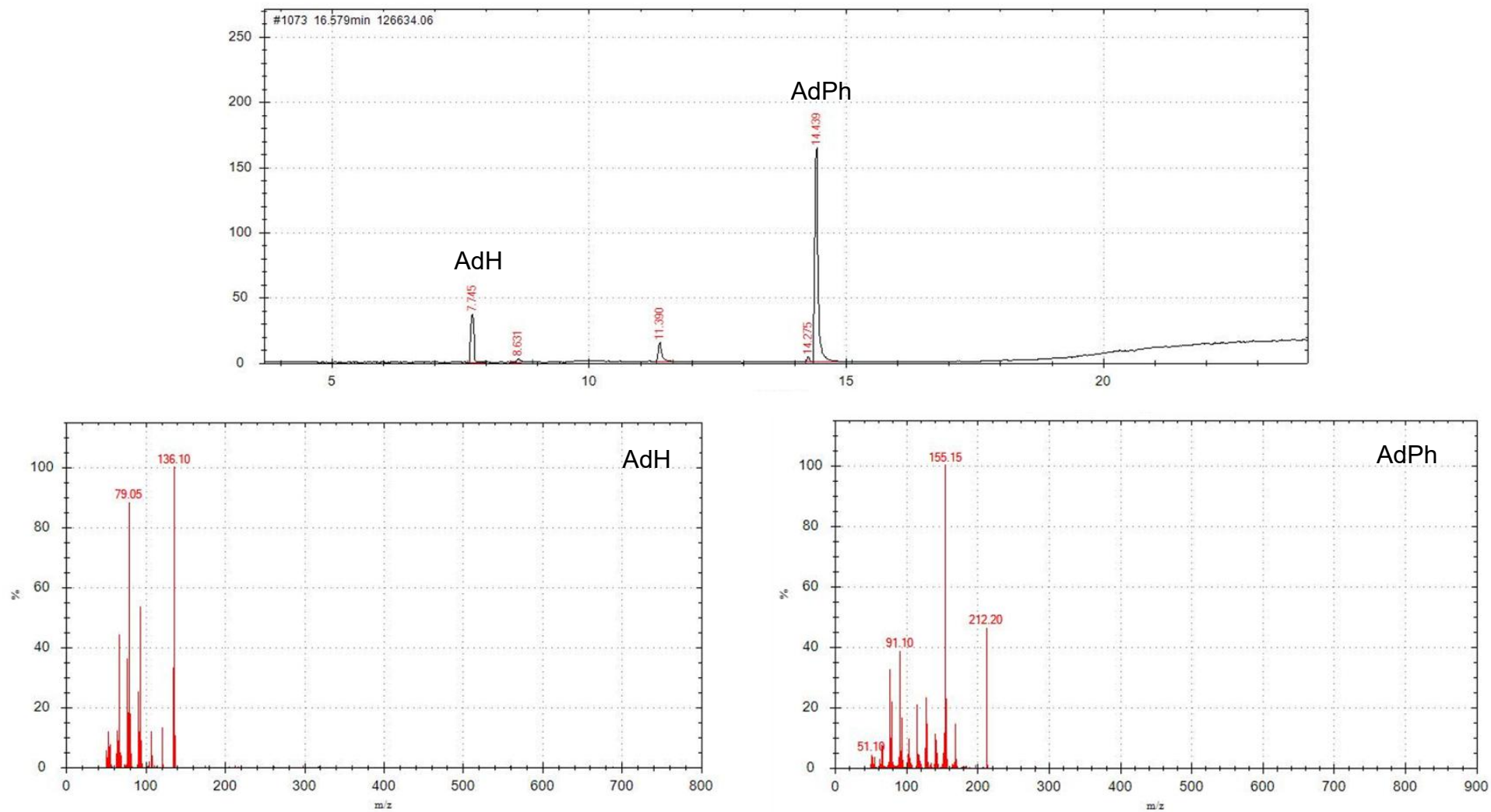


Fig. S43 GC-MS analysis of the hexane wash from the reaction of Complex **4** with 10 equiv. of AdNC in C₆H₆.

Magnetic measurements

Magnetic measurements were carried out using a Quantum Design MPMS3 SQUID magnetometer. Crystalline samples were handled and loaded into quartz tubes inside a glovebox under an inert atmosphere. A measured amount of eicosane was added to immobilize the crystallites, prevent sample torquing, and ensure good thermal contact between the sample and the temperature bath. The quartz tubes were subsequently sealed with silicone stoppers.

Direct-current (dc) magnetic susceptibility measurements were performed in the temperature range of 1.9–300 K under an applied magnetic field of 1000 Oe (0.1 T). All magnetic data were corrected for diamagnetic contributions arising from both the sample and the eicosane, estimated using Pascal's constants. The diamagnetic correction for the sample was calculated to be $\chi_{\text{Di}} = -1.38 \times 10^{-3} \text{ cm}^3 \text{ mol}^{-1}$, while that for eicosane was taken as $-2.43 \times 10^{-4} \text{ cm}^3 \text{ mol}^{-1}$.

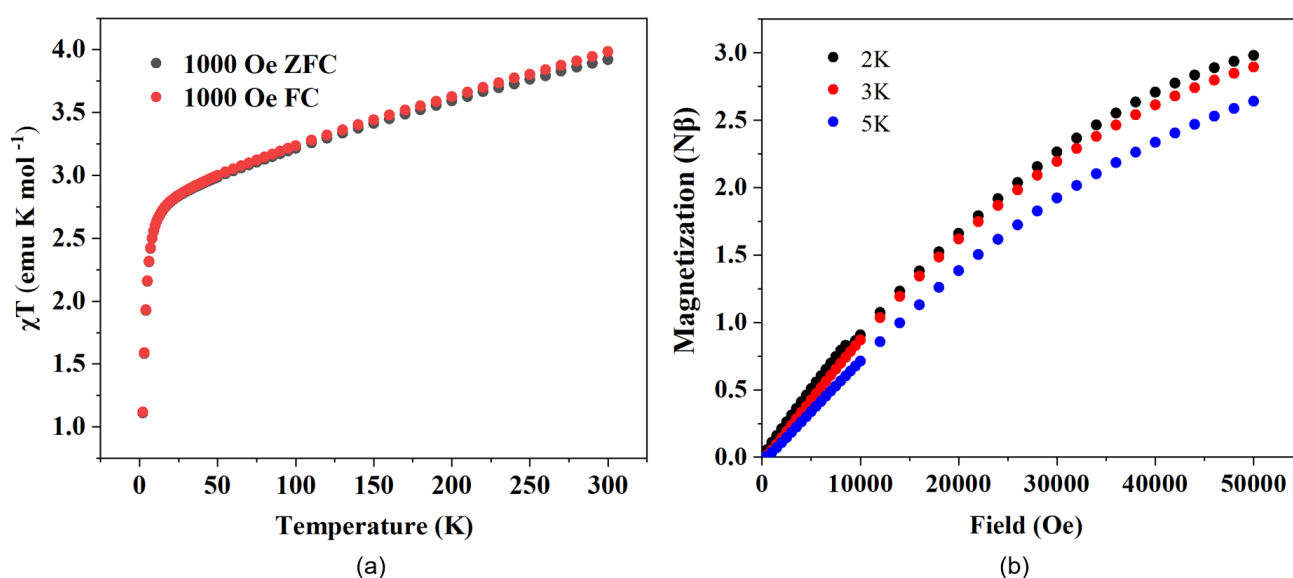


Fig. S44 (a) Field-cooled (FC) and zero-field-cooled (ZFC) χT versus T curves for complex **7**, which almost completely overlap, indicating the absence of magnetic hysteresis or long-range magnetic ordering. (b) Field dependence of the magnetization, $M(H)$, measured at selected temperatures for complex **7**.

UV/vis/NIR spectra

UV-Vis-NIR spectra were collected on solutions of complex **2**, **3**, **4**, **6**, and **7** in toluene.

Spectral fits in the UV/vis region of the electronic absorption spectra of complex **7** were performed using the peak analysis module in Origin. Gaussian functions were used for the deconvolution analysis of the observed features. Fits were conducted in units of molar absorptivity ($M^{-1} cm^{-1}$) and energy (cm^{-1}). A table of the optimized Gaussian parameters is provided below.

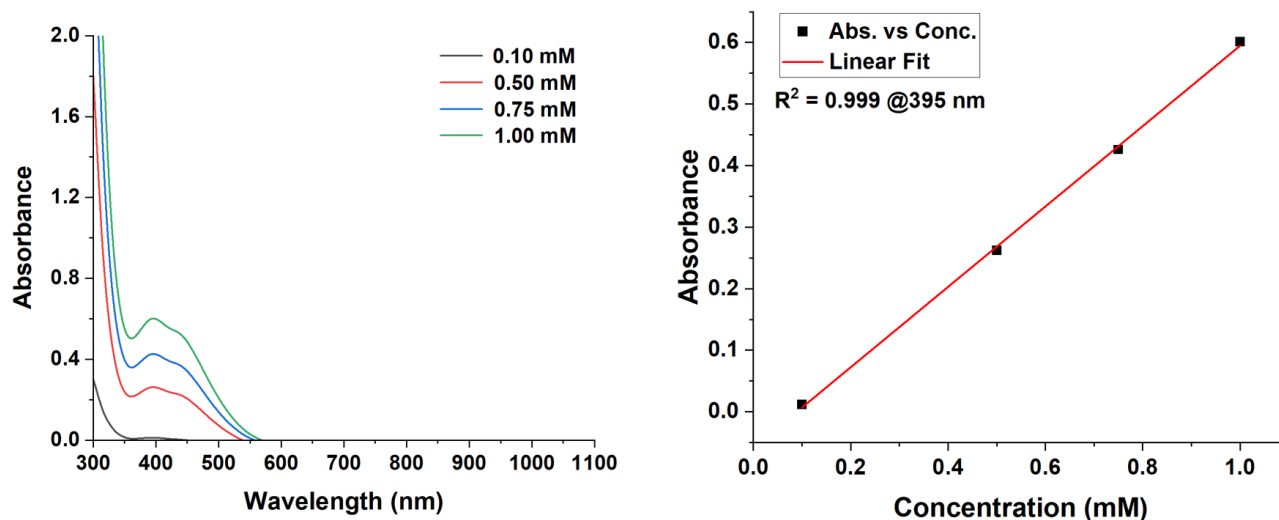


Fig. S45 UV/Vis/NIR spectra of complex **2** in toluene.

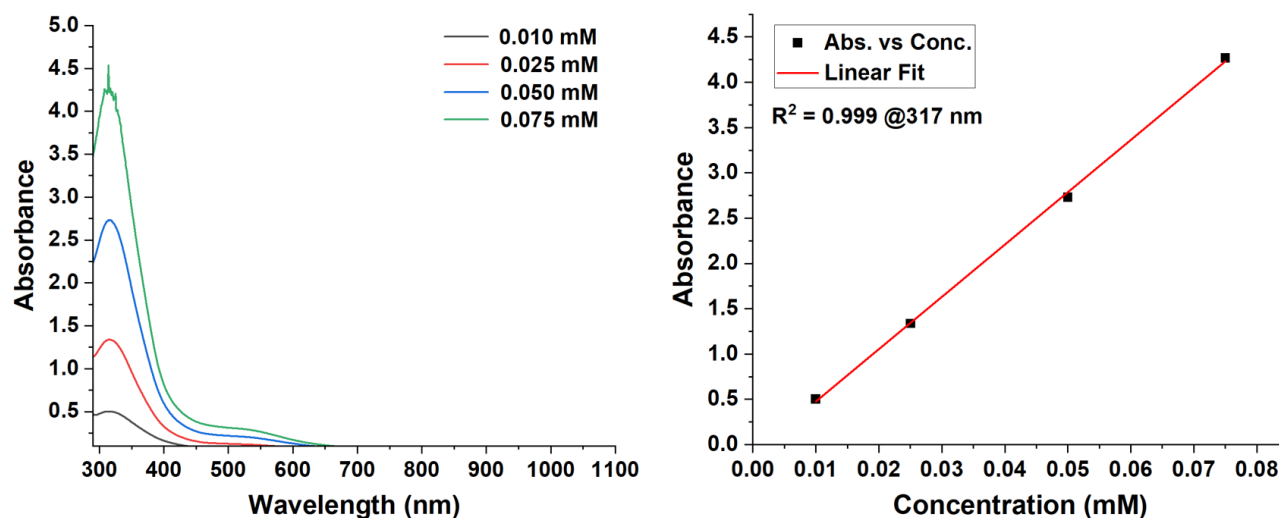


Fig. S46 UV/Vis/NIR spectra of complex **3** in toluene.

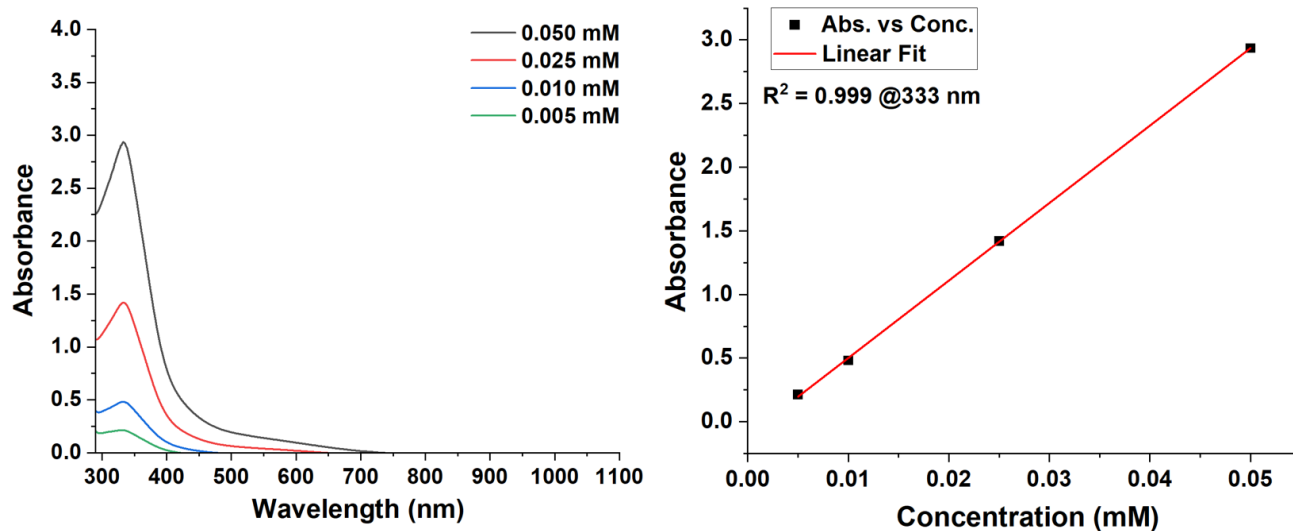


Fig. S47 UV/Vis/NIR spectra of complex 4 in toluene.

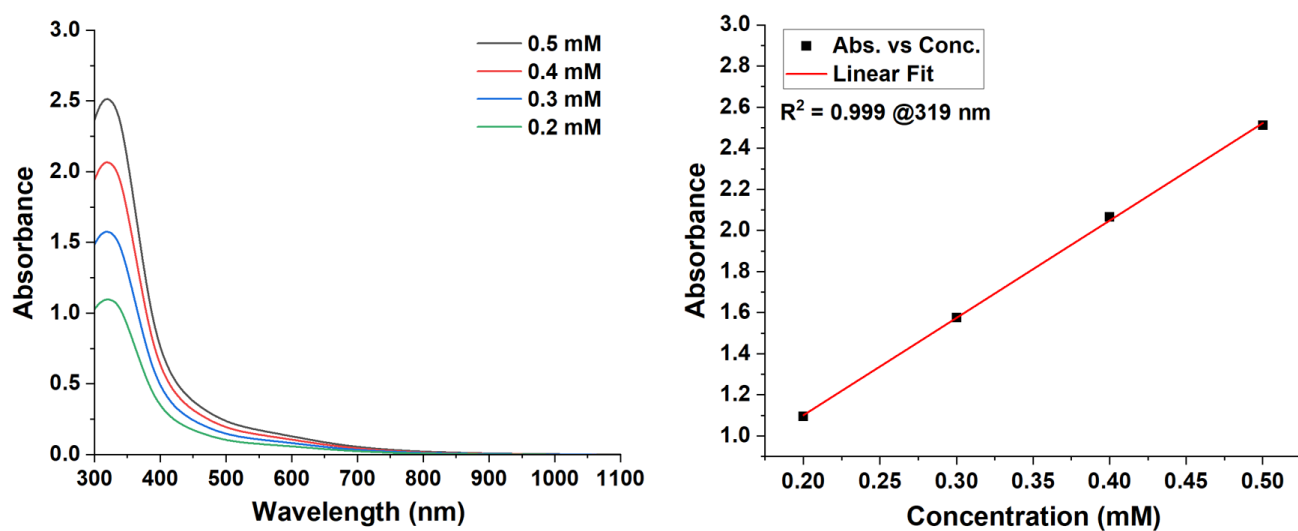


Fig. S48 UV/Vis/NIR spectra of complex 6 in toluene.

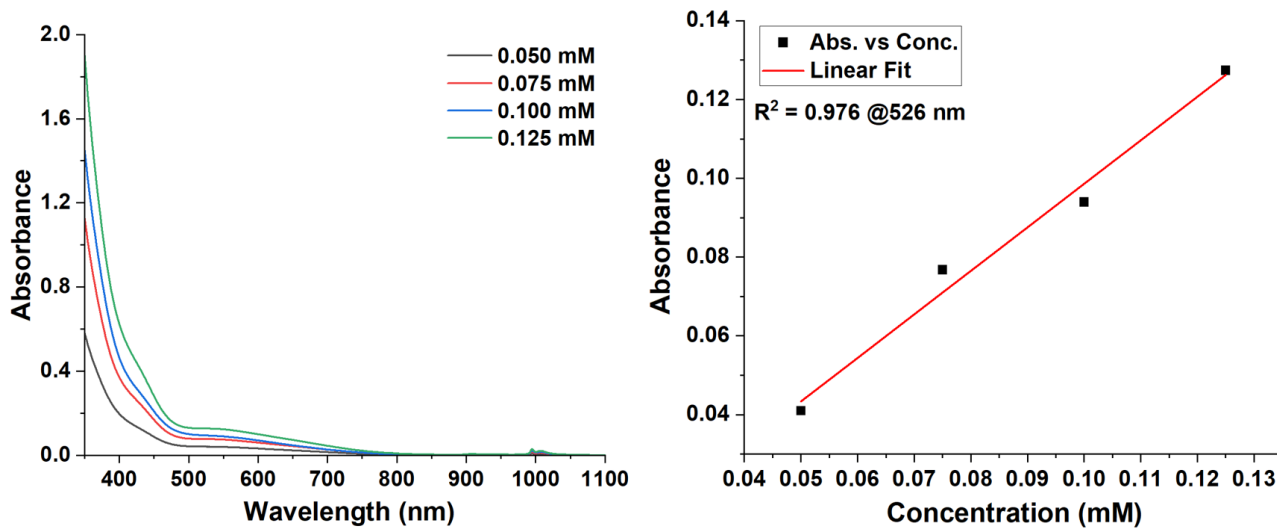


Fig. S49 UV/Vis/NIR spectra of complex 7 in toluene.

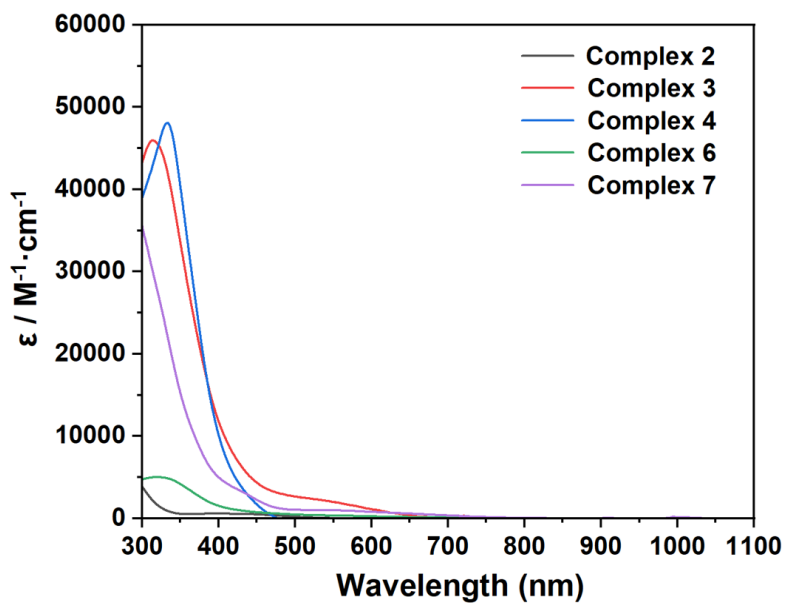


Fig. S50 Co-plotted UV/Vis/NIR spectra of complexes 2, 3, 4, 6 and 7 in toluene.

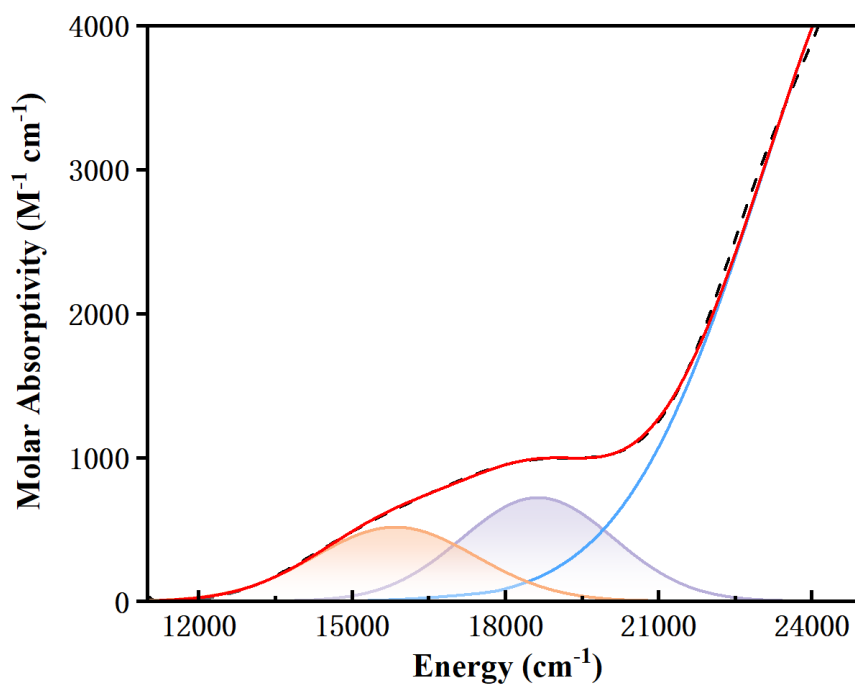


Fig. S51 Gaussian fit for complex **7** in toluene at 27 °C. The orange, purple, and blue lines represent the individual Gaussian peaks which are added together in the overall fit (red line).

Table S2 Fit parameters electronic absorption spectra of complex **7**.

Temp (°C)	ϵ ($M^{-1} \text{ cm}^{-1}$)	ν_{max} (cm^{-1})	$\Delta\nu_{1/2}$ (cm^{-1})	Γ
27 °C	722.9	18634	3500	0.47
27 °C	517.1	15846	3709	0.39

Computational details

DFT calculations were carried out by employing hybrid functional (B3PW91)¹² along with small core pseudopotential Stuttgart basis set^{13,14} for ytterbium, phosphorus and silicon atoms (polarization functions¹⁵ were added for phosphorus and silicon atoms), and Pople basis set^{16–18} (6-31G**) for the rest of the atoms. Dispersion corrections were included in our calculations by employing D3 version of Grimme's dispersion with Becke-Johnson damping¹⁹. Frequency calculations were performed to locate minima for the optimized structures. All the calculations were performed using Gaussian 09 suite of programs.²⁰ Natural bond order analysis was carried out by employing NBO 6.0 version, as implemented in gaussian program.²¹ AIM analysis was performed using Multiwfn software.²² TDDFT was carried out to obtain the UV-Visible spectrum of complex **7** by computing 200 states.

Table S3 Comparison of bond distances (Å) between selected atoms in DFT optimized and X-ray structure for complex **3**.

Atom labels	DFT		X-ray
	No dispersion	dispersion	
Yb3-P1	3.04	2.94	2.99
Yb1-P1	3.02	2.92	2.94
Yb2-P1	2.97	2.88	2.95
Yb4-P1	2.99	2.87	2.94
Yb1-P2	3.01	2.90	2.93
Yb2-P2	2.98	2.87	2.92
Yb3-P4	3.04	2.89	2.95
Yb4-P4	2.99	2.86	2.92
Yb3-P3	3.00	2.87	2.94
Yb2-P3	2.94	2.83	2.90
Yb1-P5	2.97	2.92	2.94
Yb4-P5	2.97	2.85	2.92
Yb3-O2	2.50	2.44	2.45
Yb1-O4	2.50	2.44	2.46
Yb2-O1	2.48	2.40	2.42
Yb4-O3	2.48	2.42	2.44
Yb1-C5	2.62	2.58	2.61
Yb4-C5	2.62	2.56	2.59

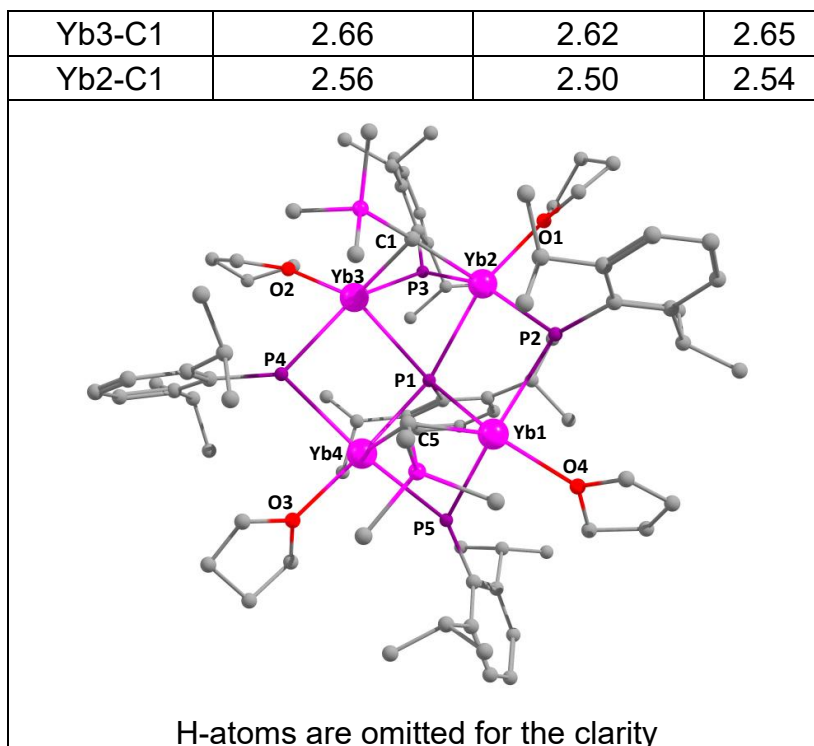


Table S4 Computed natural charges for selected atoms in complex **3**.

Atom labels	Natural charges	
	No dispersion	dispersion
Yb3	1.22352	1.00080
Yb1	1.17483	1.02860
Yb2	1.07593	0.92036
Yb4	1.16898	1.01752
P1	-0.71955	-0.51637
P2	-0.26898	-0.18763
P4	-0.28365	-0.20384
P3	-0.24846	-0.14636
P5	-0.26728	-0.18341
O2	-0.63811	-0.62721
O4	-0.63812	-0.62781
O1	-0.63381	-0.62895
O3	-0.63950	-0.63503
C5	-1.63170	-1.60305
C1	-1.61859	-1.58681

Table S5 Computed Wiberg bond index between selected atoms in complex **3**.

Atom labels	Wiberg bond index	
	No dispersion	dispersion
Yb3-P1	0.3121	0.3590

Yb1-P1	0.2687	0.3312
Yb2-P1	0.2993	0.3601
Yb4-P1	0.1313	0.1534
Yb1-P2	0.2085	0.2365
Yb2-P2	0.3316	0.3656
Yb3-P4	0.2807	0.3174
Yb4-P4	0.3155	0.3194
Yb3-P3	0.1330	0.1470
Yb2-P3	0.2411	0.2523
Yb1-P5	0.3611	0.3946
Yb4-P5	0.3045	0.3454
Yb3-O2	0.3433	0.3856
Yb1-O4	0.1414	0.1517
Yb2-O1	0.2808	0.3068
Yb4-O3	0.3315	0.3876
Yb1-C5	0.2866	0.3160
Yb4-C5	0.3235	0.3798
Yb3-C1	0.1339	0.1454
Yb2-C1	0.2410	0.2490

Bonding orbitals between ytterbium and atoms in the first coordination sphere of metal in complex 3 (dispersion)

(1.69952) BD (1)Yb 3- P 1

(9.10%) 0.3016*Yb 1 s(16.17%)p 0.00(0.07%)d 5.17(83.62%) f 0.01(0.12%)g 0.00(0.02%)

(90.90%) 0.9534* P 5 s(38.75%)p 1.58(61.23%)d 0.00(0.02%)

(1.72628) BD (1)Yb 1- P 1

(9.38%) 0.3062*Yb 2 s(15.62%)p 0.00(0.05%)d 5.39(84.19%) f 0.01(0.12%)g 0.00(0.02%)

(90.62%) 0.9520* P 5 s(42.56%)p 1.35(57.42%)d 0.00(0.02%)

Bonding orbitals between ytterbium and atoms in the first coordination sphere of metal in complex 3 (no dispersion)

(1.75316) BD (1)Yb 3- P 1

(7.25%) 0.2693*Yb 1 s(25.04%)p 0.01(0.15%)d 2.98(74.66%) f 0.01(0.13%)g 0.00(0.02%)

(92.75%) 0.9631* P 5 s(38.73%)p 1.58(61.25%)d 0.00(0.02%)

(1.77783) BD (1)Yb 1- P 1

(8.16%) 0.2857*Yb 2 s(23.68%)p 0.01(0.12%)d 3.21(76.05%) f 0.01(0.13%)g 0.00(0.02%)

(91.84%) 0.9583* P 5 s(42.23%)p 1.37(57.75%)d 0.00(0.02%)

Table S6 NBO Second order perturbation analysis for complex **3** (dispersion).

Donor NBO	Acceptor NBO	E(2) kcal/ mol
(1.65103) LP (1) P 1 s(1.58%)p62.12(98.41%)d 0.01(0.01%)	(0.12810) LV (3)Yb 3 s(0.83%)p 0.11(0.09%)d99.99(98.99%)f 0.08(0.06%)g 0.02(0.01%)	6.10
(1.65103) LP (1) P 1 s(1.58%)p62.12(98.41%)d 0.01(0.01%)	(0.10992) LV (4)Yb 3 s(27.19%)p 0.01(0.16%)d 2.67(72.56%)f 0.00(0.08%)g 0.00(0.01%)	8.89
(1.65103) LP (1) P 1 s(1.58%)p62.12(98.41%)d 0.01(0.01%)	(0.12041) LV (3)Yb 1 s(13.90%)p 0.01(0.13%)d 6.18(85.91%)f 0.00(0.06%)g 0.00(0.01%)	6.99
(1.65103) LP (1) P 1 s(1.58%)p62.12(98.41%)d 0.01(0.01%)	(0.23261) LV (2)Yb 2 s(33.01%)p 0.00(0.05%)d 2.02(66.81%)f 0.00(0.12%)g 0.00(0.01%)	8.07
(1.65103) LP (1) P 1 s(1.58%)p62.12(98.41%)d 0.01(0.01%)	(0.12845) LV (4)Yb 2 s(24.20%)p 0.00(0.05%)d 3.12(75.61%)f 0.01(0.12%)g 0.00(0.02%)	4.71
(1.69952) BD (1)Yb 3- P 1 (9.10%) 0.3016*Yb 3 s(16.17%)p 0.00(0.07%)d 5.17(83.62%) f 0.01(0.12%)g 0.00(0.02%) (90.90%) 0.9534* P 1 s(38.75%)p 1.58(61.23%)d 0.00(0.02%)	(0.36958) LV (1)Yb 2 s(11.98%)p 0.00(0.01%)d 7.34(87.93%)f 0.01(0.07%)g 0.00(0.01%)	10.39
(1.69952) BD (1)Yb 3- P 1 (9.10%) 0.3016*Yb 3 s(16.17%)p 0.00(0.07%)d 5.17(83.62%) f 0.01(0.12%)g 0.00(0.02%) (90.90%) 0.9534* P 1 s(38.75%)p 1.58(61.23%)d 0.00(0.02%)	(0.23261) LV (2)Yb 2 s(33.01%)p 0.00(0.05%)d 2.02(66.81%)f 0.00(0.12%)g 0.00(0.01%)	75.81
(1.69952) BD (1)Yb 3- P 1 (9.10%) 0.3016*Yb 3 s(16.17%)p 0.00(0.07%)d 5.17(83.62%) f 0.01(0.12%)g 0.00(0.02%) (90.90%) 0.9534* P 1 s(38.75%)p 1.58(61.23%)d 0.00(0.02%)	(0.19211) LV (3)Yb 2 s(11.53%)p 0.00(0.05%)d 7.66(88.31%)f 0.01(0.10%)g 0.00(0.01%)	12.88

(1.69952) BD (1)Yb 3- P 1 (9.10%) 0.3016*Yb 3 s(16.17%)p 0.00(0.07%)d 5.17(83.62%) f 0.01(0.12%)g 0.00(0.02%) (90.90%) 0.9534* P 1 s(38.75%)p 1.58(61.23%)d 0.00(0.02%)	(0.11786) LV (5)Yb 2 s(14.24%)p 0.01(0.12%)d 6.00(85.50%)f 0.01(0.13%)g 0.00(0.01%)	5.09
(1.72628) BD (1)Yb 1- P 1 (9.38%) 0.3062*Yb 1 s(15.62%)p 0.00(0.05%)d 5.39(84.19%) f 0.01(0.12%)g 0.00(0.02%) (90.62%) 0.9520* P 1 s(42.56%)p 1.35(57.42%)d 0.00(0.02%)	(0.23261) LV (2)Yb 2 s(33.01%)p 0.00(0.05%)d 2.02(66.81%)f 0.00(0.12%)g 0.00(0.01%)	15.42
(1.65103) LP (1) P 1 s(1.58%)p62.12(98.41%)d 0.01(0.01%)	(0.20778) LV (2)Yb 4 s(30.64%)p 0.00(0.10%)d 2.26(69.16%)f 0.00(0.09%)g 0.00(0.02%)	13.23
(1.69952) BD (1)Yb 3- P 1 (9.10%) 0.3016*Yb 3 s(16.17%)p 0.00(0.07%)d 5.17(83.62%) f 0.01(0.12%)g 0.00(0.02%) (90.90%) 0.9534* P 1 s(38.75%)p 1.58(61.23%)d 0.00(0.02%)	(0.20778) LV (2)Yb 4 s(30.64%)p 0.00(0.10%)d 2.26(69.16%)f 0.00(0.09%)g 0.00(0.02%)	7.32
(1.72628) BD (1)Yb 1- P 1 (9.38%) 0.3062*Yb 1 s(15.62%)p 0.00(0.05%)d 5.39(84.19%) f 0.01(0.12%)g 0.00(0.02%) (90.62%) 0.9520* P 1 s(42.56%)p 1.35(57.42%)d 0.00(0.02%)	(0.33310) LV (1)Yb 4 s(10.64%)p 0.00(0.02%)d 8.39(89.26%)f 0.01(0.07%)g 0.00(0.01%)	9.92
(1.72628) BD (1)Yb 1- P 1 (9.38%) 0.3062*Yb 1 s(15.62%)p 0.00(0.05%)d 5.39(84.19%) f 0.01(0.12%)g 0.00(0.02%) (90.62%) 0.9520* P 1 s(42.56%)p 1.35(57.42%)d 0.00(0.02%)	(0.20778) LV (2)Yb 4 s(30.64%)p 0.00(0.10%)d 2.26(69.16%)f 0.00(0.09%)g 0.00(0.02%)	56.60
(1.72628) BD (1)Yb 1- P 1 (9.38%) 0.3062*Yb 1 s(15.62%)p 0.00(0.05%)d 5.39(84.19%) f 0.01(0.12%)g 0.00(0.02%) (90.62%) 0.9520* P 1 s(42.56%)p 1.35(57.42%)d 0.00(0.02%)	(0.18191) LV (3)Yb 4 s(18.43%)p 0.00(0.07%)d 4.42(81.39%)f 0.01(0.10%)g 0.00(0.01%)	16.23
(1.74295) LP (1) P 2 s(1.58%)p62.12(98.41%)d 0.01(0.01%)	(0.30513) LV (1)Yb 1 s(36.57%)p 0.00(0.07%)d 1.73(63.24%)f 0.00(0.10%)g	77.22

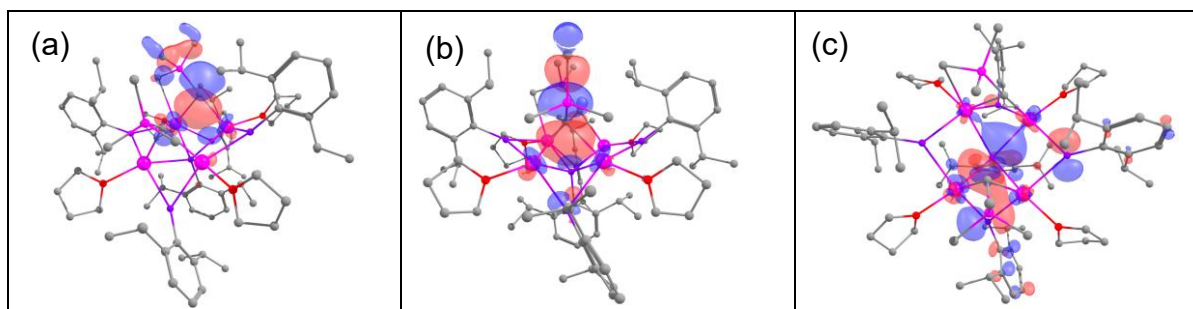
	0.00(0.02%)	
(1.74295) LP (1) P 2 s(1.58%)p62.12(98.41%)d 0.01(0.01%)	(0.09927) LV (4)Yb 1 s(16.15%)p 0.01(0.22%)d 5.17(83.46%)f 0.01(0.16%)g 0.00(0.01%)	4.75
(1.69941) LP (2) P 2 s(49.50%)p 1.02(50.46%)d 0.00(0.04%)	(0.30138) LV (1)Yb 3 s(37.20%)p 0.00(0.03%)d 1.68(62.67%)f 0.00(0.08%)g 0.00(0.01%)	6.48
(1.69941) LP (2) P 2 s(49.50%)p 1.02(50.46%)d 0.00(0.04%)	(0.30513) LV (1)Yb 1 s(36.57%)p 0.00(0.07%)d 1.73(63.24%)f 0.00(0.10%)g 0.00(0.02%)	18.37
(1.69941) LP (2) P 2 s(49.50%)p 1.02(50.46%)d 0.00(0.04%)	(0.12041) LV (3)Yb 1 s(13.90%)p 0.01(0.13%)d 6.18(85.91%)f 0.00(0.06%)g 0.00(0.01%)	9.97
(1.69941) LP (2) P 2 s(49.50%)p 1.02(50.46%)d 0.00(0.04%)	(0.07178) BD*(1)Yb 1- P 1 (90.62%) 0.9520*Yb 1 s(15.62%)p 0.00(0.05%)d 5.39(84.19%)f 0.01(0.12%)g 0.00(0.02%) (9.38%) -0.3062* P 1 s(42.56%)p 1.35(57.42%)d 0.00(0.02%)	5.86
(1.74295) LP (1) P 2 s(1.58%)p62.12(98.41%)d 0.01(0.01%)	(0.19211) LV (3)Yb 2 s(11.53%)p 0.00(0.05%)d 7.66(88.31%)f 0.01(0.10%)g 0.00(0.01%)	10.92
(1.74295) LP (1) P 2 s(1.58%)p62.12(98.41%)d 0.01(0.01%)	(0.08130) LV (6)Yb 2 s(4.83%)p 0.03(0.12%)d19.62(94.86%)f 0.03(0.15%)g 0.01(0.03%)	5.97
(1.69941) LP (2) P 2 s(49.50%)p 1.02(50.46%)d 0.00(0.04%)	(0.36958) LV (1)Yb 2 s(11.98%)p 0.00(0.01%)d 7.34(87.93%)f 0.01(0.07%)g 0.00(0.01%)	121.7 3
(1.69941) LP (2) P 2 s(49.50%)p 1.02(50.46%)d 0.00(0.04%)	(0.23261) LV (2)Yb 2 s(33.01%)p 0.00(0.05%)d 2.02(66.81%)f 0.00(0.12%)g 0.00(0.01%)	12.10
(1.74295) LP (1) P 2 s(1.58%)p62.12(98.41%)d 0.01(0.01%)	(0.33310) LV (1)Yb 4 s(10.64%)p 0.00(0.02%)d 8.39(89.26%)f 0.01(0.07%)g 0.00(0.01%)	5.17

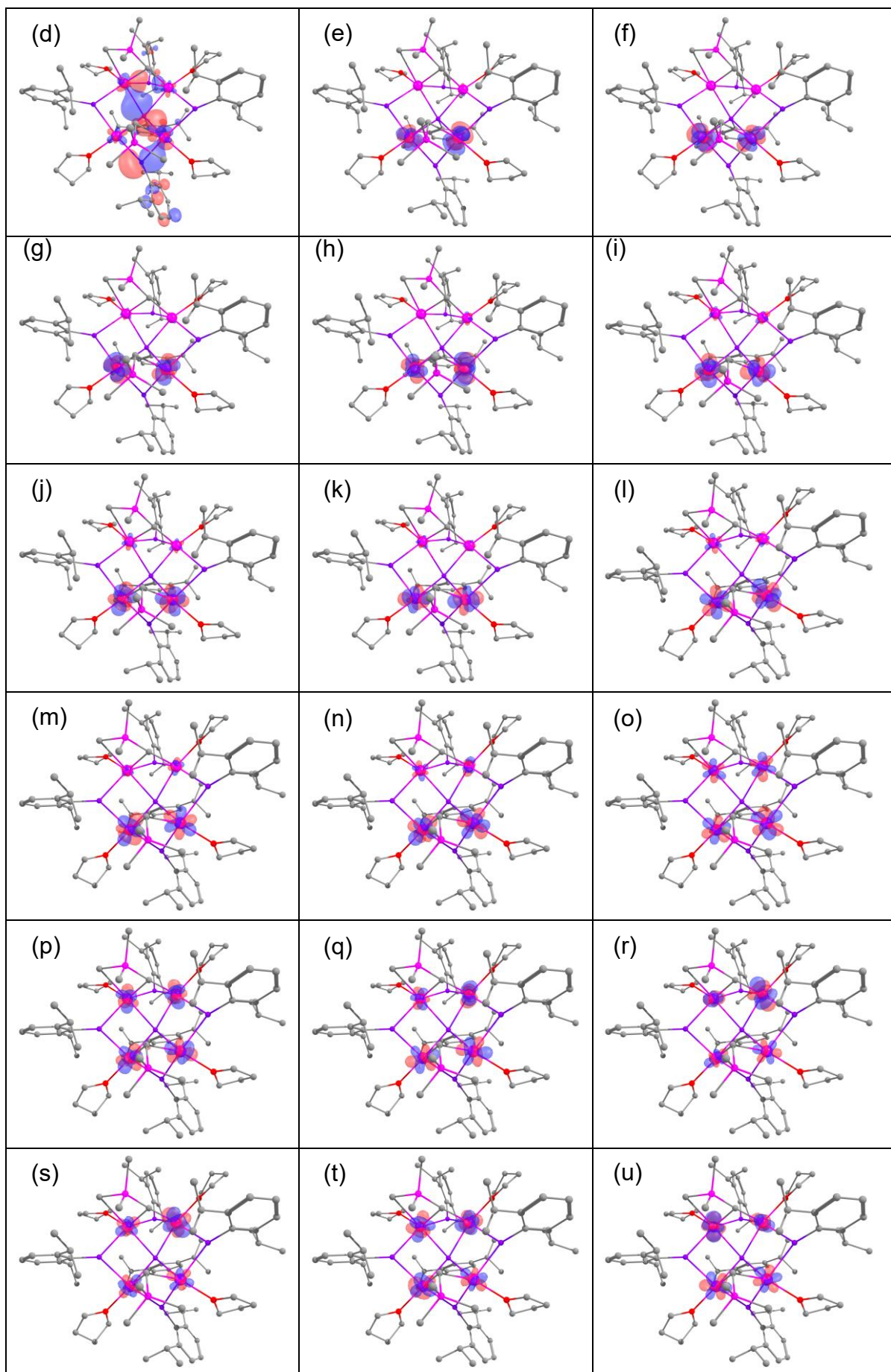
(1.74616) LP (1) P 4 s(9.24%)p 9.82(90.72%)d 0.00(0.04%)	(0.30138) LV (1)Yb 3 s(37.20%)p 0.00(0.03%)d 1.68(62.67%)f 0.00(0.08%)g 0.00(0.01%)	5.87
(1.74616) LP (1) P 4 s(9.24%)p 9.82(90.72%)d 0.00(0.04%)	(0.18423) LV (2)Yb 3 s(18.35%)p 0.00(0.05%)d 4.44(81.40%)f 0.01(0.19%)g 0.00(0.02%)	9.24
(1.74616) LP (1) P 4 s(9.24%)p 9.82(90.72%)d 0.00(0.04%)	(0.30513) LV (1)Yb 1 s(36.57%)p 0.00(0.07%)d 1.73(63.24%)f 0.00(0.10%)g 0.00(0.02%)	7.27
(1.72329) LP (2) P 4 s(54.92%)p 0.82(45.04%)d 0.00(0.04%)	(0.30138) LV (1)Yb 3 s(37.20%)p 0.00(0.03%)d 1.68(62.67%)f 0.00(0.08%)g 0.00(0.01%)	93.26
(1.72329) LP (2) P 4 s(54.92%)p 0.82(45.04%)d 0.00(0.04%)	(0.12810) LV (3)Yb 3 s(0.83%)p 0.11(0.09%)d99.99(98.99%)f 0.08(0.06%)g 0.02(0.01%)	19.46
(1.72329) LP (2) P 4 s(54.92%)p 0.82(45.04%)d 0.00(0.04%)	(0.07855) LV (5)Yb 3 s(0.16%)p 0.93(0.15%)d99.99(99.62%)f 0.44(0.07%)g 0.09(0.01%)	6.07
(1.72329) LP (2) P 4 s(54.92%)p 0.82(45.04%)d 0.00(0.04%)	(0.08408) BD*(1)Yb 3- P 1 (90.90%) 0.9534*Yb 3 s(16.17%)p 0.00(0.07%)d 5.17(83.62%) f 0.01(0.12%)g 0.00(0.02%) (9.10%) -0.3016* P 1 s(38.75%)p 1.58(61.23%)d 0.00(0.02%)	11.15
(1.72329) LP (2) P 4 s(54.92%)p 0.82(45.04%)d 0.00(0.04%)	(0.36958) LV (1)Yb 2 s(11.98%)p 0.00(0.01%)d 7.34(87.93%)f 0.01(0.07%)g 0.00(0.01%)	5.36
(1.74616) LP (1) P 4 s(9.24%)p 9.82(90.72%)d 0.00(0.04%)	(0.33310) LV (1)Yb 4 s(10.64%)p 0.00(0.02%)d 8.39(89.26%)f 0.01(0.07%)g 0.00(0.01%)	77.68
(1.74616) LP (1) P 4 s(9.24%)p 9.82(90.72%)d 0.00(0.04%)	(0.20778) LV (2)Yb 4 s(30.64%)p 0.00(0.10%)d 2.26(69.16%)f 0.00(0.09%)g 0.00(0.02%)	7.55
(1.74616) LP (1) P 4	(0.18191) LV (3)Yb 4	5.73

s(9.24%)p 9.82(90.72%)d 0.00(0.04%)	s(18.43%)p 0.00(0.07%)d 4.42(81.39%)f 0.01(0.10%)g 0.00(0.01%)	
(1.74616) LP (1) P 4 s(9.24%)p 9.82(90.72%)d 0.00(0.04%)	(0.06354) LV (6) Yb 4 s(8.14%)p 0.03(0.21%)d11.24(91.58%)f 0.01(0.05%)g 0.00(0.01%)	5.55
(1.72329) LP (2) P 4 s(54.92%)p 0.82(45.04%)d 0.00(0.04%)	(0.33310) LV (1) Yb 4 s(10.64%)p 0.00(0.02%)d 8.39(89.26%)f 0.01(0.07%)g 0.00(0.01%)	28.88
(1.70288) LP (1) P 3 s(0.15%)p99.99(99.84%)d 0.07(0.01%)	(0.30138) LV (1) Yb 3 s(37.20%)p 0.00(0.03%)d 1.68(62.67%)f 0.00(0.08%)g 0.00(0.01%)	7.24
(1.70288) LP (1) P 3 s(0.15%)p99.99(99.84%)d 0.07(0.01%)	(0.10992) LV (4) Yb 3 s(27.19%)p 0.01(0.16%)d 2.67(72.56%)f 0.00(0.08%)g 0.00(0.01%)	16.94
(1.66634) LP (2) P 3 s(61.72%)p 0.62(38.24%)d 0.00(0.05%)	(0.30138) LV (1) Yb 3 s(37.20%)p 0.00(0.03%)d 1.68(62.67%)f 0.00(0.08%)g 0.00(0.01%)	62.67
(1.70288) LP (1) P 3 s(0.15%)p99.99(99.84%)d 0.07(0.01%)	(0.36958) LV (1) Yb 2 s(11.98%)p 0.00(0.01%)d 7.34(87.93%)f 0.01(0.07%)g 0.00(0.01%)	21.64
(1.70288) LP (1) P 3 s(0.15%)p99.99(99.84%)d 0.07(0.01%)	(0.19211) LV (3) Yb 2 s(11.53%)p 0.00(0.05%)d 7.66(88.31%)f 0.01(0.10%)g 0.00(0.01%)	5.68
(1.70288) LP (1) P 3 s(0.15%)p99.99(99.84%)d 0.07(0.01%)	(0.12845) LV (4) Yb 2 s(24.20%)p 0.00(0.05%)d 3.12(75.61%)f 0.01(0.12%)g 0.00(0.02%)	5.31
(1.70288) LP (1) P 3 s(0.15%)p99.99(99.84%)d 0.07(0.01%)	(0.11786) LV (5) Yb 2 s(14.24%)p 0.01(0.12%)d 6.00(85.50%)f 0.01(0.13%)g 0.00(0.01%)	7.91
(1.66634) LP (2) P 3 s(61.72%)p 0.62(38.24%)d 0.00(0.05%)	(0.36958) LV (1) Yb 2 s(11.98%)p 0.00(0.01%)d 7.34(87.93%)f 0.01(0.07%)g 0.00(0.01%)	78.10

(1.66634) LP (2) P 3 s(61.72%)p 0.62(38.24%)d 0.00(0.05%)	(0.23261) LV (2)Yb 2 s(33.01%)p 0.00(0.05%)d 2.02(66.81%)f 0.00(0.12%)g 0.00(0.01%)	8.05
(1.64639) LP (2) P 5 s(31.01%)p 2.22(68.94%)d 0.00(0.06%)	(0.30513) LV (1)Yb 1 s(36.57%)p 0.00(0.07%)d 1.73(63.24%)f 0.00(0.10%)g 0.00(0.02%)	59.05
(1.64639) LP (2) P 5 s(31.01%)p 2.22(68.94%)d 0.00(0.06%)	(0.07178) BD*(1)Yb 1- P 1 (90.62%) 0.9520*Yb 1 s(15.62%)p 0.00(0.05%)d 5.39(84.19%)f 0.01(0.12%)g 0.00(0.02%) (9.38%) -0.3062* P 1 s(42.56%)p 1.35(57.42%)d 0.00(0.02%)	9.89
(1.76459) LP (1) P 5 s(30.30%)p 2.30(69.69%)d 0.00(0.01%)	(0.33310) LV (1)Yb 4 s(10.64%)p 0.00(0.02%)d 8.39(89.26%)f 0.01(0.07%)g 0.00(0.01%)	56.03
(1.76459) LP (1) P 5 s(30.30%)p 2.30(69.69%)d 0.00(0.01%)	(0.13146) LV (4)Yb 4 s(31.79%)p 0.01(0.23%)d 2.13(67.80%)f 0.00(0.15%)g 0.00(0.02%)	10.52
(1.64639) LP (2) P 5 s(31.01%)p 2.22(68.94%)d 0.00(0.06%)	(0.33310) LV (1)Yb 4 s(10.64%)p 0.00(0.02%)d 8.39(89.26%)f 0.01(0.07%)g 0.00(0.01%)	27.99
(1.64639) LP (2) P 5 s(31.01%)p 2.22(68.94%)d 0.00(0.06%)	(0.20778) LV (2)Yb 4 s(30.64%)p 0.00(0.10%)d 2.26(69.16%)f 0.00(0.09%)g 0.00(0.02%)	5.41
(1.92073) LP (2) O 2 s(39.73%)p 1.52(60.25%)d 0.00(0.02%)	(0.07855) LV (5)Yb 3 s(0.16%)p 0.93(0.15%)d99.99(99.62%)f 0.44(0.07%)g 0.09(0.01%)	26.22
(1.92073) LP (2) O 2 s(39.73%)p 1.52(60.25%)d 0.00(0.02%)	(0.08408) BD*(1)Yb 3- P 1 (90.90%) 0.9534*Yb 3 s(16.17%)p 0.00(0.07%)d 5.17(83.62%) f 0.01(0.12%)g 0.00(0.02%) (9.10%) -0.3016* P 1 s(38.75%)p 1.58(61.23%)d 0.00(0.02%)	16.33
(1.92302) LP (1) O 4 s(28.44%)p 2.51(71.53%)d 0.00(0.03%)	(0.18107) LV (2)Yb 1 s(11.35%)p 0.01(0.08%)d 7.79(88.46%)f 0.01(0.10%)g	18.49

	0.00(0.01%)	
(1.92302) LP (1) O 4 s(28.44%)p 2.51(71.53%)d 0.00(0.03%)	(0.07091) LV (5)Yb 1 s(6.16%)p 0.01(0.06%)d15.20(93.71%)f 0.01(0.05%)g 0.00(0.01%)	7.57
(1.92302) LP (1) O 4 s(28.44%)p 2.51(71.53%)d 0.00(0.03%)	(0.07178) BD*(1)Yb 1- P 1 (90.62%) 0.9520*Yb 1 s(15.62%)p 0.00(0.05%)d 5.39(84.19%)f 0.01(0.12%)g 0.00(0.02%) (9.38%) -0.3062* P 1 s(42.56%)p 1.35(57.42%)d 0.00(0.02%)	9.78
(1.92130) LP (2) O 4 s(11.81%)p 7.47(88.15%)d 0.00(0.04%)	(0.07091) LV (5)Yb 1 s(6.16%)p 0.01(0.06%)d15.20(93.71%)f 0.01(0.05%)g 0.00(0.01%)	6.13
(1.92130) LP (2) O 4 s(11.81%)p 7.47(88.15%)d 0.00(0.04%)	(0.07178) BD*(1)Yb 1- P 1 (90.62%) 0.9520*Yb 1 s(15.62%)p 0.00(0.05%)d 5.39(84.19%)f 0.01(0.12%)g 0.00(0.02%) (9.38%) -0.3062* P 1 s(42.56%)p 1.35(57.42%)d 0.00(0.02%)	10.79
(1.91963) LP (2) O 1 s(32.51%)p 2.08(67.47%)d 0.00(0.02%)	(0.36958) LV (1)Yb 2 s(11.98%)p 0.00(0.01%)d 7.34(87.93%)f 0.01(0.07%)g 0.00(0.01%)	8.53
(1.91963) LP (2) O 1 s(32.51%)p 2.08(67.47%)d 0.00(0.02%)	(0.23261) LV (2)Yb 2 s(33.01%)p 0.00(0.05%)d 2.02(66.81%)f 0.00(0.12%)g 0.00(0.01%)	26.22
(1.91963) LP (2) O 1 s(32.51%)p 2.08(67.47%)d 0.00(0.02%)	(0.08130) LV (6)Yb 2 s(4.83%)p 0.03(0.12%)d19.62(94.86%)f 0.03(0.15%)g 0.01(0.03%)	7.23





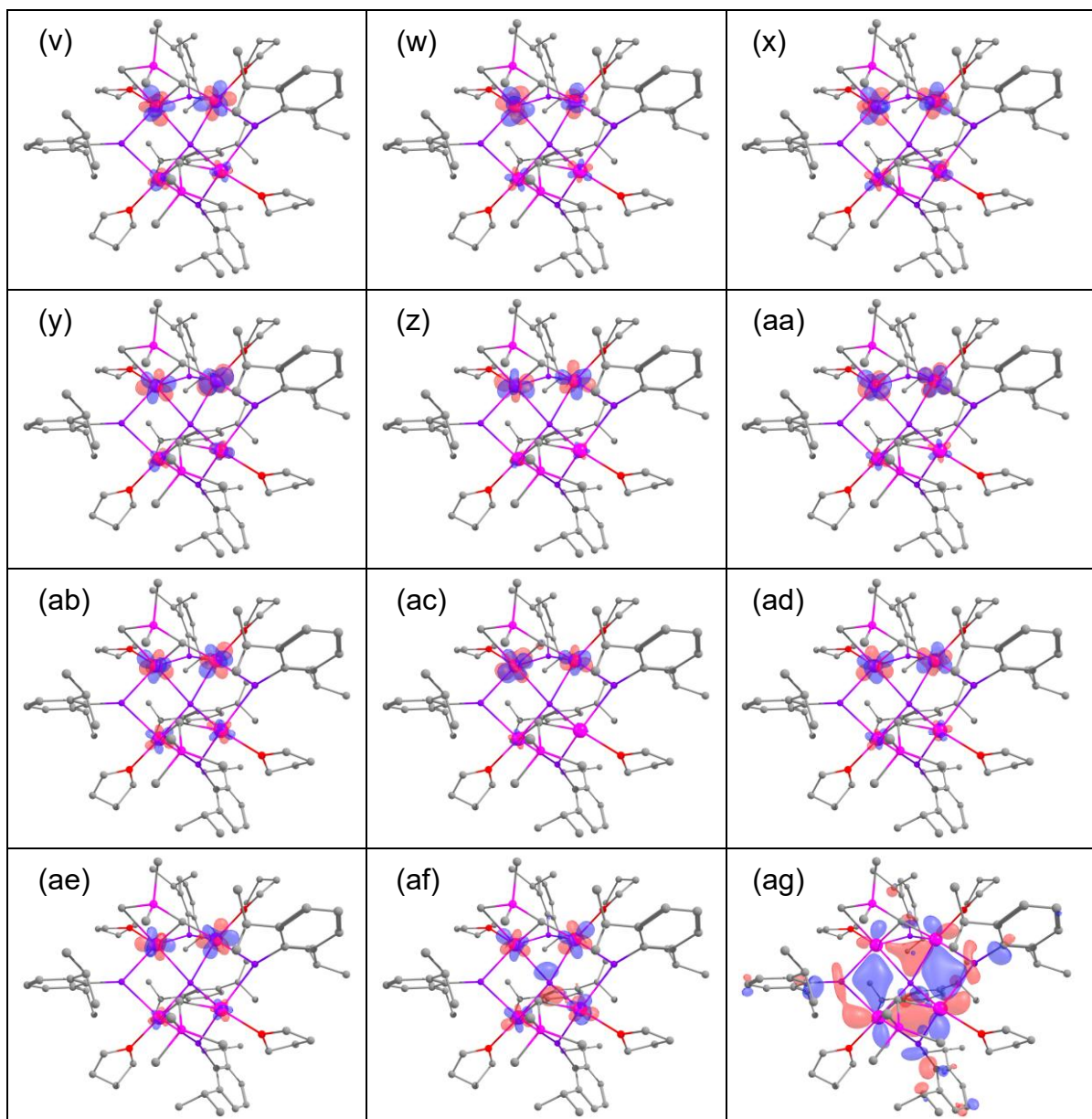


Fig. S52 Computed MOs for complex **3** (dispersion). (a)HOMO-35 (b)HOMO-34 (c)HOMO-30 (d)HOMO-28 (e)HOMO-27 (f)HOMO-26 (g)HOMO-25 (h)HOMO-24 (i)HOMO-23 (j)HOMO-22 (k)HOMO-21 (l)HOMO-20 (m)HOMO-19 (n)HOMO-18 (o)HOMO-17 (p)HOMO-16 (q)HOMO-15 (r)HOMO-14 (s)HOMO-13 (t)HOMO-12 (u)HOMO-11 (v)HOMO-10 (w)HOMO-9 (x)HOMO-8 (y)HOMO-7 (z)HOMO-6 (aa)HOMO-5 (ab)HOMO-4 (ac)HOMO-3 (ad)HOMO-2 (ae)HOMO-1 (af)HOMO (ag)LUMO.

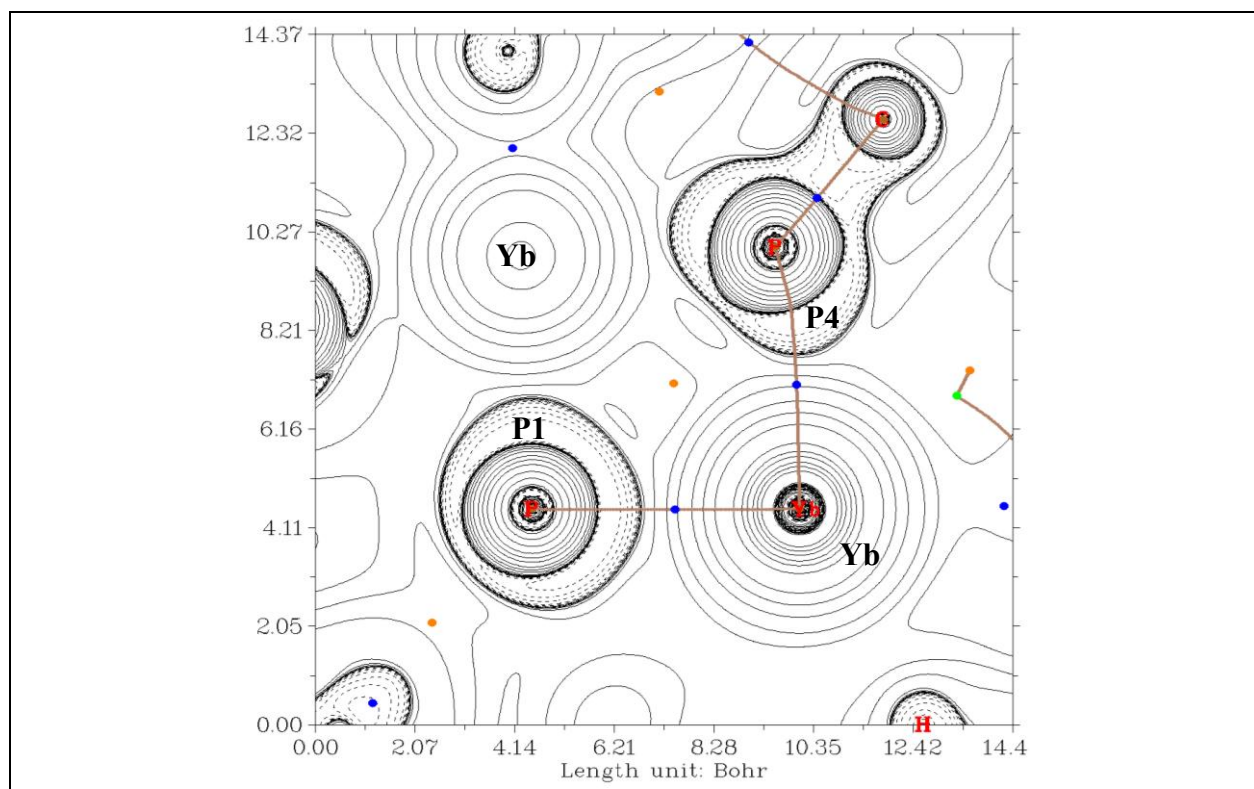
Table S7 NBO analysis of canonical molecular orbitals for complex **3** (dispersion).

MO 410 (occ): orbital energy = - 0.16339 a.u. 0.419*[169]: LP (1) P 1(lp)	(1.65103) LP (1) P 1 s(1.58%)p62.12(98.41%)d 0.01(0.01%)
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<p>-0.369*[191]: BD (1)Yb 3- P 1 -0.296*[176]: LP (1) P 5(lp) 0.269*[192]: BD (1)Yb 1- P 1 -0.229*[170]: LP (1) P 2(lp)</p>	<p><u>(1.69952) BD (1)Yb 3- P 1</u> (9.10%) 0.3016*Yb 3 s(16.17%)p 0.00(0.07%)d 5.17(83.62%)f 0.01(0.12%)g 0.00(0.02%) (90.90%) 0.9534* P 1 s(38.75%)p 1.58(61.23%)d 0.00(0.02%) <u>(1.76459) LP (1) P 5</u> s(30.30%)p 2.30(69.69%)d 0.00(0.01%) <u>(1.72628) BD (1)Yb 1- P 1</u> (9.38%) 0.3062*Yb 1 s(15.62%)p 0.00(0.05%)d 5.39(84.19%)f 0.01(0.12%)g 0.00(0.02%) (90.62%) 0.9520* P 1 s(42.56%)p 1.35(57.42%)d 0.00(0.02%) <u>(1.74295) LP (1) P 2</u> s(13.74%)p 6.28(86.25%)d 0.00(0.01%)</p>
<p>MO 412 (occ): orbital energy = - 0.15267 a.u. 0.355*[192]: BD (1)Yb 1- P 1 -0.320*[177]: LP (2) P 5(lp) 0.306*[176]: LP (1) P 5(lp) -0.300*[191]: BD (1)Yb 3- P 1 -0.297*[174]: LP (1) P 3(lp) -0.294*[169]: LP (1) P 1(lp)</p>	<p><u>(1.72628) BD (1)Yb 1- P 1</u> (9.38%) 0.3062*Yb 1 s(15.62%)p 0.00(0.05%)d 5.39(84.19%)f 0.01(0.12%)g 0.00(0.02%) (90.62%) 0.9520* P 1 s(42.56%)p 1.35(57.42%)d 0.00(0.02%) <u>(1.64639) LP (2) P 5</u> s(31.01%)p 2.22(68.94%)d 0.00(0.06%) <u>(1.76459) LP (1) P 5</u> s(30.30%)p 2.30(69.69%)d 0.00(0.01%) <u>(1.69952) BD (1)Yb 3- P 1</u> (9.10%) 0.3016*Yb 3 s(16.17%)p 0.00(0.07%)d 5.17(83.62%)f 0.01(0.12%)g 0.00(0.02%) (90.90%) 0.9534* P 1 s(38.75%)p 1.58(61.23%)d 0.00(0.02%) <u>(1.70288) LP (1) P 3</u> s(0.15%)p99.99(99.84%)d 0.07(0.01%) <u>(1.65103) LP (1) P 1</u> s(1.58%)p62.12(98.41%)d 0.01(0.01%)</p>

Table S8 Computed BCP descriptors for complex **3** (dispersion).

Atom labels	$\rho(r)$	$\nabla^2\rho(r)$	$G(r)$	$V(r)$	$H(r)$	ε
Yb3-P1	0.03	0.07	0.02	-0.02	-0.003	0.21
Yb1-P1	0.03	0.07	0.02	-0.02	-0.004	0.26
Yb2-P1	0.03	0.07	0.02	-0.03	-0.004	0.22
Yb4-P1	0.04	0.07	0.02	-0.03	-0.005	0.23
Yb1-P2	0.03	0.07	0.02	-0.02	-0.003	0.05
Yb2-P2	0.03	0.08	0.02	-0.03	-0.004	0.05
Yb3-P4	0.03	0.07	0.02	-0.03	-0.004	0.05
Yb4-P4	0.03	0.08	0.02	-0.03	-0.004	0.05
Yb3-P3	0.03	0.08	0.02	-0.03	-0.004	0.10
Yb2-P3	0.04	0.08	0.03	-0.03	-0.005	0.15
Yb1-P5	0.03	0.07	0.02	-0.03	-0.004	0.09
Yb4-P5	0.03	0.08	0.02	-0.03	-0.003	0.25
Yb3-O2	0.04	0.19	0.04	-0.04	0.003	0.18
Yb1-O4	0.04	0.18	0.04	-0.04	0.003	0.19
Yb2-O1	0.04	0.21	0.05	-0.05	0.003	0.15
Yb4-O3	0.04	0.20	0.05	-0.04	0.003	0.15
Yb1-C5	0.04	0.12	0.03	-0.04	-0.003	0.13
Yb4-C5	0.04	0.12	0.04	-0.04	-0.004	0.18
Yb3-C1	0.04	0.11	0.03	-0.03	-0.003	0.13
Yb2-C1	0.04	0.14	0.04	-0.04	-0.005	0.09



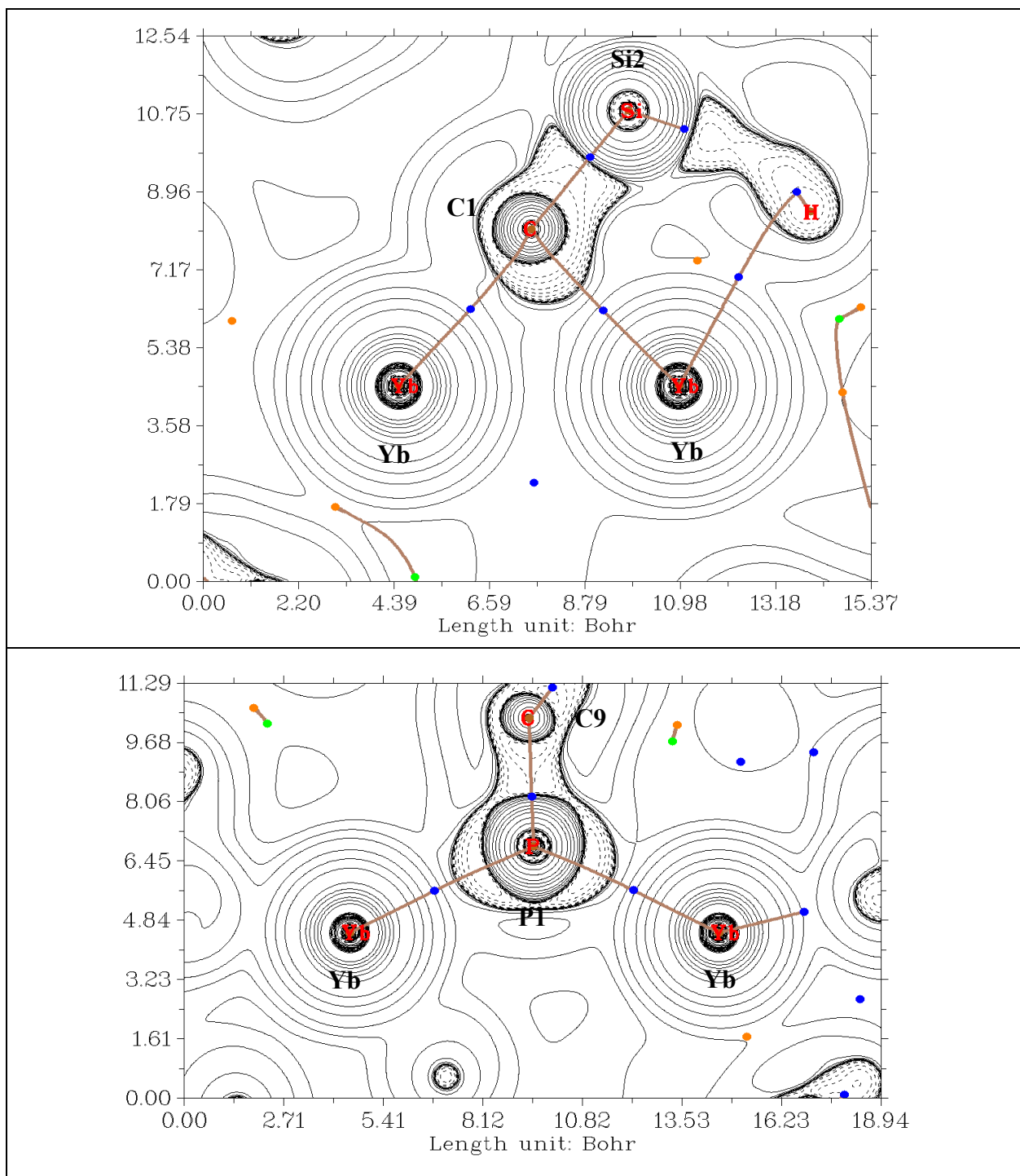


Fig. S53 Computed Laplacian distribution for complex **3** (dispersion).

Table S9 Comparison of bond distance (Å) between selected atoms in DFT optimized and X-ray structure for complex **4**.

Atom labels	DFT		X-ray
	No dispersion	dispersion	
Yb3-P4	2.90	2.86	2.87
Yb3-P3	2.97	2.88	2.92
Yb3-P1	2.83	2.78	2.80

Yb3-P5	2.99	2.88	2.94
Yb5-P4	3.07	2.92	3.02
Yb5-P3	2.93	2.87	2.87
Yb5-P5	3.04	2.92	3.01
Yb5-P6	2.95	2.87	2.93
Yb5-O5	2.47	2.41	2.45
Yb4-P4	2.93	2.88	2.89
Yb4-P3	3.04	2.96	3.00
Yb4-P2	2.91	2.80	2.84
Yb4-P6	3.12	2.96	3.01
Yb4-O4	2.49	2.43	2.46
Yb1-P3	3.12	2.95	3.02
Yb1-P1	2.97	2.92	2.97
Yb1-P2	2.86	2.77	2.80
Yb1-O1	2.56	2.45	2.53
Yb1-O2	2.51	2.43	2.44
Yb2-P4	2.96	2.91	2.95
Yb2-P1	2.82	2.75	2.77
Yb2-P2	2.87	2.81	2.86
Yb2-O3	2.48	2.41	2.45

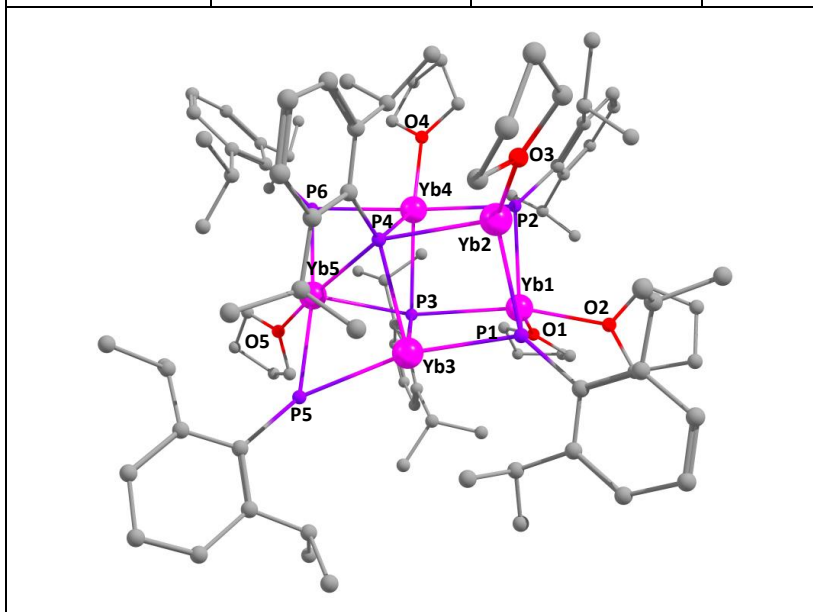


Table S10 Computed natural charges for selected atoms in complex **4**.

Atom label	Natural charges	
	No dispersion	dispersion
Yb3	0.88406	0.68428
Yb5	1.09155	0.89216
Yb4	1.04482	0.83444

Yb1	1.26986	1.12859
Yb2	1.14286	0.89307
P4	-0.68038	-0.48833
P3	-0.70277	-0.51057
P1	-0.79518	-0.62173
P2	-0.83910	-0.64910
P5	-0.28579	-0.19929
P6	-0.25616	-0.17992
O3	-0.64712	-0.63204
O1	-0.63961	-0.63321
O4	-0.63400	-0.62486
O5	-0.63622	-0.61224
O2	-0.64182	-0.63808

Table S11 Computed Wiberg bond index for selected atoms in complex **4**.

Atom labels	DFT	
	No dispersion	dispersion
Yb3-P4	0.4276	0.4484
Yb3-P3	0.4017	0.4438
Yb3-P1	0.4732	0.5096
Yb3-P5	0.3577	0.3892
Yb5-P4	0.2816	0.3501
Yb5-P3	0.3751	0.4120
Yb5-P5	0.2920	0.3252
Yb5-P6	0.3218	0.3514
Yb5-O5	0.1318	0.1520
Yb4-P4	0.3610	0.3886
Yb4-P3	0.3241	0.3643
Yb4-P2	0.3889	0.4451
Yb4-P6	0.2726	0.3304
Yb4-O4	0.1358	0.1478
Yb1-P3	0.2372	0.2853
Yb1-P1	0.3232	0.3453
Yb1-P2	0.3819	0.4442
Yb1-O1	0.1090	0.1270
Yb1-O2	0.1027	0.1145
Yb2-P4	0.3103	0.3489
Yb2-P1	0.4444	0.5285
Yb2-P2	0.4167	0.4730
Yb2-O3	0.1259	0.1530

Bonding orbitals between ytterbium and atoms in the first coordination sphere of metal in complex **4** (dispersion)

(0.89146) BD (1)Yb 3- P 4

(11.12%) 0.3335*Yb 3 s(28.38%)p 0.00(0.08%)d 2.52(71.39%) f 0.00(0.14%)g 0.00(0.01%)

(88.88%) 0.9428* P 4 s(37.05%)p 1.70(62.92%)d 0.00(0.03%)

(0.88787) BD (1)Yb 3- P 3

(10.95%) 0.3310*Yb 3 s(33.39%)p 0.00(0.10%)d 1.99(66.36%) f 0.00(0.13%)g 0.00(0.02%)

(89.05%) 0.9436* P 3 s(39.21%)p 1.55(60.76%)d 0.00(0.04%)

(0.92690) BD (1)Yb 3- P 5

(10.78%) 0.3283*Yb 3 s(34.20%)p 0.00(0.14%)d 1.92(65.55%) f 0.00(0.09%)g 0.00(0.01%)

(89.22%) 0.9446* P 5 s(59.50%)p 0.68(40.47%)d 0.00(0.04%)

(0.94500) BD (1)Yb 5- P 6

(9.30%) 0.3050*Yb 5 s(19.62%)p 0.01(0.11%)d 4.09(80.15%) f 0.01(0.10%)g 0.00(0.01%)

(90.70%) 0.9523* P 6 s(31.12%)p 2.21(68.85%)d 0.00(0.03%)

(0.88647) BD (1)Yb 4- P 4

(9.86%) 0.3140*Yb 4 s(31.54%)p 0.01(0.21%)d 2.16(68.08%) f 0.00(0.15%)g 0.00(0.02%)

(90.14%) 0.9494* P 4 s(43.78%)p 1.28(56.19%)d 0.00(0.03%)

(0.88176) BD (1)Yb 4- P 3

(9.66%) 0.3108*Yb 4 s(31.05%)p 0.00(0.08%)d 2.21(68.75%) f 0.00(0.11%)g 0.00(0.01%)

(90.34%) 0.9505* P 3 s(40.67%)p 1.46(59.30%)d 0.00(0.03%)

(0.88027) BD (1)Yb 4- P 2

(6.18%) 0.2486*Yb 4 s(8.65%)p 0.06(0.54%)d 10.45(90.36%) f 0.05(0.43%)g 0.00(0.02%)

(93.82%) 0.9686* P 2 s(44.32%)p 1.26(55.65%)d 0.00(0.03%)

(0.91230) BD (1)Yb 4- P 6

(7.65%) 0.2766*Yb 4 s(24.39%)p 0.03(0.65%)d 3.06(74.58%) f 0.01(0.36%)g 0.00(0.01%)

(92.35%) 0.9610* P 6 s(30.78%)p 2.25(69.20%)d 0.00(0.02%)

(0.92718) BD (1)Yb 2- P 1

(9.98%) 0.3160*Yb 2 s(23.72%)p 0.01(0.28%)d 3.19(75.77%) f 0.01(0.20%)g 0.00(0.02%)

(90.02%) 0.9488* P 1 s(26.99%)p 2.70(72.99%)d 0.00(0.02%)

(0.90240) BD (1)Yb 2- P 2

(10.88%) 0.3298*Yb 2 s(18.32%)p 0.01(0.14%)d 4.44(81.40%) f 0.01(0.13%)g 0.00(0.01%)

(89.12%) 0.9440* P 2 s(34.84%)p 1.87(65.13%)d 0.00(0.03%)

Bonding orbitals between ytterbium and atoms in the first coordination sphere of metal in complex **4** (no dispersion)

(0.91018) BD (1)Yb 3- P 4
 (9.83%) 0.3135*Yb 3 s(27.76%)p 0.00(0.08%)d 2.59(72.01%) f 0.01(0.14%)g
 0.00(0.01%)
 (90.17%) 0.9496* P 4 s(36.64%)p 1.73(63.32%)d 0.00(0.03%)
 (0.91004) BD (1)Yb 3- P 3
 (8.70%) 0.2949*Yb 3 s(31.32%)p 0.00(0.13%)d 2.18(68.42%) f 0.00(0.11%)g
 0.00(0.01%)
 (91.30%) 0.9555* P 3 s(24.38%)p 3.10(75.59%)d 0.00(0.03%)
 (0.91679) BD (1)Yb 3- P 1
 (8.61%) 0.2934*Yb 3 s(18.04%)p 0.03(0.59%)d 4.50(81.10%) f 0.01(0.26%)g
 0.00(0.02%)
 (91.39%) 0.9560* P 1 s(38.06%)p 1.63(61.91%)d 0.00(0.03%)
 (0.93791) BD (1)Yb 3- P 5
 (7.46%) 0.2731*Yb 3 s(21.88%)p 0.04(0.91%)d 3.52(76.92%) f 0.01(0.27%)g
 0.00(0.02%)
 (92.54%) 0.9620* P 5 s(29.26%)p 2.42(70.71%)d 0.00(0.03%)
 (0.93649) BD (1)Yb 5- P 5
 (5.77%) 0.2401*Yb 5 s(17.82%)p 0.10(1.84%)d 4.47(79.74%) f 0.03(0.56%)g
 0.00(0.03%)
 (94.23%) 0.9707* P 5 s(32.13%)p 2.11(67.85%)d 0.00(0.02%)
 (0.91005) BD (1)Yb 4- P 4
 (8.49%) 0.2913*Yb 4 s(22.24%)p 0.01(0.26%)d 3.48(77.35%) f 0.01(0.14%)g
 0.00(0.02%)
 (91.51%) 0.9566* P 4 s(43.47%)p 1.30(56.50%)d 0.00(0.03%)
 (0.91377) BD (1)Yb 1- P 2
 (7.14%) 0.2673*Yb 1 s(22.47%)p 0.01(0.32%)d 3.43(76.98%) f 0.01(0.20%)g
 0.00(0.03%)
 (92.86%) 0.9636* P 2 s(34.19%)p 1.92(65.78%)d 0.00(0.03%)
 (0.93134) BD (1)Yb 2- P 1
 (8.51%) 0.2917*Yb 2 s(26.52%)p 0.01(0.33%)d 2.75(72.92%) f 0.01(0.21%)g
 0.00(0.02%)
 (91.49%) 0.9565* P 1 s(35.65%)p 1.80(64.32%)d 0.00(0.02%)
 (0.92500) BD (1)Yb 2- P 2
 (8.21%) 0.2865*Yb 1 s(26.16%)p 0.01(0.28%)d 2.80(73.35%) f 0.01(0.19%)g
 0.00(0.02%)
 (91.79%) 0.9581* P 2 s(35.49%)p 1.82(64.48%)d 0.00(0.03%)

Table S12 NBO Second order perturbation analysis for complex **4** (dispersion).

Donor NBO	Acceptor NBO	E(2) kcal/mol
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(0.78188) LP (1) P 4 s(1.78%)p55.04(98.21%)d 0.00(0.01%)	(0.10239) LV (1)Yb 3 s(0.45%)p 0.15(0.07%)d99.99(99.41%) f 0.14(0.06%)g 0.01(0.00%)	8.59
(0.78188) LP (1) P 4 s(1.78%)p55.04(98.21%)d 0.00(0.01%)	(0.13059) LV (1)Yb 5 s(0.42%)p 0.05(0.02%)d99.99(99.47%) f 0.20(0.08%)g 0.01(0.01%)	8.82
(0.78188) LP (1) P 4 s(1.78%)p55.04(98.21%)d 0.00(0.01%)	(0.10058) LV (1)Yb 2 s(33.70%)p 0.00(0.03%)d 1.96(66.19%)f 0.00(0.06%)g 0.00(0.01%)	18.05
(0.78188) LP (1) P 4 s(1.78%)p55.04(98.21%)d 0.00(0.01%)	(0.05643) LV (4)Yb 2 s(0.19%)p 0.14(0.03%)d99.99(99.68%)f 0.46(0.09%)g 0.09(0.02%)	7.24
(0.79533) LP (1) P 3 s(1.94%)p50.56(98.06%)d 0.00(0.00%)	(0.10239) LV (1)Yb 3 s(0.45%)p 0.15(0.07%)d99.99(99.41%) f 0.14(0.06%)g 0.01(0.00%)	11.03
(0.79533) LP (1) P 3 s(1.94%)p50.56(98.06%)d 0.00(0.00%)	(0.13059) LV (1)Yb 5 s(0.42%)p 0.05(0.02%)d99.99(99.47%) f 0.20(0.08%)g 0.01(0.01%)	13.62
(0.79533) LP (1) P 3 s(1.94%)p50.56(98.06%)d 0.00(0.00%)	(0.06873) LV (1)Yb 4 s(0.05%)p 0.78(0.04%)d99.99(99.85%) f 1.02(0.05%)g 0.04(0.00%)	8.32
(0.80028) LP (1) P 1 s(48.32%)p 1.07(51.65%)d 0.00(0.03%)	(0.10413) BD*(1)Yb 3- P 5 (89.22%) 0.9446*Yb 3 s(34.20%)p 0.00(0.14%)d 1.92(65.55%) f 0.00(0.09%)g 0.00(0.01%) (10.78%) -0.3283* P 5 s(59.50%)p 0.68(40.47%)d 0.00(0.04%)	72.09
(0.88670) LP (1) P 5 s(3.00%)p32.27(96.98%)d 0.01(0.02%)	(0.10239) LV (1)Yb 3 s(0.45%)p 0.15(0.07%)d99.99(99.41%) f 0.14(0.06%)g 0.01(0.00%)	9.18
(0.88670) LP (1) P 5 s(3.00%)p32.27(96.98%)d 0.01(0.02%)	(0.09614) LV (2)Yb 5 s(2.52%)p 0.03(0.07%)d38.56(97.34%)f 0.03(0.06%)g 0.00(0.00%)	13.31

(0.88670) LP (1) P 5 s(3.00%)p32.27(96.98%)d 0.01(0.02%)	(0.09419) BD*(1)Yb 5- P 6 (90.70%) 0.9523*Yb 5 s(19.62%)p 0.01(0.11%)d 4.09(80.15%) f 0.01(0.10%)g 0.00(0.01%) (9.30%) -0.3050* P 6 s(31.12%)p 2.21(68.85%)d 0.00(0.03%)	20.30
(0.89146) BD (1)Yb 3- P 4 (11.12%) 0.3335*Yb 3 s(28.38%)p 0.00(0.08%)d 2.52(71.39%) f 0.00(0.14%)g 0.00(0.01%) (88.88%) 0.9428* P 4 s(37.05%)p 1.70(62.92%)d 0.00(0.03%)	(0.13059) LV (1)Yb 5 s(0.42%)p 0.05(0.02%)d99.99(99.47%) f 0.20(0.08%)g 0.01(0.01%)	14.24
(0.89146) BD (1)Yb 3- P 4 (11.12%) 0.3335*Yb 3 s(28.38%)p 0.00(0.08%)d 2.52(71.39%) f 0.00(0.14%)g 0.00(0.01%) (88.88%) 0.9428* P 4 s(37.05%)p 1.70(62.92%)d 0.00(0.03%)	(0.09614) LV (2)Yb 5 s(2.52%)p 0.03(0.07%)d38.56(97.34%)f 0.03(0.06%)g 0.00(0.00%)	14.28
(0.89146) BD (1)Yb 3- P 4 (11.12%) 0.3335*Yb 1 s(28.38%)p 0.00(0.08%)d 2.52(71.39%) f 0.00(0.14%)g 0.00(0.01%) (88.88%) 0.9428* P 4 s(37.05%)p 1.70(62.92%)d 0.00(0.03%)	(0.09060) LV (3)Yb 5 s(65.35%)p 0.00(0.09%)d 0.53(34.49%)f 0.00(0.06%)g 0.00(0.01%)	8.44
(0.89146) BD (1)Yb 3- P 4 (11.12%) 0.3335*Yb 3 s(28.38%)p 0.00(0.08%)d 2.52(71.39%) f 0.00(0.14%)g 0.00(0.01%) (88.88%) 0.9428* P 4 s(37.05%)p 1.70(62.92%)d 0.00(0.03%)	(0.10058) LV (1)Yb 2 s(33.70%)p 0.00(0.03%)d 1.96(66.19%)f 0.00(0.06%)g 0.00(0.01%)	7.64
(0.92690) BD (1)Yb 3- P 5 (10.78%) 0.3283*Yb 3 s(34.20%)p 0.00(0.14%)d 1.92(65.55%) f 0.00(0.09%)g	(0.09419) BD*(1)Yb 5- P 6 (90.70%) 0.9523*Yb 5 s(19.62%)p 0.01(0.11%)d 4.09(80.15%) f 0.01(0.10%)g	57.28

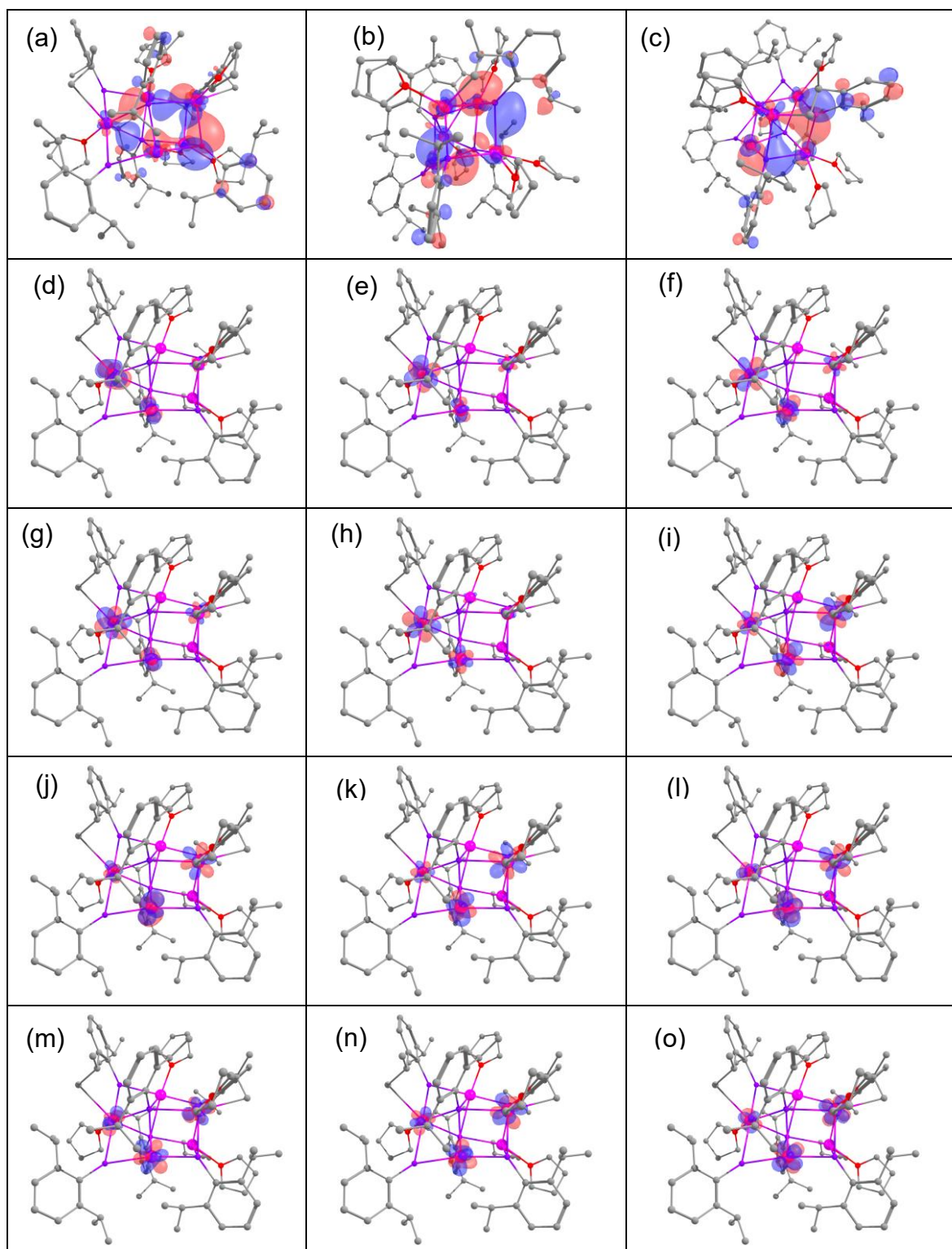
0.00(0.01%) (89.22%) 0.9446* P 5 s(59.50%)p 0.68(40.47%)d 0.00(0.04%)	0.00(0.01%) (9.30%) -0.3050* P 6 s(31.12%)p 2.21(68.85%)d 0.00(0.03%)	
(0.94500) BD (1)Yb 5- P 6 (9.30%) 0.3050*Yb 5 s(19.62%)p 0.01(0.11%)d 4.09(80.15%) f 0.01(0.10%)g 0.00(0.01%) (90.70%) 0.9523* P 6 s(31.12%)p 2.21(68.85%)d 0.00(0.03%)	(0.05391) BD*(1)Yb 4- P 2 (93.82%) 0.9686*Yb 4 s(8.65%)p 0.06(0.54%)d10.45(90.36%)f 0.05(0.43%)g 0.00(0.02%) (6.18%) -0.2486* P 2 s(44.32%)p 1.26(55.65%)d 0.00(0.03%)	11.30
(0.88647) BD (1)Yb 4- P 4 (9.86%) 0.3140*Yb 4 s(31.54%)p 0.01(0.21%)d 2.16(68.08%) f 0.00(0.15%)g 0.00(0.02%) (90.14%) 0.9494* P 4 s(43.78%)p 1.28(56.19%)d 0.00(0.03%)	(0.09060) LV (3)Yb 5 s(65.35%)p 0.00(0.09%)d 0.53(34.49%)f 0.00(0.06%)g 0.00(0.01%)	13.55
(0.88647) BD (1)Yb 4- P 4 (9.86%) 0.3140*Yb 4 s(31.54%)p 0.01(0.21%)d 2.16(68.08%) f 0.00(0.15%)g 0.00(0.02%) (90.14%) 0.9494* P 4 s(43.78%)p 1.28(56.19%)d 0.00(0.03%)	(0.13059) LV (1)Yb 5 s(0.42%)p 0.05(0.02%)d99.99(99.47%) f 0.20(0.08%)g 0.01(0.01%)	9.60
(0.88647) BD (1)Yb 4- P 4 (9.86%) 0.3140*Yb 4 s(31.54%)p 0.01(0.21%)d 2.16(68.08%) f 0.00(0.15%)g 0.00(0.02%) (90.14%) 0.9494* P 4 s(43.78%)p 1.28(56.19%)d 0.00(0.03%)	(0.10058) LV (1)Yb 2 s(33.70%)p 0.00(0.03%)d 1.96(66.19%)f 0.00(0.06%)g 0.00(0.01%)	14.12
(0.88647) BD (1)Yb 4- P 4 (9.86%) 0.3140*Yb 4 s(31.54%)p 0.01(0.21%)d 2.16(68.08%) f 0.00(0.15%)g 0.00(0.02%) (90.14%) 0.9494* P 4 s(43.78%)p 1.28(56.19%)d	(0.09147) LV (2)Yb 2 s(15.55%)p 0.00(0.08%)d 5.42(84.27%) f 0.01(0.09%)g 0.00(0.01%)	6.71

0.00(0.03%)		
(0.88176) BD (1)Yb 4- P 3 (9.66%) 0.3108*Yb 4 s(31.05%)p 0.00(0.08%)d 2.21(68.75%) f 0.00(0.11%)g 0.00(0.01%) (90.34%) 0.9505* P 3 s(40.67%)p 1.46(59.30%)d 0.00(0.03%)	(0.09060) LV (3)Yb 5 s(65.35%)p 0.00(0.09%)d 0.53(34.49%)f 0.00(0.06%)g 0.00(0.01%)	16.33
(0.88176) BD (1)Yb 4- P 3 (9.66%) 0.3108*Yb 4 s(31.05%)p 0.00(0.08%)d 2.21(68.75%) f 0.00(0.11%)g 0.00(0.01%) (90.34%) 0.9505* P 3 s(40.67%)p 1.46(59.30%)d 0.00(0.03%)	(0.13059) LV (1)Yb 5 s(0.42%)p 0.05(0.02%)d99.99(99.47%) f 0.20(0.08%)g 0.01(0.01%)	8.64
(0.88027) BD (1)Yb 4- P 3 (6.18%) 0.2486*Yb 4 s(8.65%)p 0.06(0.54%)d10.45(90.36%) f 0.05(0.43%)g 0.00(0.02%) (93.82%) 0.9686* P 3 s(44.32%)p 1.26(55.65%)d 0.00(0.03%)	(0.08570) BD*(1)Yb 4- P 6 (92.35%) 0.9610*Yb 4 s(24.39%)p 0.03(0.65%)d 3.06(74.58%) f 0.01(0.36%)g 0.00(0.01%) (7.65%) -0.2766* P 6 s(30.78%)p 2.25(69.20%)d 0.00(0.02%)	13.05
(0.91230) BD (1)Yb 4- P 6 (7.65%) 0.2766*Yb 4 s(24.39%)p 0.03(0.65%)d 3.06(74.58%) f 0.01(0.36%)g 0.00(0.01%) (92.35%) 0.9610* P 6 s(30.78%)p 2.25(69.20%)d 0.00(0.02%)	(0.09614) LV (2)Yb 5 s(2.52%)p 0.03(0.07%)d38.56(97.34%)f 0.03(0.06%)g 0.00(0.00%)	7.53
(0.91230) BD (1)Yb 4- P 6 (7.65%) 0.2766*Yb 4 s(24.39%)p 0.03(0.65%)d 3.06(74.58%) f 0.01(0.36%)g 0.00(0.01%) (92.35%) 0.9610* P 6 s(30.78%)p 2.25(69.20%)d 0.00(0.02%)	(0.09419) BD*(1)Yb 5- P 6 (90.70%) 0.9523*Yb 5 s(19.62%)p 0.01(0.11%)d 4.09(80.15%) f 0.01(0.10%)g 0.00(0.01%) (9.30%) -0.3050* P 6 s(31.12%)p 2.21(68.85%)d 0.00(0.03%)	8.54
(0.90240) BD (1)Yb 2- P 2 (10.88%) 0.3298*Yb 2	(0.08570) BD*(1)Yb 4- P 6 (92.35%) 0.9610*Yb 4	27.75

s(18.32%)p 0.01(0.14%)d 4.44(81.40%) f 0.01(0.13%)g 0.00(0.01%) (89.12%) 0.9440* P 2 s(34.84%)p 1.87(65.13%)d 0.00(0.03%)	s(24.39%)p 0.03(0.65%)d 3.06(74.58%) f 0.01(0.36%)g 0.00(0.01%) (7.65%) -0.2766* P 6 s(30.78%)p 2.25(69.20%)d 0.00(0.02%)	
(0.80028) LP (1) P 1 s(48.32%)p 1.07(51.65%)d 0.00(0.03%)	(0.11165) LV (1)Yb 1 s(3.91%)p 0.03(0.10%)d24.53(95.86%)f 0.03(0.12%)g 0.00(0.01%)	11.68
(0.80028) LP (1) P 1 s(48.32%)p 1.07(51.65%)d 0.00(0.03%)	(0.10475) LV (2)Yb 1 s(1.06%)p 0.15(0.16%)d93.24(98.67%)f 0.10(0.10%)g 0.01(0.01%)	12.05
(0.88787) BD (1)Yb 3- P 3 (10.95%) 0.3310*Yb 3 s(33.39%)p 0.00(0.10%)d 1.99(66.36%) f 0.00(0.13%)g 0.00(0.02%) (89.05%) 0.9436* P 3 s(39.21%)p 1.55(60.76%)d 0.00(0.04%)	(0.11165) LV (1)Yb 1 s(3.91%)p 0.03(0.10%)d24.53(95.86%)f 0.03(0.12%)g 0.00(0.01%)	8.25
(0.88787) BD (1)Yb 3- P 3 (10.95%) 0.3310*Yb 3 s(33.39%)p 0.00(0.10%)d 1.99(66.36%) f 0.00(0.13%)g 0.00(0.02%) (89.05%) 0.9436* P 3 s(39.21%)p 1.55(60.76%)d 0.00(0.04%)	(0.07962) LV (3)Yb 1 s(84.79%)p 0.00(0.02%)d 0.18(15.02%)f 0.00(0.15%)g 0.00(0.02%)	9.37
(0.88176) BD (1)Yb 4- P 3 (9.66%) 0.3108*Yb 4 s(31.05%)p 0.00(0.08%)d 2.21(68.75%) f 0.00(0.11%)g 0.00(0.01%) (90.34%) 0.9505* P 3 s(40.67%)p 1.46(59.30%)d 0.00(0.03%)	(0.11165) LV (1)Yb 1 s(3.91%)p 0.03(0.10%)d24.53(95.86%)f 0.03(0.12%)g 0.00(0.01%)	8.92
(0.88176) BD (1)Yb 4- P 3 (9.66%) 0.3108*Yb 4 s(31.05%)p 0.00(0.08%)d 2.21(68.75%) f 0.00(0.11%)g 0.00(0.01%)	(0.07962) LV (3)Yb 1 s(84.79%)p 0.00(0.02%)d 0.18(15.02%)f 0.00(0.15%)g 0.00(0.02%)	9.14

(90.34%) 0.9505* P 3 s(40.67%)p 1.46(59.30%)d 0.00(0.03%)		
(0.88027) BD (1)Yb 4- P 2 (6.18%) 0.2486*Yb 4 s(8.65%)p 0.06(0.54%)d10.45(90.36%) f 0.05(0.43%)g 0.00(0.02%) (93.82%) 0.9686* P 2 s(44.32%)p 1.26(55.65%)d 0.00(0.03%)	(0.10475) LV (2)Yb 1 s(1.06%)p 0.15(0.16%)d93.24(98.67%)f 0.10(0.10%)g 0.01(0.01%)	20.97
(0.90240) BD (1)Yb 2- P 2 (10.88%) 0.3298*Yb 2 s(18.32%)p 0.01(0.14%)d 4.44(81.40%) f 0.01(0.13%)g 0.00(0.01%) (89.12%) 0.9440* P 2 s(34.84%)p 1.87(65.13%)d 0.00(0.03%)	(0.10475) LV (2)Yb 1 s(1.06%)p 0.15(0.16%)d93.24(98.67%)f 0.10(0.10%)g 0.01(0.01%)	8.77
(0.96087) LP (2) O 3 s(38.14%)p 1.62(61.85%)d 0.00(0.02%)	(0.09147) LV (2)Yb 2 s(15.55%)p 0.00(0.08%)d 5.42(84.27%) f 0.01(0.09%)g 0.00(0.01%)	9.06
(0.96087) LP (2) O 3 s(38.14%)p 1.62(61.85%)d 0.00(0.02%)	(0.05643) LV (4)Yb 2 s(0.19%)p 0.14(0.03%)d99.99(99.68%)f 0.46(0.09%)g 0.09(0.02%)	12.12
(0.95963) LP (2) O 4 s(36.37%)p 1.75(63.61%)d 0.00(0.02%)	(0.03564) BD*(1)Yb 4- P 3 (90.34%) 0.9505*Yb 4 s(31.05%)p 0.00(0.08%)d 2.21(68.75%) f 0.00(0.11%)g 0.00(0.01%) (9.66%) -0.3108* P 3 s(40.67%)p 1.46(59.30%)d 0.00(0.03%)	12.42
(0.96029) LP (1) O 5 s(40.18%)p 1.49(59.80%)d 0.00(0.02%)	(0.13059) LV (1)Yb 5 s(0.42%)p 0.05(0.02%)d99.99(99.47%) f 0.20(0.08%)g 0.01(0.01%)	16.25
(0.96409) LP (2) O 2 s(25.02%)p 3.00(74.96%)d 0.00(0.02%)	(0.11165) LV (1)Yb 1 s(3.91%)p 0.03(0.10%)d24.53(95.86%)f 0.03(0.12%)g 0.00(0.01%)	8.17

<p>(0.96409) LP (2) O 2 s(25.02%)p 3.00(74.96%)d 0.00(0.02%)</p>	<p>(0.07962) LV (3)Yb 1 s(84.79%)p 0.00(0.02%)d 0.18(15.02%)f 0.00(0.15%)g 0.00(0.02%)</p>	<p>6.10</p>
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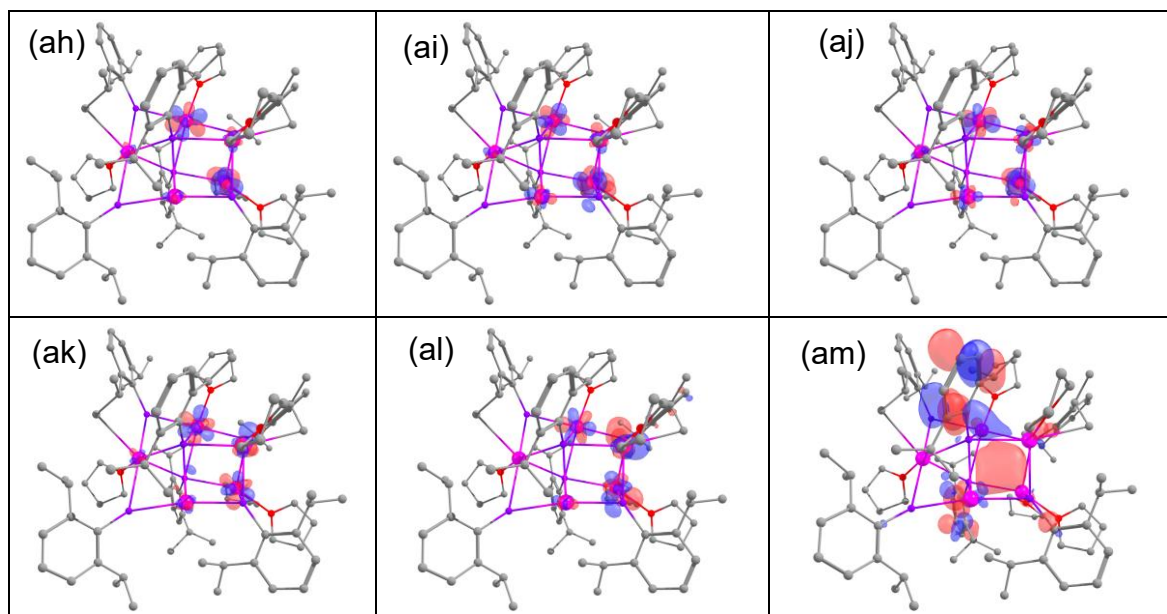


Fig. S54 Computed MOs for complex **4** (dispersion). (a)HOMO-37 (b)HOMO-36 (c)HOMO-35 (d)HOMO-34 (e)HOMO-33 (f)HOMO-32 (g)HOMO-31 (h)HOMO-30 (i)HOMO-29 (j)HOMO-28 (k)HOMO-27 (l)HOMO-26 (m)HOMO-25 (n)HOMO-24 (o)HOMO-23 (p)HOMO-22 (q)HOMO-21 (r)HOMO-20 (s)HOMO-19 (t)HOMO-18 (u)HOMO-17 (v)HOMO-16 (w)HOMO-15 (x)HOMO-14 (y)HOMO-13 (z)HOMO-12 (aa)HOMO-11 (ab)HOMO-10 (ac)HOMO-9 (ad)HOMO-8 (ae)HOMO-7 (af)HOMO-6 (ag)HOMO-5 (ah)HOMO-4 (ai)HOMO-3 (aj)HOMO-2 (ak)HOMO-1 (al)HOMO (am)LUMO.

Table S13 NBO analysis of canonical molecular orbitals for complex **4** (dispersion).

MO 451 (occ): orbital energy = -0.14888 a.u. (HOMO-37)	(0.79533) LP (1) P 3
-0.328*[199]: LP (1) P 3(lp)	s(1.94%)p50.56(98.06%)d 0.00(0.00%)
-0.318*[198]: LP (1) P 4(lp)	(0.78188) LP (1) P 4
0.283*[222]: BD (1)Yb 2- P	s(1.78%)p55.04(98.21%)d 0.00(0.01%)
1	(0.92718) BD (1)Yb 2- P 1
0.274*[227]: BD (2) P 1- C1	(9.98%) 0.3160*Yb 2 s(23.72%)p
-0.236*[229]: BD (2) P 2- C13	0.01(0.28%)d 3.19(75.77%) f
	0.01(0.20%)g 0.00(0.02%)
	(90.02%) 0.9488* P 1 s(26.99%)p
	2.70(72.99%)d 0.00(0.02%)
	(0.88173) BD (2) P 1- C 1
	(81.30%) 0.9017* P 1
	s(0.27%)p99.99(99.71%)d 0.06(0.02%)
	(18.70%) 0.4325* C 1 s(0.00%)p
	1.00(99.95%)d 0.00(0.05%)
	(0.89241) BD (2) P 2- C 13

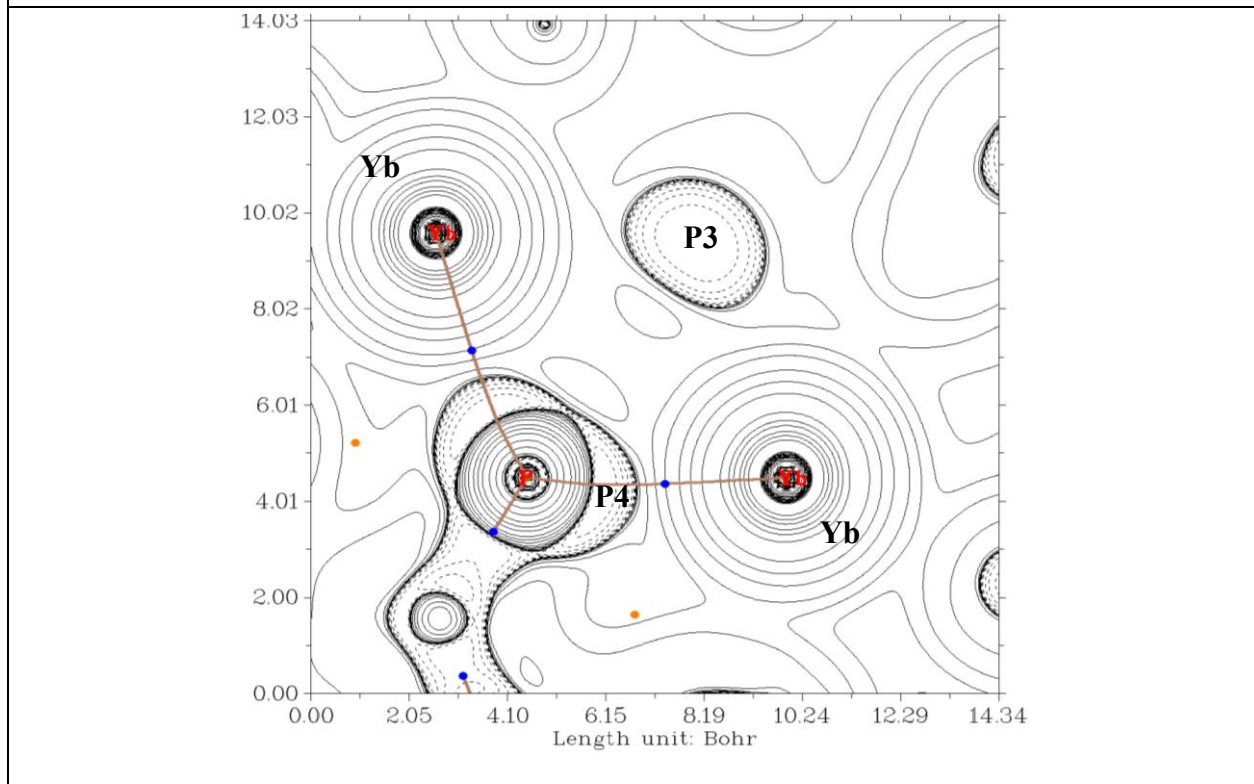
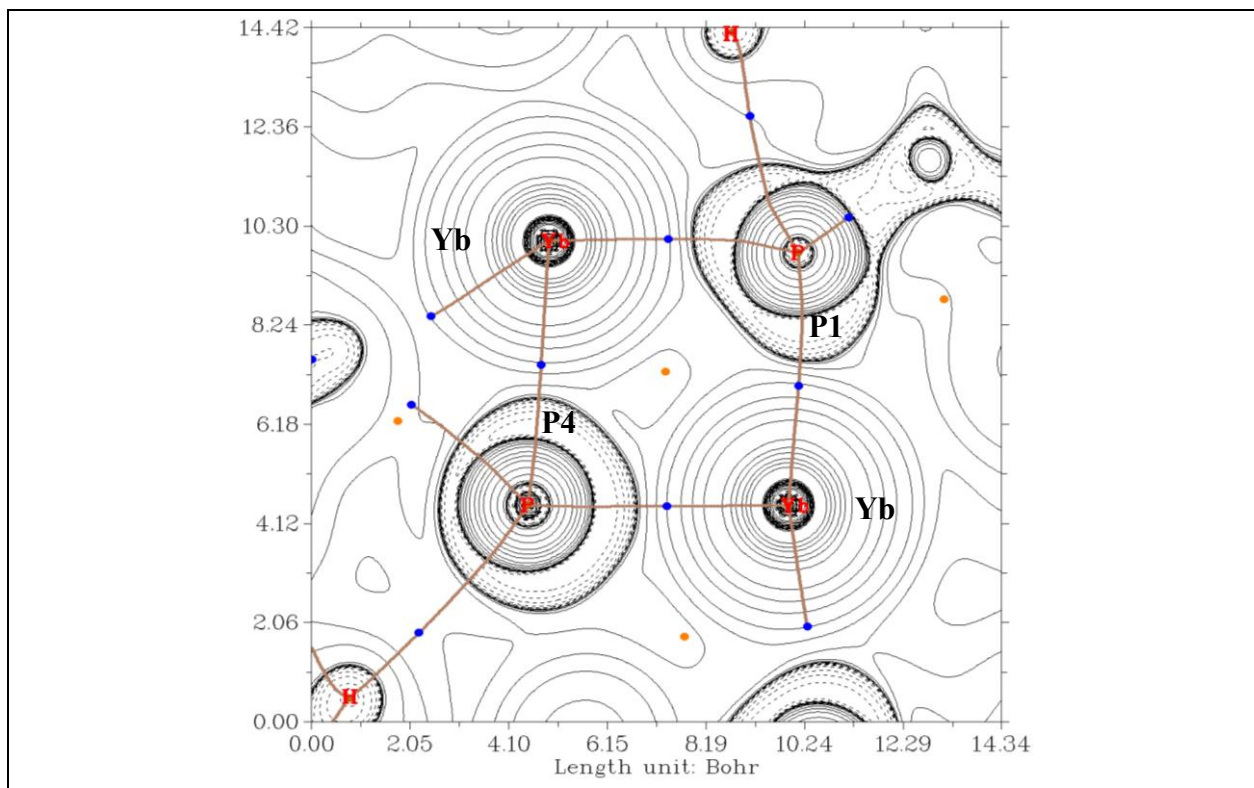
	(83.15%) 0.9119* P 2 s(0.29%)p99.99(99.70%)d 0.02(0.00%) (16.85%) 0.4105* C 13 s(0.03%)p99.99(99.92%)d 1.77(0.05%)
MO 452 (occ): orbital energy = -0.14493 a.u. (HOMO-36) 2 0.430*[223]: BD (1)Yb 2- P -0.387*[220]: BD (1)Yb 4- P 2 -0.253*[229]: BD (2) P 2- C13 -0.251*[227]: BD (2) P 1- C1 -0.240*[222]: BD (1)Yb 2- P 1	<u>(0.90240) BD (1)Yb 2- P 2</u> (10.88%) 0.3298*Yb 2 s(18.32%)p 0.01(0.14%)d 4.44(81.40%) f 0.01(0.13%)g 0.00(0.01%) (89.12%) 0.9440* P 2 s(34.84%)p 1.87(65.13%)d 0.00(0.03%) <u>(0.88027) BD (1)Yb 4- P 2</u> (6.18%) 0.2486*Yb 4 s(8.65%)p 0.06(0.54%)d10.45(90.36%) f 0.05(0.43%)g 0.00(0.02%) (93.82%) 0.9686* P 2 s(44.32%)p 1.26(55.65%)d 0.00(0.03%) <u>(0.89241) BD (2) P 2- C 13</u> (83.15%) 0.9119* P 2 s(0.29%)p99.99(99.70%)d 0.02(0.00%) (16.85%) 0.4105* C 13 s(0.03%)p99.99(99.92%)d 1.77(0.05%) <u>(0.88173) BD (2) P 1- C 1</u> (81.30%) 0.9017* P 1 s(0.27%)p99.99(99.71%)d 0.06(0.02%) (18.70%) 0.4325* C 1 s(0.00%)p 1.00(99.95%)d 0.00(0.05%) <u>(0.92718) BD (1)Yb 2- P 1</u> (9.98%) 0.3160*Yb 2 s(23.72%)p 0.01(0.28%)d 3.19(75.77%) f 0.01(0.20%)g 0.00(0.02%) (90.02%) 0.9488* P 1 s(26.99%)p 2.70(72.99%)d 0.00(0.02%)
MO 453 (occ): orbital energy = -0.13978 a.u. (HOMO-35) C13 0.346*[229]: BD (2) P 2- 0.300*[227]: BD (2) P 1- C1 0.259*[191]: LP (1)Yb 2(lp) 0.226*[194]: LP (4)Yb 2(lp) -0.225*[222]: BD (1)Yb 2- P 1 -0.224*[220]: BD (1)Yb 4- P 2	<u>(0.89241) BD (2) P 2- C 13</u> (83.15%) 0.9119* P 2 s(0.29%)p99.99(99.70%)d 0.02(0.00%) (16.85%) 0.4105* C 13 s(0.03%)p99.99(99.92%)d 1.77(0.05%) <u>(0.88173) BD (2) P 1- C 1</u> (81.30%) 0.9017* P 1 s(0.27%)p99.99(99.71%)d 0.06(0.02%) (18.70%) 0.4325* C 1 s(0.00%)p 1.00(99.95%)d 0.00(0.05%) <u>(0.99898) LP (1)Yb 2</u>

	<p>s(0.00%)p 0.00(0.00%)d 0.00(0.01%)f 1.00(99.99%)g 0.00(0.00%) <u>(0.99796) LP (4)Yb 2</u> s(0.01%)p 0.00(0.00%)d 1.00(0.03%)f99.99(99.96%)g 0.01(0.00%) <u>(0.92718) BD (1)Yb 2- P 1</u> (9.98%) 0.3160*Yb 2 s(23.72%)p 0.01(0.28%)d 3.19(75.77%) f 0.01(0.20%)g 0.00(0.02%) (90.02%) 0.9488* P 1 s(26.99%)p 2.70(72.99%)d 0.00(0.02%) <u>(0.88027) BD (1)Yb 4- P 2</u> (6.18%) 0.2486*Yb 4 s(8.65%)p 0.06(0.54%)d10.45(90.36%) f 0.05(0.43%)g 0.00(0.02%) (93.82%) 0.9686* P 2 s(44.32%)p 1.26(55.65%)d 0.00(0.03%)</p>
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Table S14 Computed BCP descriptors for complex **4** (dispersion).

Atom labels	$\rho(r)$	$\nabla^2\rho(r)$	$G(r)$	$V(r)$	$H(r)$	ϵ
Yb3-P4	0.04	0.08	0.02	-0.03	-0.004	0.19
Yb3-P3	0.03	0.07	0.02	-0.03	-0.004	0.22
Yb3-P1	0.04	0.09	0.03	-0.04	-0.007	0.18
Yb3-P5	0.03	0.08	0.02	-0.03	-0.004	0.13
Yb5-P4	0.03	0.07	0.02	-0.02	-0.003	0.17
Yb5-P3	0.03	0.07	0.02	-0.03	-0.004	0.23
Yb5-P5	0.03	0.07	0.02	-0.02	-0.003	0.12
Yb5-P6	0.04	0.08	0.02	-0.03	-0.004	0.14
Yb5-O5	0.04	0.19	0.05	-0.04	0.002	0.13
Yb4-P4	0.03	0.08	0.02	-0.03	-0.004	0.16
Yb4-P3	0.03	0.07	0.02	-0.02	-0.003	0.16
Yb4-P2	0.04	0.08	0.03	-0.03	-0.005	0.21
Yb4-P6	0.03	0.07	0.02	-0.02	-0.003	0.11
Yb4-O4	0.04	0.19	0.04	-0.04	0.003	0.17
Yb1-P3	0.03	0.06	0.02	-0.02	-0.003	0.19
Yb1-P1	0.03	0.07	0.02	-0.02	-0.003	0.20
Yb1-P2	0.04	0.09	0.03	-0.03	-0.006	0.18
Yb1-O1	0.04	0.18	0.04	-0.04	0.003	0.15
Yb1-O2	0.04	0.19	0.04	-0.04	0.002	0.07
Yb2-P4	0.03	0.07	0.02	-0.02	-0.004	0.18

Yb2-P1	0.04	0.09	0.03	-0.04	-0.007	0.16
Yb2-P2	0.04	0.09	0.03	-0.03	-0.006	0.16
Yb2-O3	0.04	0.20	0.05	-0.04	0.002	0.10



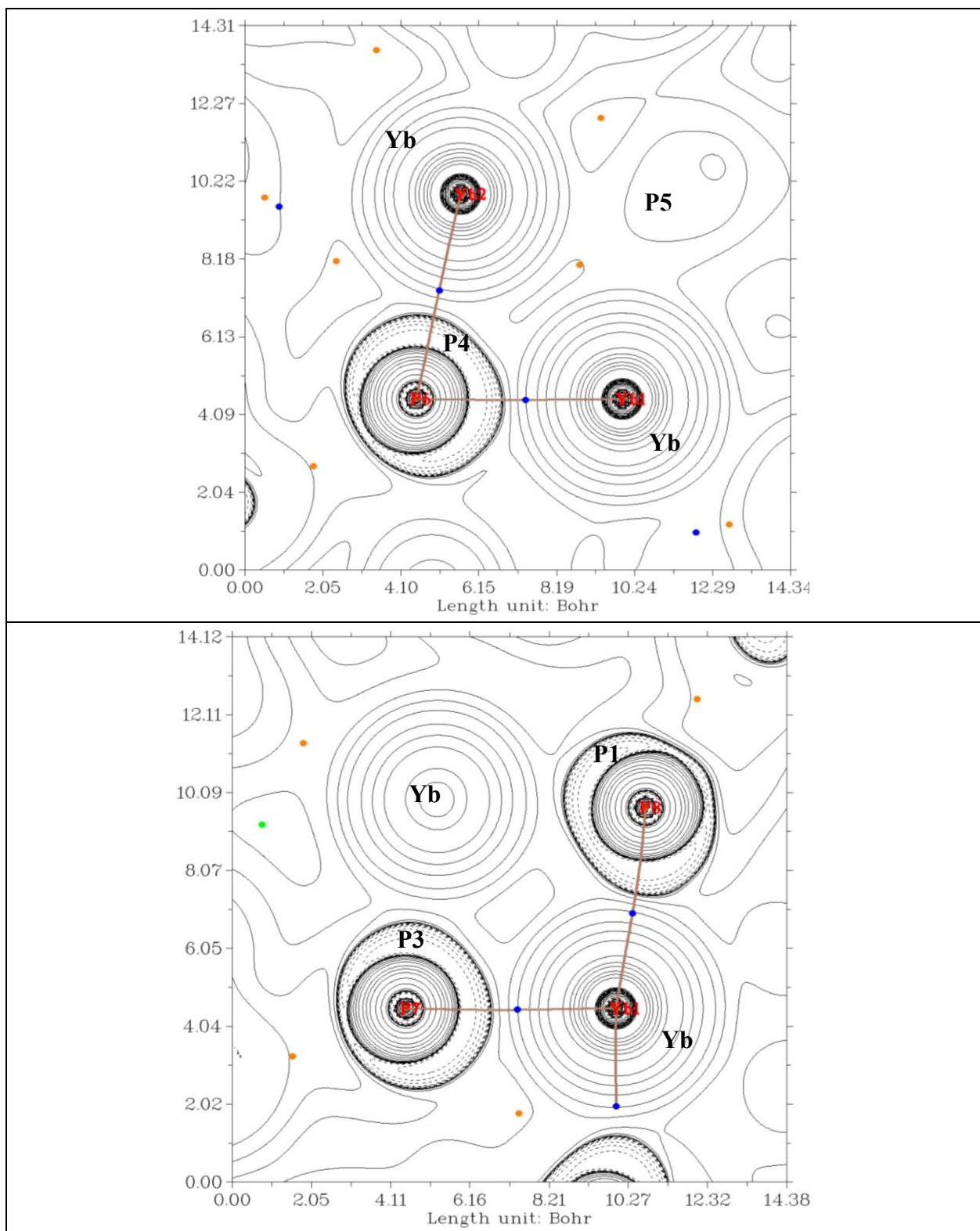


Fig. S55 Computed Laplacian distribution for complex 4 (dispersion).

Table S15 Comparison of bond distance (Å) between selected atoms in DFT optimized and X-ray structure for complex 5.

Atom labels	DFT	X-ray	
	dispersion		

Yb1-P4	2.85	2.83
Yb1-P5	2.85	2.89
Yb1-P139	2.87	2.85
Yb1-P141	2.81	2.86
Yb2-P4	2.80	2.82
Yb2-P5	2.78	2.82
Yb2-P6	2.82	2.85
Yb2-C10	2.54	2.56
Yb3-P4	2.83	2.83
Yb3-C71	2.55	2.63
Yb3-P140	2.79	2.88
Yb3-P141	2.83	2.87
Yb136-P4	2.85	2.85
Yb136-P6	2.81	2.86
Yb136-P139	2.86	2.83
Yb136-P140	2.86	2.89
Yb137-P139	2.84	2.82
Yb137-P140	2.80	2.82
Yb137-P141	2.84	2.85
Yb137-C145	2.55	2.56
Yb138-P5	2.81	2.88
Yb138-P6	2.83	2.87
Yb138-P139	2.86	2.83
Yb138-C206	2.57	2.63

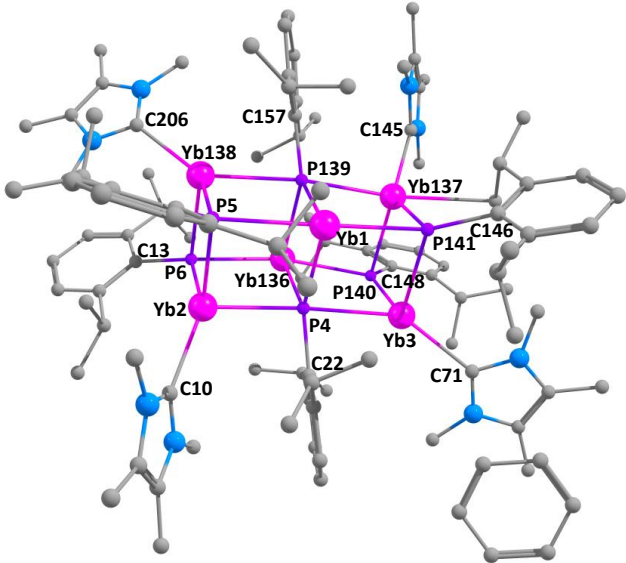


Table S16 Computed natural charges for selected atoms in complex **5** (dispersion).

Atom labels	Natural charges
Yb1	0.76217
Yb2	0.82570
Yb3	1.02957
P4	-0.48169
P5	-0.64084

P6	-0.64607
C10	0.03951
C71	-0.00183
Yb136	0.83212
Yb137	0.85262
Yb138	1.02151
P139	-0.51198
P140	-0.64048
P141	-0.65000
C145	0.03774
C206	0.01734

Table S17 Computed Wiberg bond index between selected atoms in complex **5** (dispersion).

Atom labels	Wiberg bond index
Yb1-P4	0.4263
Yb1-P5	0.4037
Yb1-P139	0.4205
Yb1-P141	0.4594
Yb2-P4	0.3920
Yb2-P5	0.5102
Yb2-P6	0.4756
Yb2-C10	0.3039
Yb3-P4	0.3119
Yb3-C71	0.2544
Yb3-P140	0.4360
Yb3-P141	0.4210
Yb136-P4	0.4096
Yb136-P6	0.4389
Yb136-P139	0.4054
Yb136-P140	0.3903
Yb137-P139	0.3877
Yb137- P140	0.4753
Yb137-P141	0.4569
Yb137-C145	0.2973
Yb138-P5	0.4235
Yb138-P6	0.4172
Yb138-P139	0.3195
Yb138-C206	0.2733

Bonding orbitals between ytterbium and atoms in the first coordination sphere of metal in complex **5** (dispersion)

(1.79565) BD (1)Yb 1- P139

(10.46%) 0.3234*Yb 1 s(21.01%)p 0.01(0.21%)d 3.74(78.63%) f 0.01(0.14%)g 0.00(0.01%)

(89.54%) 0.9463* P139 s(29.99%)p 2.33(69.98%)d 0.00(0.03%)

(1.72768) BD (1)Yb 2- P 4

(7.31%) 0.2704*Yb 2 s(19.32%)p 0.00(0.05%)d 4.17(80.51%) f 0.01(0.11%)g 0.00(0.02%)

(92.69%) 0.9628* P 4 s(23.35%)p 3.28(76.62%)d 0.00(0.03%)

(1.70063) BD (2)Yb 2- P 4

(6.25%) 0.2501*Yb 2 s(10.42%)p 0.02(0.19%)d 8.57(89.26%) f 0.01(0.12%)g 0.00(0.01%)

(93.75%) 0.9682* P 4 s(22.14%)p 3.52(77.84%)d 0.00(0.02%)

(1.79409) BD (1)Yb 2- P 6

(9.74%) 0.3121*Yb 2 s(29.67%)p 0.00(0.09%)d 2.36(70.04%) f 0.01(0.19%)g 0.00(0.01%)

(90.26%) 0.9500* P 6 s(43.16%)p 1.32(56.79%)d 0.00(0.05%)

(1.68407) BD (1)Yb 3- P 4

(8.51%) 0.2917*Yb 3 s(15.99%)p 0.01(0.12%)d 5.24(83.73%) f 0.01(0.13%)g 0.00(0.03%)

(91.49%) 0.9565* P 4 s(39.03%)p 1.56(60.94%)d 0.00(0.03%)

(1.73327) BD (1)Yb 3- P141

(8.73%) 0.2955*Yb 3 s(31.64%)p 0.00(0.10%)d 2.15(68.00%) f 0.01(0.23%)g 0.00(0.02%)

(91.27%) 0.9553* P141 s(21.16%)p 3.73(78.81%)d 0.00(0.03%)

(1.71296) BD (1) P 6-Yb138

(90.51%) 0.9514* P 6 s(22.47%)p 3.45(77.48%)d 0.00(0.05%)

(9.49%) 0.3081*Yb138 s(31.32%)p 0.00(0.08%)d 2.18(68.38%) f 0.01(0.19%)g 0.00(0.02%)

(1.75731) BD (1)Yb137- P139

(9.07%) 0.3012*Yb137 s(27.58%)p 0.00(0.10%)d 2.62(72.21%) f 0.00(0.09%)g 0.00(0.02%)

(90.93%) 0.9536* P139 s(29.82%)p 2.35(70.16%)d 0.00(0.02%)

(1.73063) BD (1)Yb137- P140

(10.87%) 0.3296*Yb137 s(31.42%)p 0.00(0.08%)d 2.17(68.27%) f 0.01(0.21%)g 0.00(0.02%)

(89.13%) 0.9441* P140 s(67.49%)p 0.48(32.47%)d 0.00(0.04%)

(1.77290) BD (1)Yb137- P141

(9.57%) 0.3093*Yb137 s(31.09%)p 0.00(0.10%)d 2.21(68.59%) f 0.01(0.21%)g 0.00(0.01%)

(90.43%) 0.9510* P141 s(46.01%)p 1.17(53.96%)d 0.00(0.03%)

(1.69325) BD (1)Yb138- P139

(7.83%) 0.2798*Yb138 s(19.74%)p 0.00(0.07%)d 4.05(80.03%) f 0.01(0.13%)g
 0.00(0.02%)
 (92.17%) 0.9601* P139 s(23.55%)p 3.25(76.43%)d 0.00(0.02%)

Table S18 NBO Second order perturbation analysis for complex **5** (dispersion).

Donor NBO	Acceptor NBO	E(2) kcal/mol
(1.71108) LP (1) P140 s(1.82%)p53.78(98.13%)d 0.02(0.04%)	(0.21839) LV (1)Yb 3 s(46.49%)p 0.00(0.14%)d 1.14(53.07%)f 0.01(0.28%)g 0.00(0.01%)	21.07
(1.71108) LP (1) P140 s(1.82%)p53.78(98.13%)d 0.02(0.04%)	(0.15060) LV (2)Yb 3 s(0.43%)p 0.10(0.04%)d99.99(99.46%)f 0.16(0.07%)g 0.01(0.00%)	13.86
(1.71108) LP (1) P140 s(1.82%)p53.78(98.13%)d 0.02(0.04%)	(0.21254) LV (1)Yb137 s(7.66%)p 0.01(0.07%)d12.03(92.12%)f 0.02(0.15%)g 0.00(0.01%)	21.75
(1.70260) LP (1) P141 s(12.95%)p 6.72(87.02%)d 0.00(0.03%)	(0.36817) LV (1)Yb 1 s(23.99%)p 0.00(0.06%)d 3.16(75.87%) f 0.00(0.07%)g 0.00(0.01%)	80.02
(1.70260) LP (1) P141 s(12.95%)p 6.72(87.02%)d 0.00(0.03%)	(0.15363) LV (4)Yb 1 s(0.09%)p 0.65(0.06%)d99.99(99.81%)f 0.44(0.04%)g 0.03(0.00%)	12.85
(1.70260) LP (1) P141 s(12.95%)p 6.72(87.02%)d 0.00(0.03%)	(0.15060) LV (2)Yb 3 s(0.43%)p 0.10(0.04%)d99.99(99.46%)f 0.16(0.07%)g 0.01(0.00%)	12.33
(1.79565) BD (1)Yb 1- P139 (10.46%) 0.3234*Yb 1 s(21.01%)p 0.01(0.21%)d 3.74(78.63%) f 0.01(0.14%)g 0.00(0.01%) (89.54%) 0.9463* P139 s(29.99%)p 2.33(69.98%)d 0.00(0.03%)	(0.14791) LV (2)Yb137 s(1.50%)p 0.09(0.14%)d65.40(98.31%)f 0.03(0.04%)g 0.01(0.01%)	18.44
(1.79565) BD (1)Yb 1- P139 (10.46%) 0.3234*Yb 1 s(21.01%)p 0.01(0.21%)d 3.74(78.63%) f 0.01(0.14%)g 0.00(0.01%) (89.54%) 0.9463* P139 s(29.99%)p	(0.16930) LV (2)Yb138 s(0.80%)p 0.09(0.07%)d99.99(99.00%)f 0.14(0.11%)g 0.01(0.01%)	10.65

2.33(69.98%)d 0.00(0.03%)		
(1.72768) BD (1)Yb 2- P 4 (7.31%) 0.2704*Yb 2 s(19.32%)p 0.00(0.05%)d 4.17(80.51%) f 0.01(0.11%)g 0.00(0.02%) (92.69%) 0.9628* P 4 s(23.35%)p 3.28(76.62%)d 0.00(0.03%)	(0.19502) LV (3)Yb 1 s(46.25%)p 0.00(0.10%)d 1.16(53.56%)f 0.00(0.07%)g 0.00(0.01%)	42.75
(1.68407) BD (1)Yb 3- P 4 (8.51%) 0.2917*Yb 3 s(15.99%)p 0.01(0.12%)d 5.24(83.73%) f 0.01(0.13%)g 0.00(0.03%) (91.49%) 0.9565* P 4 s(39.03%)p 1.56(60.94%)d 0.00(0.03%)	(0.22505) LV (2)Yb 1 s(7.92%)p 0.00(0.03%)d11.61(91.98%)f 0.01(0.05%)g 0.00(0.01%)	42.77
(1.68407) BD (1)Yb 3- P 4 (8.51%) 0.2917*Yb 3 s(15.99%)p 0.01(0.12%)d 5.24(83.73%) f 0.01(0.13%)g 0.00(0.03%) (91.49%) 0.9565* P 4 s(39.03%)p 1.56(60.94%)d 0.00(0.03%)	(0.19502) LV (3)Yb 1 s(46.25%)p 0.00(0.10%)d 1.16(53.56%)f 0.00(0.07%)g 0.00(0.01%)	15.42
(1.73327) BD (1)Yb 3- P141 (8.73%) 0.2955*Yb 3 s(31.64%)p 0.00(0.10%)d 2.15(68.00%) f 0.01(0.23%)g 0.00(0.02%) (91.27%) 0.9553* P141 s(21.16%)p 3.73(78.81%)d 0.00(0.03%)	(0.36817) LV (1)Yb 1 s(23.99%)p 0.00(0.06%)d 3.16(75.87%) f 0.00(0.07%)g 0.00(0.01%)	18.07
(1.73327) BD (1)Yb 3- P141 (8.73%) 0.2955*Yb 3 s(31.64%)p 0.00(0.10%)d 2.15(68.00%) f 0.01(0.23%)g 0.00(0.02%) (91.27%) 0.9553* P141 s(21.16%)p 3.73(78.81%)d 0.00(0.03%)	(0.21254) LV (1)Yb137 s(7.66%)p 0.01(0.07%)d12.03(92.12%)f 0.02(0.15%)g 0.00(0.01%)	17.51
(1.73327) BD (1)Yb 3- P141 (8.73%) 0.2955*Yb 3 s(31.64%)p 0.00(0.10%)d 2.15(68.00%) f 0.01(0.23%)g 0.00(0.02%) (91.27%) 0.9553* P141 s(21.16%)p 3.73(78.81%)d 0.00(0.03%)	(0.14791) LV (2)Yb137 s(1.50%)p 0.09(0.14%)d65.40(98.31%)f 0.03(0.04%)g 0.01(0.01%)	11.76
(1.71296) BD (1) P 6-Yb138 (90.51%) 0.9514* P 6 s(22.47%)p 3.45(77.48%)d 0.00(0.05%) (9.49%) 0.3081*Yb138 s(31.32%)p 0.00(0.08%)d 2.18(68.38%) f 0.01(0.19%)g 0.00(0.02%)	(0.21832) LV (2)Yb 2 s(7.92%)p 0.01(0.06%)d11.60(91.85%)f 0.02(0.16%)g 0.00(0.01%)	25.91

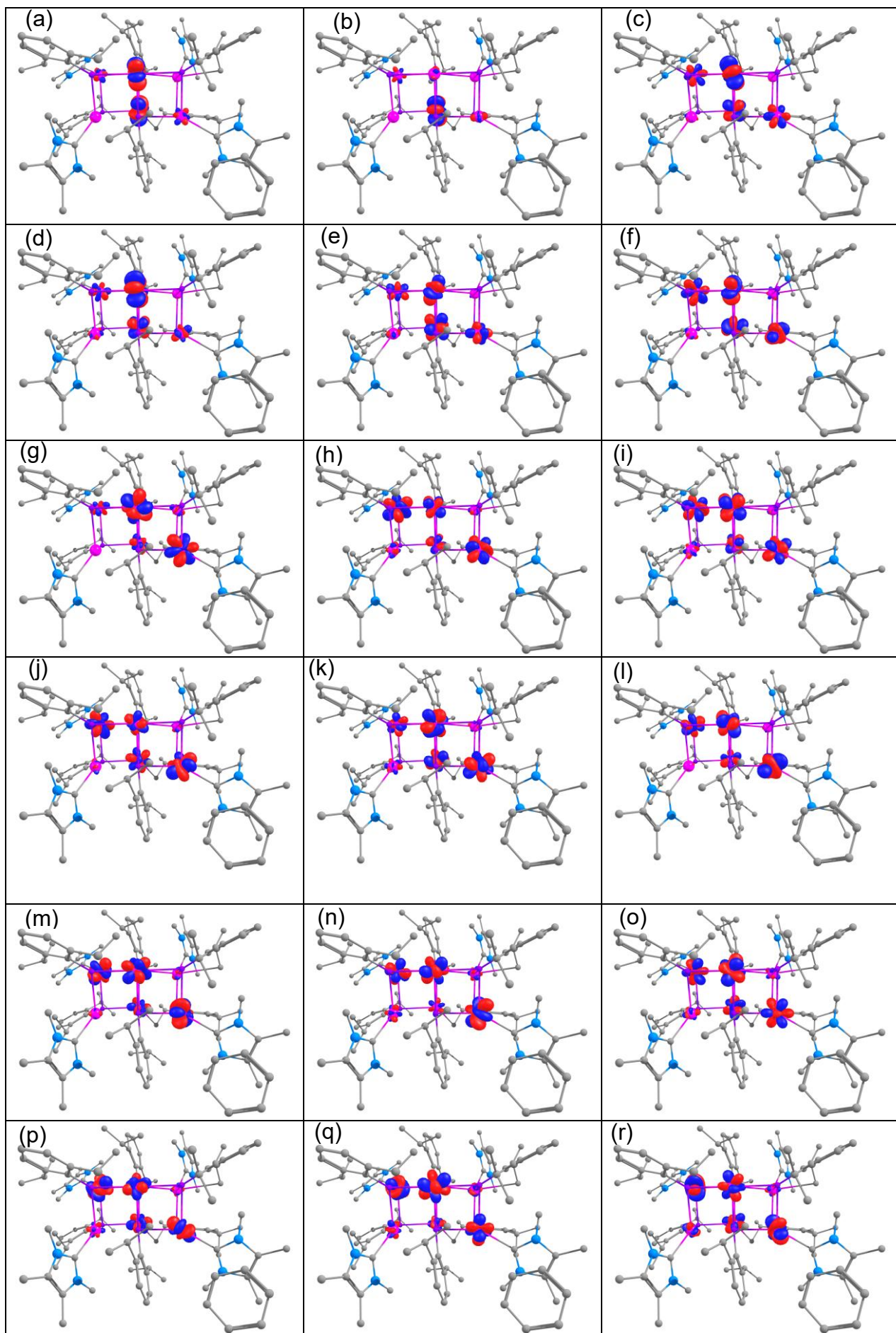
(1.73063) BD (1)Yb137- P140 (10.87%) 0.3296*Yb137 s(31.42%)p 0.00(0.08%)d 2.17(68.27%) f 0.01(0.21%)g 0.00(0.02%) (89.13%) 0.9441* P140 s(67.49%)p 0.48(32.47%)d 0.00(0.04%)	(0.21839) LV (1)Yb 3 s(46.49%)p 0.00(0.14%)d 1.14(53.07%)f 0.01(0.28%)g 0.00(0.01%)	50.98
(1.77290) BD (1)Yb137- P141 (9.57%) 0.3093*Yb137 s(31.09%)p 0.00(0.10%)d 2.21(68.59%) f 0.01(0.21%)g 0.00(0.01%) (90.43%) 0.9510* P141 s(46.01%)p 1.17(53.96%)d 0.00(0.03%)	(0.36817) LV (1)Yb 1 s(23.99%)p 0.00(0.06%)d 3.16(75.87%) f 0.00(0.07%)g 0.00(0.01%)	86.35
(1.77290) BD (1)Yb137- P141 (9.57%) 0.3093*Yb137 s(31.09%)p 0.00(0.10%)d 2.21(68.59%) f 0.01(0.21%)g 0.00(0.01%) (90.43%) 0.9510* P141 s(46.01%)p 1.17(53.96%)d 0.00(0.03%)	(0.22505) LV (2)Yb 1 s(7.92%)p 0.00(0.03%)d11.61(91.98%)f 0.01(0.05%)g 0.00(0.01%)	18.68
(1.77290) BD (1)Yb137- P141 (9.57%) 0.3093*Yb137 s(31.09%)p 0.00(0.10%)d 2.21(68.59%) f 0.01(0.21%)g 0.00(0.01%) (90.43%) 0.9510* P141 s(46.01%)p 1.17(53.96%)d 0.00(0.03%)	(0.19502) LV (3)Yb 1 s(46.25%)p 0.00(0.10%)d 1.16(53.56%)f 0.00(0.07%)g 0.00(0.01%)	24.33
(1.71788) LP (1) P 6 s(14.86%)p 5.73(85.12%)d 0.00(0.03%)	(0.37247) LV (1)Yb136 s(14.35%)p 0.00(0.03%)d 5.97(85.59%)f 0.00(0.03%)g 0.00(0.01%)	81.41
(1.71788) LP (1) P 6 s(14.86%)p 5.73(85.12%)d 0.00(0.03%)	(0.17535) LV (4)Yb136 s(79.67%)p 0.00(0.21%)d 0.25(19.97%)f 0.00(0.13%)g 0.00(0.02%)	12.46
(1.71108) LP (1) P140 s(1.82%)p53.78(98.13%)d 0.02(0.04%)	(0.37247) LV (1)Yb136 s(14.35%)p 0.00(0.03%)d 5.97(85.59%)f 0.00(0.03%)g 0.00(0.01%)	15.72
(1.70063) BD (2)Yb 2- P 4 (6.25%) 0.2501*Yb 2 s(10.42%)p 0.02(0.19%)d 8.57(89.26%) f 0.01(0.12%)g 0.00(0.01%) (93.75%) 0.9682* P 4 s(22.14%)p 3.52(77.84%)d 0.00(0.02%)	(0.24368) LV (2)Yb136 s(0.73%)p 0.11(0.08%)d99.99(99.07%)f 0.15(0.11%)g 0.01(0.00%)	32.55
(1.70063) BD (2)Yb 2- P 4	(0.17535) LV (4)Yb136	13.85

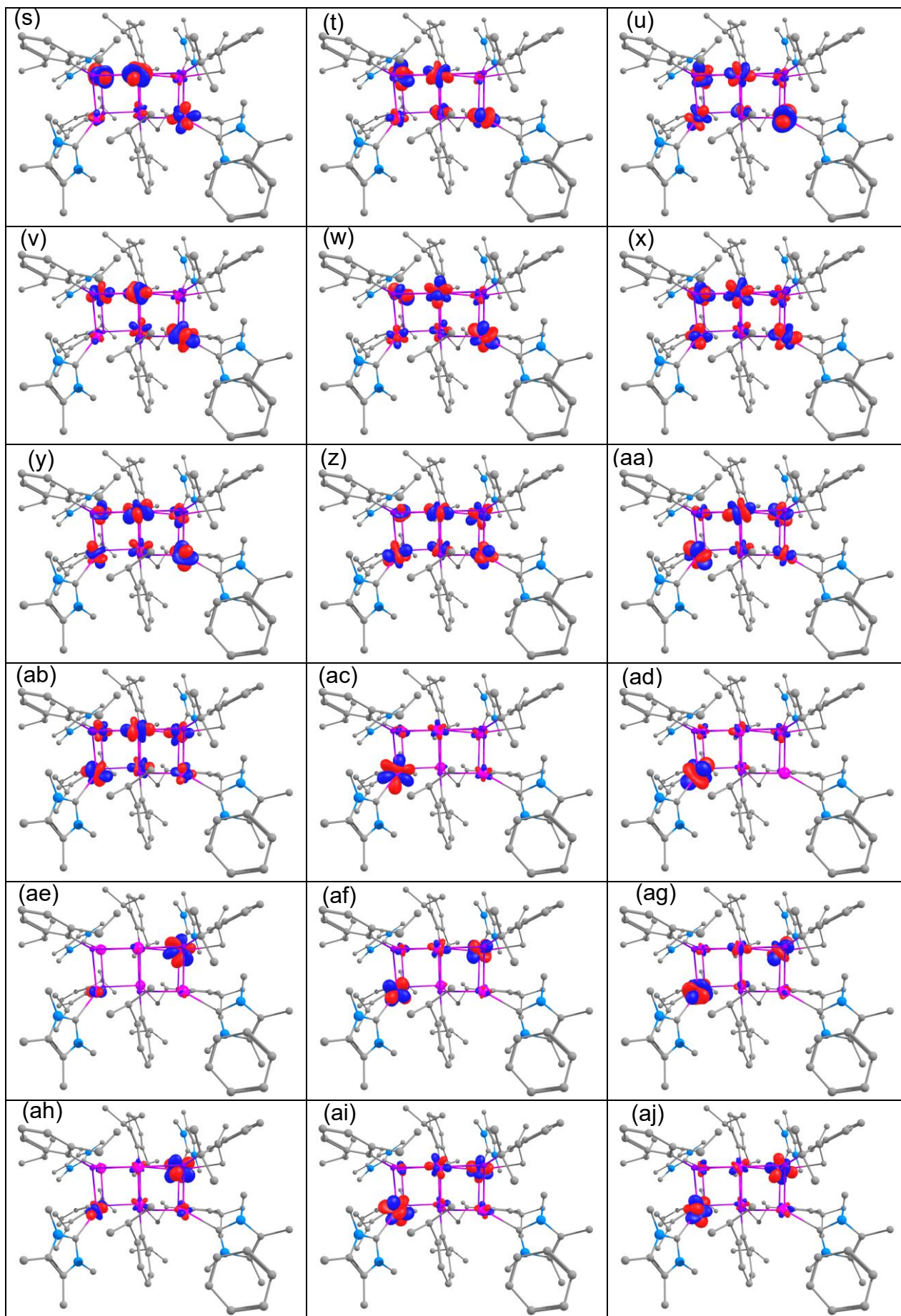
(6.25%) 0.2501*Yb 2 s(10.42%)p 0.02(0.19%)d 8.57(89.26%) f 0.01(0.12%)g 0.00(0.01%) (93.75%) 0.9682* P 4 s(22.14%)p 3.52(77.84%)d 0.00(0.02%)	s(79.67%)p 0.00(0.21%)d 0.25(19.97%)f 0.00(0.13%)g 0.00(0.02%)	
(1.70063) BD (2)Yb 2- P 4 (6.25%) 0.2501*Yb 2 s(10.42%)p 0.02(0.19%)d 8.57(89.26%) f 0.01(0.12%)g 0.00(0.01%) (93.75%) 0.9682* P 4 s(22.14%)p 3.52(77.84%)d 0.00(0.02%)	(0.13950) LV (5)Yb136 s(2.68%)p 0.02(0.05%)d36.26(97.24%)f 0.01(0.03%)g 0.00(0.00%)	14.43
(1.79409) BD (1)Yb 2- P 6 (9.74%) 0.3121*Yb 2 s(29.67%)p 0.00(0.09%)d 2.36(70.04%) f 0.01(0.19%)g 0.00(0.01%) (90.26%) 0.9500* P 6 s(43.16%)p 1.32(56.79%)d 0.00(0.05%)	(0.37247) LV (1)Yb136 s(14.35%)p 0.00(0.03%)d 5.97(85.59%)f 0.00(0.03%)g 0.00(0.01%)	65.81
(1.79409) BD (1)Yb 2- P 6 (9.74%) 0.3121*Yb 2 s(29.67%)p 0.00(0.09%)d 2.36(70.04%) f 0.01(0.19%)g 0.00(0.01%) (90.26%) 0.9500* P 6 s(43.16%)p 1.32(56.79%)d 0.00(0.05%)	(0.19166) LV (3)Yb136 s(1.91%)p 0.01(0.02%)d51.28(98.03%)f 0.01(0.02%)g 0.00(0.01%)	14.42
(1.68407) BD (1)Yb 3- P 4 (8.51%) 0.2917*Yb 3 s(15.99%)p 0.01(0.12%)d 5.24(83.73%) f 0.01(0.13%)g 0.00(0.03%) (91.49%) 0.9565* P 4 s(39.03%)p 1.56(60.94%)d 0.00(0.03%)	(0.24368) LV (2)Yb136 s(0.73%)p 0.11(0.08%)d99.99(99.07%)f 0.15(0.11%)g 0.01(0.00%)	14.17
(1.68407) BD (1)Yb 3- P 4 (8.51%) 0.2917*Yb 3 s(15.99%)p 0.01(0.12%)d 5.24(83.73%) f 0.01(0.13%)g 0.00(0.03%) (91.49%) 0.9565* P 4 s(39.03%)p 1.56(60.94%)d 0.00(0.03%)	(0.17535) LV (4)Yb136 s(79.67%)p 0.00(0.21%)d 0.25(19.97%)f 0.00(0.13%)g 0.00(0.02%)	12.08
(1.71296) BD (1) P 6-Yb138 (90.51%) 0.9514* P 6 s(22.47%)p 3.45(77.48%)d 0.00(0.05%) (9.49%) 0.3081*Yb138 s(31.32%)p 0.00(0.08%)d 2.18(68.38%) f 0.01(0.19%)g 0.00(0.02%)	(0.37247) LV (1)Yb136 s(14.35%)p 0.00(0.03%)d 5.97(85.59%)f 0.00(0.03%)g 0.00(0.01%)	22.41
(1.75731) BD (1)Yb137- P139 (9.07%) 0.3012*Yb137 s(27.58%)p	(0.24368) LV (2)Yb136 s(0.73%)p	14.41

0.00(0.10%)d 2.62(72.21%) f 0.00(0.09%)g 0.00(0.02%) (90.93%) 0.9536* P139 s(29.82%)p 2.35(70.16%)d 0.00(0.02%)	0.11(0.08%)d99.99(99.07%)f 0.15(0.11%)g 0.01(0.00%)	
(1.75731) BD (1)Yb137- P139 (9.07%) 0.3012*Yb137 s(27.58%)p 0.00(0.10%)d 2.62(72.21%) f 0.00(0.09%)g 0.00(0.02%) (90.93%) 0.9536* P139 s(29.82%)p 2.35(70.16%)d 0.00(0.02%)	(0.19166) LV (3)Yb136 s(1.91%)p 0.01(0.02%)d51.28(98.03%)f 0.01(0.02%)g 0.00(0.01%)	22.09
(1.75731) BD (1)Yb137- P139 (9.07%) 0.3012*Yb137 s(27.58%)p 0.00(0.10%)d 2.62(72.21%) f 0.00(0.09%)g 0.00(0.02%) (90.93%) 0.9536* P139 s(29.82%)p 2.35(70.16%)d 0.00(0.02%)	(0.17535) LV (4)Yb136 s(79.67%)p 0.00(0.21%)d 0.25(19.97%)f 0.00(0.13%)g 0.00(0.02%)	15.76
(1.73063) BD (1)Yb137- P140 (10.87%) 0.3296*Yb137 s(31.42%)p 0.00(0.08%)d 2.17(68.27%) f 0.01(0.21%)g 0.00(0.02%) (89.13%) 0.9441* P140 s(67.49%)p 0.48(32.47%)d 0.00(0.04%)	(0.37247) LV (1)Yb136 s(14.35%)p 0.00(0.03%)d 5.97(85.59%)f 0.00(0.03%)g 0.00(0.01%)	118.50
(1.73063) BD (1)Yb137- P140 (10.87%) 0.3296*Yb137 s(31.42%)p 0.00(0.08%)d 2.17(68.27%) f 0.01(0.21%)g 0.00(0.02%) (89.13%) 0.9441* P140 s(67.49%)p 0.48(32.47%)d 0.00(0.04%)	(0.17535) LV (4)Yb136 s(79.67%)p 0.00(0.21%)d 0.25(19.97%)f 0.00(0.13%)g 0.00(0.02%)	12.10
(1.69325) BD (1)Yb138- P139 (7.83%) 0.2798*Yb138 s(19.74%)p 0.00(0.07%)d 4.05(80.03%) f 0.01(0.13%)g 0.00(0.02%) (92.17%) 0.9601* P139 s(23.55%)p 3.25(76.43%)d 0.00(0.02%)	(0.24368) LV (2)Yb136 s(0.73%)p 0.11(0.08%)d99.99(99.07%)f 0.15(0.11%)g 0.01(0.00%)	39.16
(1.69325) BD (1)Yb138- P139 (7.83%) 0.2798*Yb138 s(19.74%)p 0.00(0.07%)d 4.05(80.03%) f 0.01(0.13%)g 0.00(0.02%) (92.17%) 0.9601* P139 s(23.55%)p 3.25(76.43%)d 0.00(0.02%)	(0.17535) LV (4)Yb136 s(79.67%)p 0.00(0.21%)d 0.25(19.97%)f 0.00(0.13%)g 0.00(0.02%)	23.37
(1.79265) BD (2) P140- C148 (83.20%) 0.9121* P140 s(9.84%)p 9.15(90.06%)d 0.01(0.10%)	(0.37247) LV (1)Yb136 s(14.35%)p 0.00(0.03%)d 5.97(85.59%)f 0.00(0.03%)g	21.67

(16.80%) 0.4099* C148 s(0.54%)p99.99(99.40%)d 0.11(0.06%)	0.00(0.01%)	
(1.79265) BD (2) P140- C148 (83.20%) 0.9121* P140 s(9.84%)p 9.15(90.06%)d 0.01(0.10%) (16.80%) 0.4099* C148 s(0.54%)p99.99(99.40%)d 0.11(0.06%)	(0.19166) LV (3)Yb136 s(1.91%)p 0.01(0.02%)d51.28(98.03%)f 0.01(0.02%)g 0.00(0.01%)	13.54
(1.69940) LP (1) P 5 s(0.40%)p99.99(99.57%)d 0.08(0.03%)	(0.36817) LV (1)Yb 1 s(23.99%)p 0.00(0.06%)d 3.16(75.87%) f 0.00(0.07%)g 0.00(0.01%)	19.35
(1.69940) LP (1) P 5 s(0.40%)p99.99(99.57%)d 0.08(0.03%)	(0.19502) LV (3)Yb 1 s(46.25%)p 0.00(0.10%)d 1.16(53.56%)f 0.00(0.07%)g 0.00(0.01%)	11.70
(1.69940) LP (1) P 5 s(0.40%)p99.99(99.57%)d 0.08(0.03%)	(0.21832) LV (2)Yb 2 s(7.92%)p 0.01(0.06%)d11.60(91.85%)f 0.02(0.16%)g 0.00(0.01%)	12.80
(1.69940) LP (1) P 5 s(0.40%)p99.99(99.57%)d 0.08(0.03%)	(0.16930) LV (2)Yb138 s(0.80%)p 0.09(0.07%)d99.99(99.00%)f 0.14(0.11%)g 0.01(0.01%)	27.94
(1.08256) LP (2) P 5 s(41.85%)p 0.77(32.10%)d 0.62(26.05%)	(0.36817) LV (1)Yb 1 s(23.99%)p 0.00(0.06%)d 3.16(75.87%) f 0.00(0.07%)g 0.00(0.01%)	365.73
(1.08256) LP (2) P 5 s(41.85%)p 0.77(32.10%)d 0.62(26.05%)	(0.19502) LV (3)Yb 1 s(46.25%)p 0.00(0.10%)d 1.16(53.56%)f 0.00(0.07%)g 0.00(0.01%)	95.80
(1.08256) LP (2) P 5 s(41.85%)p 0.77(32.10%)d 0.62(26.05%)	(0.24887) LV (1)Yb 2 s(31.61%)p 0.00(0.08%)d 2.15(68.04%)f 0.01(0.25%)g 0.00(0.01%)	44.02
(1.08256) LP (2) P 5 s(41.85%)p 0.77(32.10%)d 0.62(26.05%)	(0.12737) LV (3)Yb 2 s(0.86%)p 0.12(0.10%)d99.99(98.97%)f 0.07(0.06%)g 0.01(0.01%)	42.01
(1.08256) LP (2) P 5 s(41.85%)p 0.77(32.10%)d	(0.24368) LV (2)Yb136 s(0.73%)p	13.78

0.62(26.05%)	0.11(0.08%)d99.99(99.07%)f 0.15(0.11%)g 0.01(0.00%)	
(1.78165) LP (1) C 10 s(44.11%)p 1.27(55.86%)d 0.00(0.03%)	(0.21832) LV (2)Yb 2 s(7.92%)p 0.01(0.06%)d11.60(91.85%)f 0.02(0.16%)g 0.00(0.01%)	76.61
(1.78165) LP (1) C 10 s(44.11%)p 1.27(55.86%)d 0.00(0.03%)	(0.12737) LV (3)Yb 2 s(0.86%)p 0.12(0.10%)d99.99(98.97%)f 0.07(0.06%)g 0.01(0.01%)	14.59
(1.81520) LP (1) C 71 s(44.23%)p 1.26(55.75%)d 0.00(0.03%)	(0.21839) LV (1)Yb 3 s(46.49%)p 0.00(0.14%)d 1.14(53.07%)f 0.01(0.28%)g 0.00(0.01%)	20.78
(1.81520) LP (1) C 71 s(44.23%)p 1.26(55.75%)d 0.00(0.03%)	(0.15060) LV (2)Yb 3 s(0.43%)p 0.10(0.04%)d99.99(99.46%)f 0.16(0.07%)g 0.01(0.00%)	13.42
(1.81520) LP (1) C 71 s(44.23%)p 1.26(55.75%)d 0.00(0.03%)	(0.11159) LV (3)Yb 3 s(4.68%)p 0.03(0.15%)d20.30(95.06%)f 0.02(0.09%)g 0.00(0.02%)	10.05
(1.81520) LP (1) C 71 s(44.23%)p 1.26(55.75%)d 0.00(0.03%)	(0.09462) LV (4)Yb 3 s(0.51%)p 0.31(0.16%)d99.99(99.26%)f 0.13(0.07%)g 0.02(0.01%)	10.69
(1.78386) LP (1) C145 s(44.16%)p 1.26(55.81%)d 0.00(0.03%)	(0.21254) LV (1)Yb137 s(7.66%)p 0.01(0.07%)d12.03(92.12%)f 0.02(0.15%)g 0.00(0.01%)	70.59
(1.78386) LP (1) C145 s(44.16%)p 1.26(55.81%)d 0.00(0.03%)	(0.12124) LV (3)Yb137 s(0.47%)p 0.39(0.18%)d99.99(99.29%)f 0.10(0.04%)g 0.02(0.01%)	19.27
(1.80381) LP (1) C206 s(44.52%)p 1.25(55.45%)d 0.00(0.03%)	(0.24144) LV (1)Yb138 s(44.38%)p 0.00(0.12%)d 1.25(55.26%)f 0.01(0.23%)g 0.00(0.01%)	56.67
(1.80381) LP (1) C206 s(44.52%)p 1.25(55.45%)d 0.00(0.03%)	(0.16930) LV (2)Yb138 s(0.80%)p 0.09(0.07%)d99.99(99.00%)f 0.14(0.11%)g 0.01(0.01%)	28.18





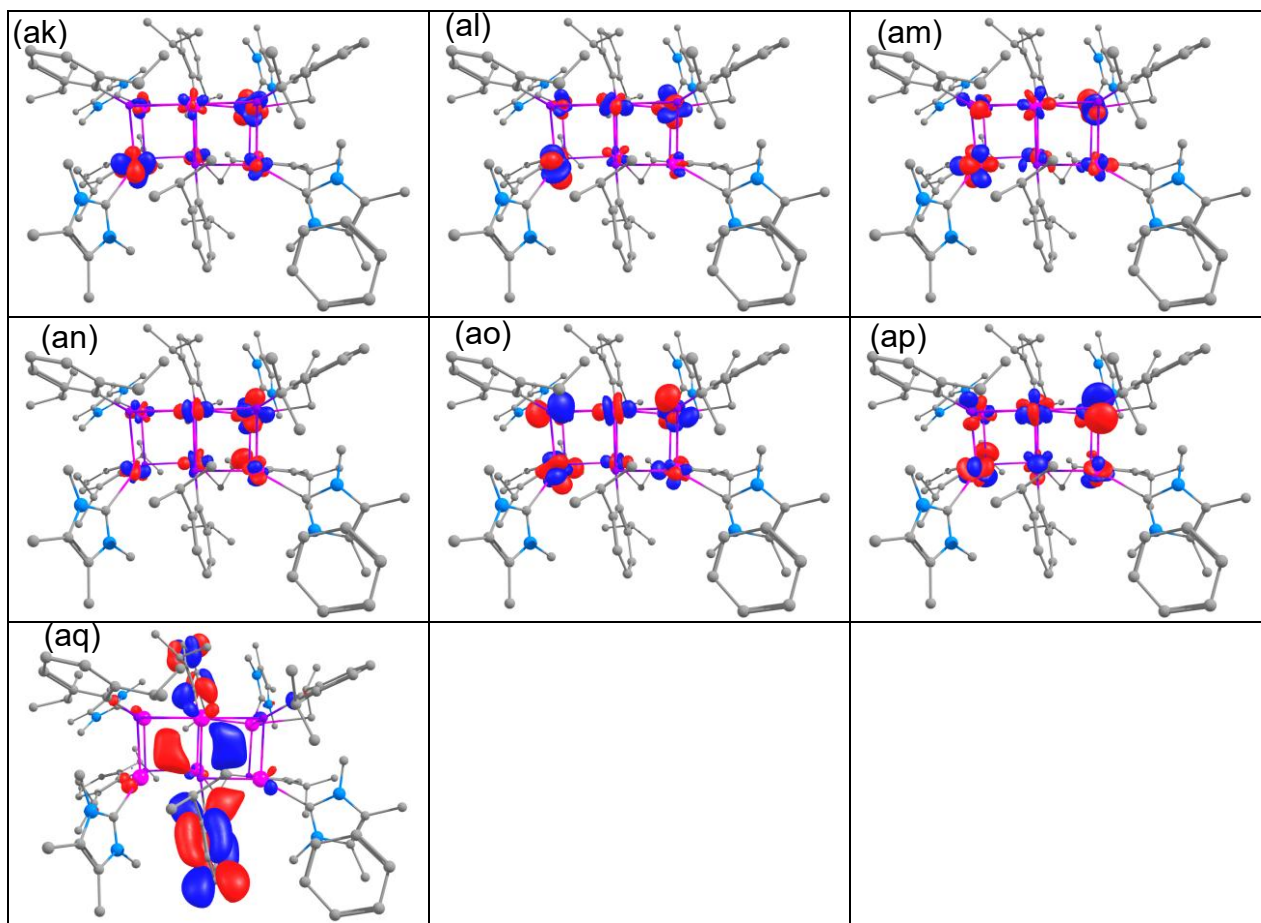
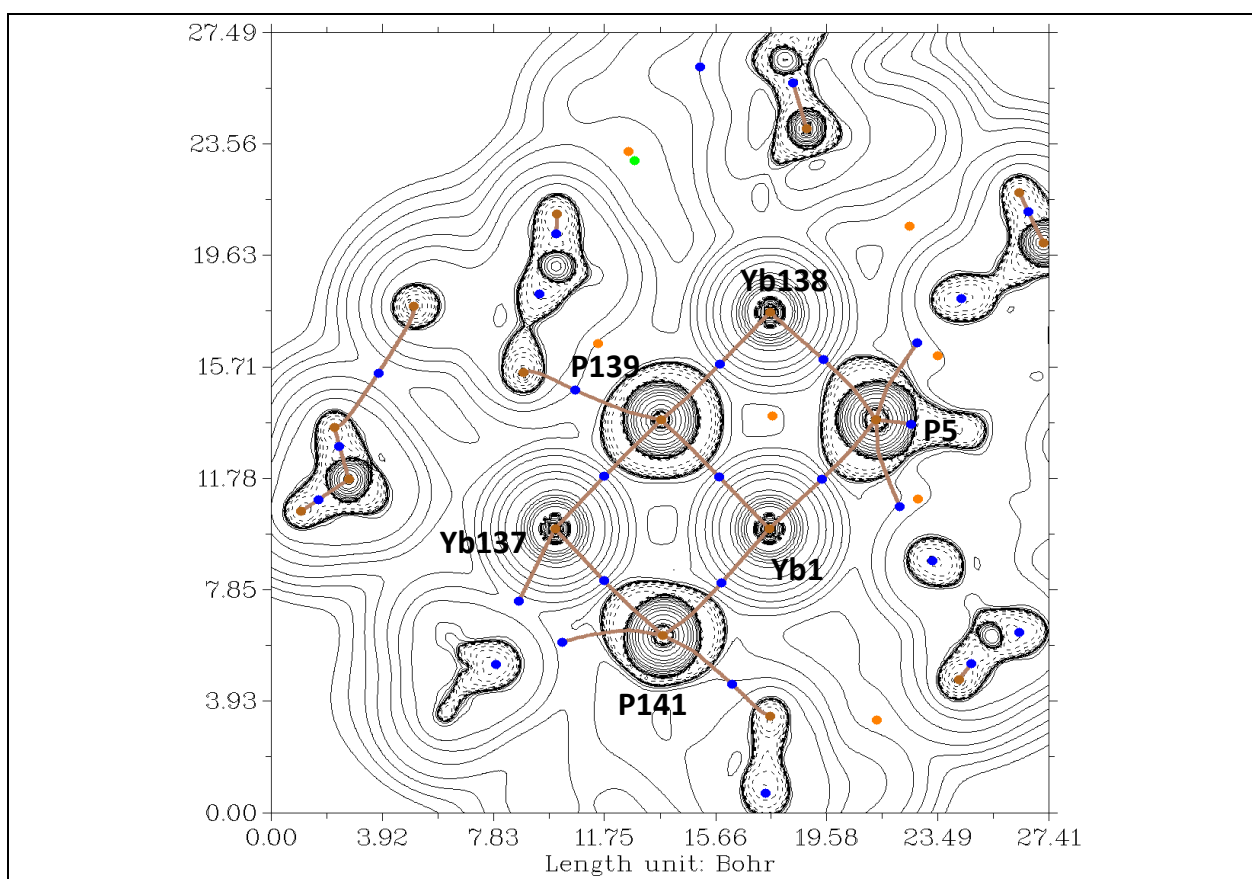


Fig. S56 Computed MOs for complex **5** (dispersion). (a)HOMO-41 (b)HOMO-40 (c)HOMO-39 (d)HOMO-38 (e)HOMO-37 (f)HOMO-36 (g)HOMO-35 (h)HOMO-34 (i)HOMO-33 (j)HOMO-32 (k)HOMO-31 (l)HOMO-30 (m)HOMO-29 (n)HOMO-28 (o)HOMO-27 (p)HOMO-26 (q)HOMO-25 (r)HOMO-24 (s)HOMO-23 (t)HOMO-22 (u)HOMO-21 (v)HOMO-20 (w)HOMO-19 (x)HOMO-18 (y)HOMO-17 (z)HOMO-16 (aa)HOMO-15 (ab)HOMO-14 (ac)HOMO-13 (ad)HOMO-12 (ae)HOMO-11 (af)HOMO-10 (ag)HOMO-9 (ah)HOMO-8 (ai)HOMO-7 (aj)HOMO-6 (ak)HOMO-5 (al)HOMO-4 (am)HOMO-3 (an)HOMO-2 (ao)HOMO-1 (ap)HOMO (aq)LUMO.

Table S19 Computed BCP descriptors for complex **5** (dispersion).

Atom labels	$\rho(r)$	$\nabla^2\rho(r)$	$G(r)$	$V(r)$	$H(r)$	ϵ
Yb1-P4	0.03	0.08	0.023	-0.027	-0.004	0.17
Yb1-P5	0.04	0.08	0.025	-0.030	-0.005	0.16
Yb1-P139	0.03	0.08	0.023	-0.027	-0.004	0.15
Yb1-P141	0.04	0.08	0.025	-0.030	-0.005	0.15
Yb2-P4	0.04	0.08	0.026	-0.032	-0.005	0.14
Yb2-P5	0.04	0.09	0.028	-0.034	-0.006	0.20

Yb2-P6	0.04	0.08	0.030	-0.033	-0.006	0.19
Yb2-C10	0.05	0.15	0.041	-0.045	-0.005	0.09
Yb3-P4	0.04	0.08	0.024	-0.029	-0.004	0.04
Yb3-C71	0.04	0.14	0.039	-0.044	-0.005	0.07
Yb3-P140	0.04	0.09	0.027	-0.033	-0.006	0.22
Yb3-P141	0.04	0.08	0.025	-0.030	-0.005	0.25
Yb136-P4	0.04	0.08	0.024	-0.029	-0.005	0.13
Yb136-P6	0.04	0.08	0.025	-0.030	-0.005	0.15
Yb136-P139	0.03	0.08	0.022	-0.026	-0.004	0.18
Yb136-P140	0.04	0.08	0.024	-0.029	-0.005	0.19
Yb137-P139	0.04	0.08	0.024	-0.029	-0.005	0.18
Yb137- P140	0.04	0.08	0.027	-0.033	-0.006	0.22
Yb137-P141	0.04	0.08	0.026	-0.032	-0.006	0.17
Yb137-C145	0.04	0.14	0.040	-0.044	-0.004	0.07
Yb138-P5	0.04	0.08	0.026	-0.031	-0.005	0.15
Yb138-P6	0.04	0.08	0.025	-0.030	-0.006	0.25
Yb138-P139	0.03	0.08	0.023	-0.027	-0.004	0.11
Yb138-C206	0.04	0.13	0.037	-0.041	-0.004	0.06



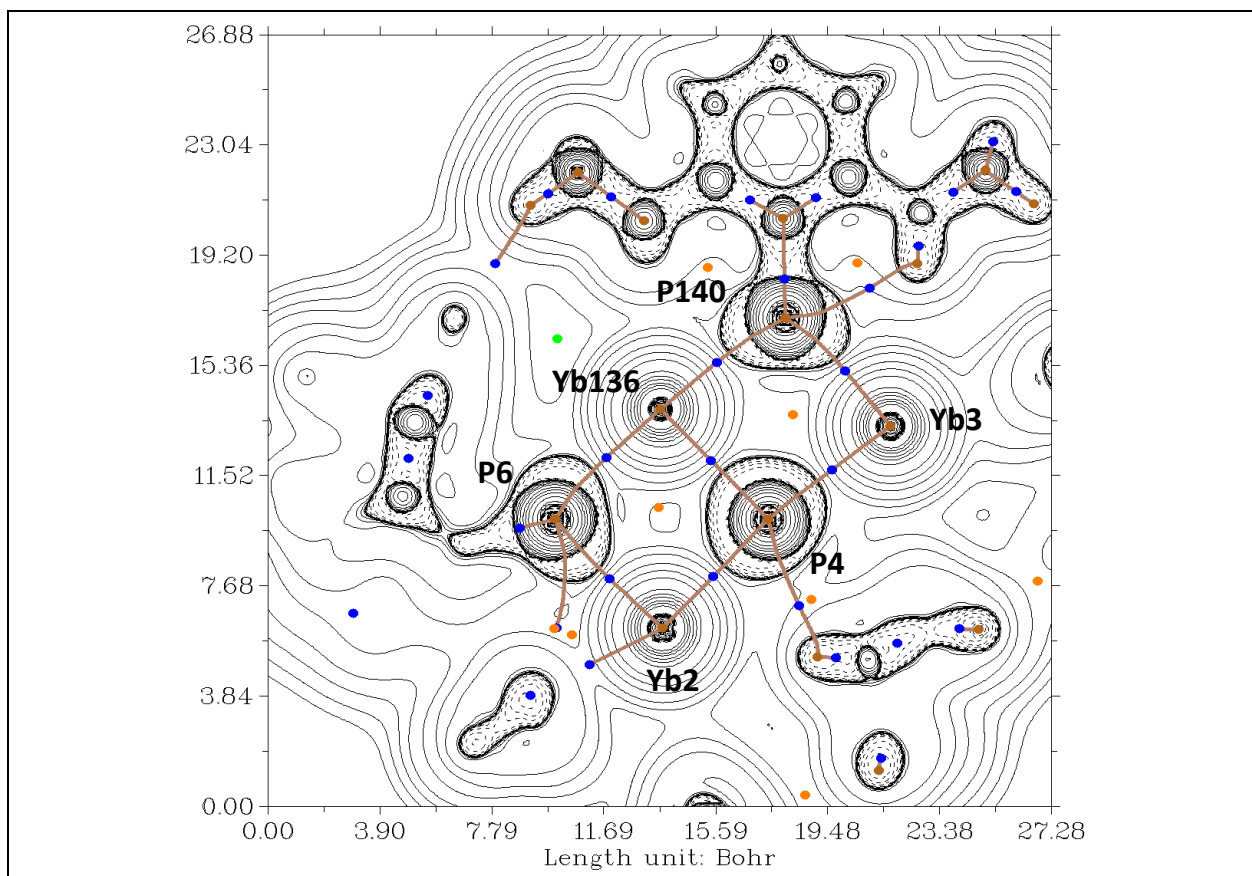


Fig. S57 Computed Laplacian distribution for complex **5** (dispersion).

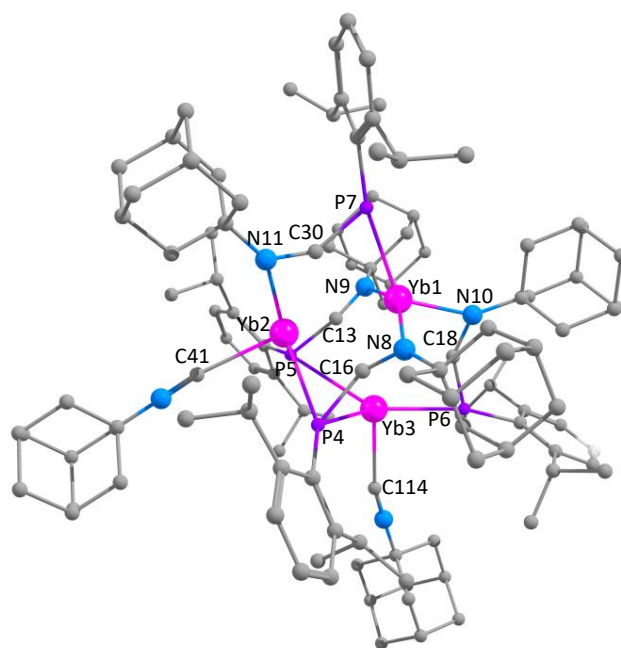
Table S20 Computed energetics (kcal/mol) for different spin states computed for complex **7**.

Spin states	ΔH	ΔG
S=1	0.1	0.8
S=0, open shell singlet	0.0	0.0

Table S21 Comparison of selected bond distances (Å) between experimental and DFT structures for complex **7**.

Atom labels	DFT		X-ray
	S=1	S=0 (open shell singlet)	
Yb3-Yb2	3.22	3.22	3.19
Yb3-P7	2.74	2.74	2.72
Yb3-N8	2.34	2.34	2.30
Yb3-N9	2.33	2.34	2.28
Yb3-N10	2.25	2.25	2.23
Yb3-C13	2.52	2.55	2.50
Yb3-C16	2.55	2.52	2.49
Yb3-C18	2.48	2.49	2.45

Yb3-C30	2.72	2.73	2.68
Yb2-Yb1	3.59	3.58	3.56
Yb2-P4	2.78	2.78	2.74
Yb2-P5	2.77	2.78	2.75
Yb2-N11	2.18	2.18	2.17
Yb2-C13	2.57	2.55	2.54
Yb2-C16	2.53	2.55	2.52
Yb2-C30	2.40	2.40	2.36
Yb2-C41	2.57	2.56	2.52
Yb1-P4	3.07	3.07	2.98
Yb1-P5	3.08	3.08	2.98
Yb1-P6	2.71	2.71	2.67
Yb1-C13	2.85	2.82	2.79
Yb1-C16	2.85	2.88	2.91
Yb1-C18	2.68	2.68	2.68
Yb1-C114	2.64	2.64	2.61



DFT structure of complex 7

Please note that there is an inconsistency between the atom labels used in the theoretical computations and those from X-ray diffraction, as detailed in the following table.

Correspondence between atom labels in theoretical computations and X-ray diffraction.

Theoretical Computations	X-ray
Yb1	Yb1
Yb2	Yb3

	Yb3	Yb2	
	P6	P1	
	P7	P2	
	P5	P3	
	P4	P4	
	N10	N1	
	N11	N2	
	N9	N3	
	N8	N4	
	C18	C1	
	C30	C2	
	C13	C3	
	C16	C4	
	C114	C5	
	C41	C6	

Table S22 Computed natural charges for selected atoms in complex **7** (S=1).

Atom labels	Natural charges
Yb3	1.25643
Yb2	1.09931
Yb1	0.93333
P4	0.28010
P5	0.27868
P6	0.23293
P7	0.36433
N8	-0.56480
N10	-0.68117
N11	-0.68925
C13	-0.46544
C16	-0.46962
C18	-0.45443
C30	-0.44698
C41	0.29941
C114	0.26721

Table S23 Computed spin densities on selected atoms in complex **7** (S=1).

Atom labels	Spin densities	
Yb3	0.903064	
Yb2	0.905779	
Yb1	0.004959	

P4	0.000425
P5	0.008581
P6	0.002128
P7	0.005177
N8	0.015512
N10	0.010594
N11	0.016792
C13	0.004327
C16	0.006411
C18	0.009347
C30	0.049838
C41	-0.001580
C114	-0.000038

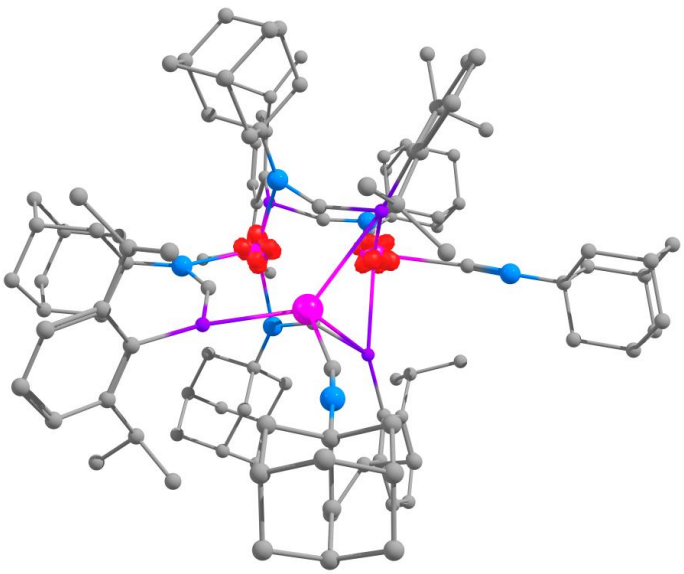


Table S24 Computed Wiberg bond index between selected atoms in complex **7** (S=1).

Atom labels	Wiberg bond index
Yb3-Yb2	0.1535
Yb3-P7	0.5214
Yb3-N8	0.2814
Yb3-N9	0.2861
Yb3-N10	0.0220
Yb3-C13	0.2827
Yb3-C16	0.2650
Yb3-C18	0.3244
Yb3-C30	0.2500
Yb2-Yb1	0.0815
Yb2-P4	0.4691
Yb2-P5	0.4776
Yb2-N11	0.4313
Yb2-C13	0.3060
Yb2-C16	0.3294
Yb2-C30	0.3915
Yb2-C41	0.3751
Yb1-P4	0.2367
Yb1-P5	0.2324
Yb1-P6	0.4787
Yb1-C13	0.1333
Yb1-C16	0.1305
Yb1-C18	0.2411
Yb1-C114	0.3256

NBO analysis (Alpha Molecular Orbitals) for bonding orbitals in Yb1 (S=1).

(0.96691) BD (1)Yb 3- P 7
 (12.74%) 0.3569*Yb 3 s(40.94%)p 0.01(0.33%)d 1.43(58.49%) f 0.01(0.21%)g
 0.00(0.04%)
 (87.26%) 0.9341* P 7 s(52.09%)p 0.92(47.88%)d 0.00(0.02%)
 (0.95810) BD (1)Yb 3- N 10
 (8.01%) 0.2829*Yb 3 s(33.96%)p 0.01(0.43%)d 1.92(65.23%) f 0.01(0.31%)g
 0.00(0.07%)
 (91.99%) 0.9591* N 10 s(29.75%)p 2.36(70.23%)d 0.00(0.02%)
 (0.96407) BD (1)Yb 2- N 11
 (9.17%) 0.3028*Yb 2 s(24.12%)p 0.01(0.19%)d 3.12(75.34%) f 0.01(0.29%)g
 0.00(0.06%)
 (90.83%) 0.9531* N 11 s(30.24%)p 2.31(69.75%)d 0.00(0.02%)
 (0.98567) BD (1)Yb 2- C 41
 (12.09%) 0.3477*Yb 2 s(35.70%)p 0.00(0.12%)d 1.79(64.05%) f 0.00(0.12%)g
 0.00(0.02%)
 (87.91%) 0.9376* C 41 s(65.11%)p 0.54(34.88%)d 0.00(0.01%)
 (0.96375) BD (1)Yb 1- P 6
 (10.25%) 0.3202*Yb 1 s(26.13%)p 0.00(0.12%)d 2.81(73.49%) f 0.01(0.24%)g
 0.00(0.01%)
 (89.75%) 0.9474* P 6 s(51.30%)p 0.95(48.67%)d 0.00(0.03%)
 (0.98727) BD (1)Yb 1- C114
 (9.28%) 0.3046*Yb 1 s(38.24%)p 0.00(0.16%)d 1.60(61.36%) f 0.01(0.23%)g
 0.00(0.01%)
 (90.72%) 0.9525* C114 s(65.15%)p 0.53(34.83%)d 0.00(0.01%)
 (0.97671) 3C (1)Yb 3- P 7- C 30
 (5.08%) 0.2255*Yb 3 s(0.22%)p 2.03(0.45%)d99.99(98.94%)f 1.37(0.30%)g
 0.37(0.08%)
 (65.78%) 0.8111* P 7 s(0.01%)p99.99(99.74%)d16.17(0.24%)
 (29.13%) 0.5398* C 30 s(0.09%)p99.99(99.82%)d 1.13(0.10%)

Table S25 DFT computed NBO second order perturbation analysis (Alpha Molecular Orbitals)

for complex **7** (S=1).

Donor NBO	Acceptor NBO	E(2) kcal/mol
(0.73591) LP (1) P 6 s(0.00%)p 1.00(99.87%)d 0.00(0.13%)	(0.12034) LV (1)Yb 1 s(0.01%)p 1.00(0.12%)d99.99(99.81%)f 0.48(0.06%)g 0.10(0.01%)	13.76
(0.73902) LP (1) N 11 s(0.00%)p 1.00(99.94%)d 0.00(0.06%)	(0.16225) LV (1)Yb 2	4.94

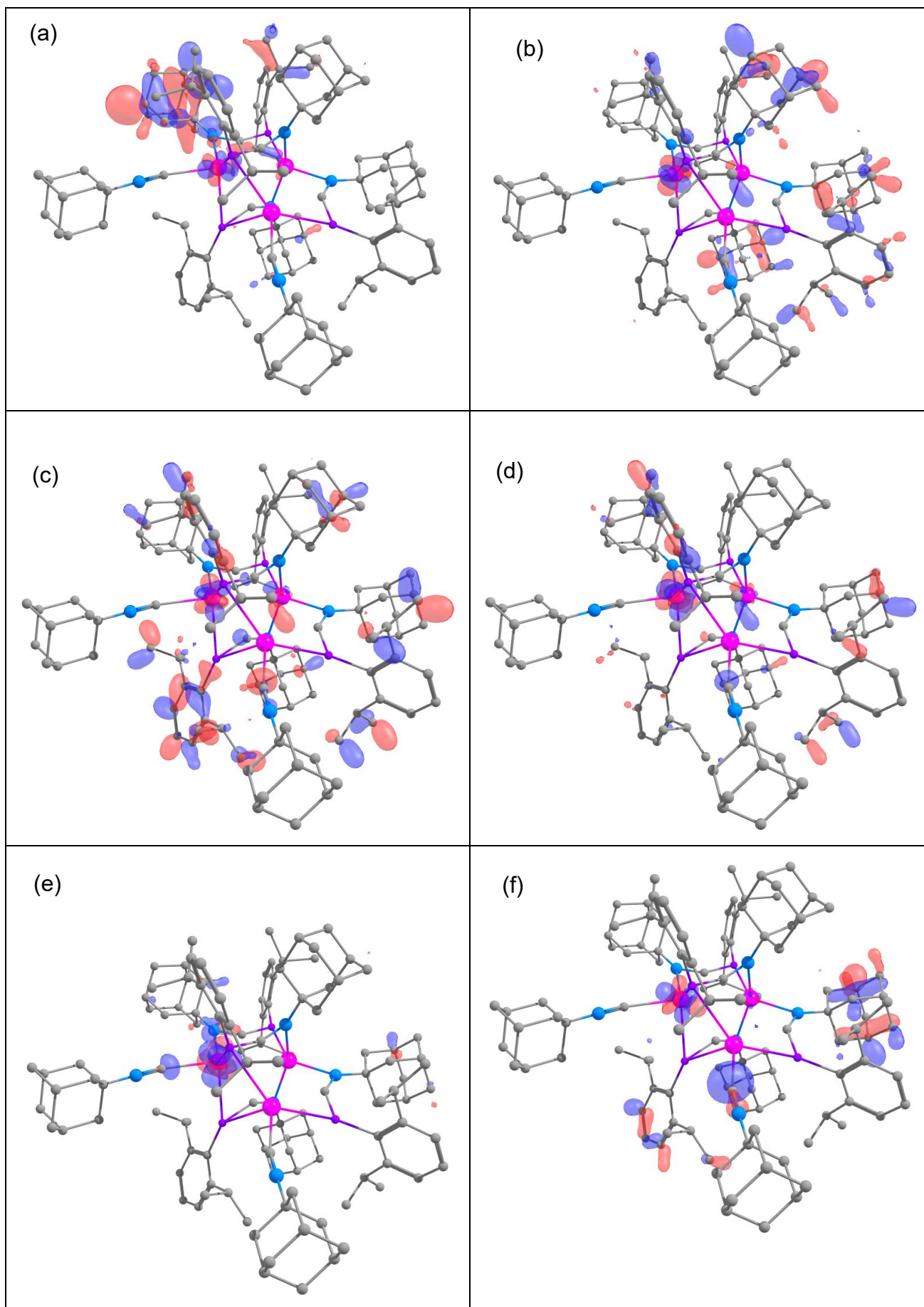
	s(0.06%)p 2.08(0.12%)d99.99(99.74%)f 1.38(0.08%)g 0.25(0.01%)	
(0.73902) LP (1) N 11 s(0.00%)p 1.00(99.94%)d 0.00(0.06%)	(0.12161) LV (3)Yb 2 s(0.85%)p 0.60(0.51%)d99.99(98.50%)f 0.15(0.13%)g 0.01(0.01%)	5.56
(0.75989) LP (1) C 18 s(38.50%)p 1.60(61.49%)d 0.00(0.01%)	(0.11979) LV (2)Yb 3 s(0.06%)p 1.75(0.11%)d99.99(99.68%)f 2.17(0.13%)g 0.20(0.01%)	26.27
(0.75989) LP (1) C 18 s(38.50%)p 1.60(61.49%)d 0.00(0.01%)	(0.07509) LV (2)Yb 1 s(17.64%)p 0.03(0.54%)d 4.62(81.48%)f 0.02(0.31%)g 0.00(0.03%)	12.82
(0.75989) LP (1) C 18 s(38.50%)p 1.60(61.49%)d 0.00(0.01%)	(0.09241) BD*(1)Yb 3- P 7 (87.26%) 0.9341*Yb 3 s(40.94%)p 0.01(0.33%)d 1.43(58.49%)f 0.01(0.21%)g 0.00(0.04%) (12.74%) -0.3569* P 7 s(52.09%)p 0.92(47.88%)d 0.00(0.02%)	28.69
(0.74780) LP (1) C 30 s(40.14%)p 1.49(59.85%)d 0.00(0.02%)	(0.11979) LV (2)Yb 3 s(0.06%)p 1.75(0.11%)d99.99(99.68%)f 2.17(0.13%)g 0.20(0.01%)	21.04
(0.74780) LP (1) C 30 s(40.14%)p 1.49(59.85%)d 0.00(0.02%)	(0.14701) LV (2)Yb 2 s(23.61%)p 0.01(0.32%)d 3.21(75.82%)f 0.01(0.24%)g 0.00(0.01%)	18.22
(0.74780) LP (1) C 30 s(40.14%)p 1.49(59.85%)d 0.00(0.02%)	(0.10856) LV (4)Yb 2 s(13.33%)p 0.02(0.33%)d 6.47(86.22%)f 0.01(0.11%)g 0.00(0.02%)	11.10
(0.74780) LP (1) C 30 s(40.14%)p 1.49(59.85%)d 0.00(0.02%)	(0.08874) BD*(1)Yb 3- N 10 (91.99%) 0.9591*Yb 3 s(33.96%)p 0.01(0.43%)d 1.92(65.23%)f 0.01(0.31%)g 0.00(0.07%) (8.01%) -0.2829* N 10 s(29.75%)p 2.36(70.23%)d 0.00(0.02%)	15.44

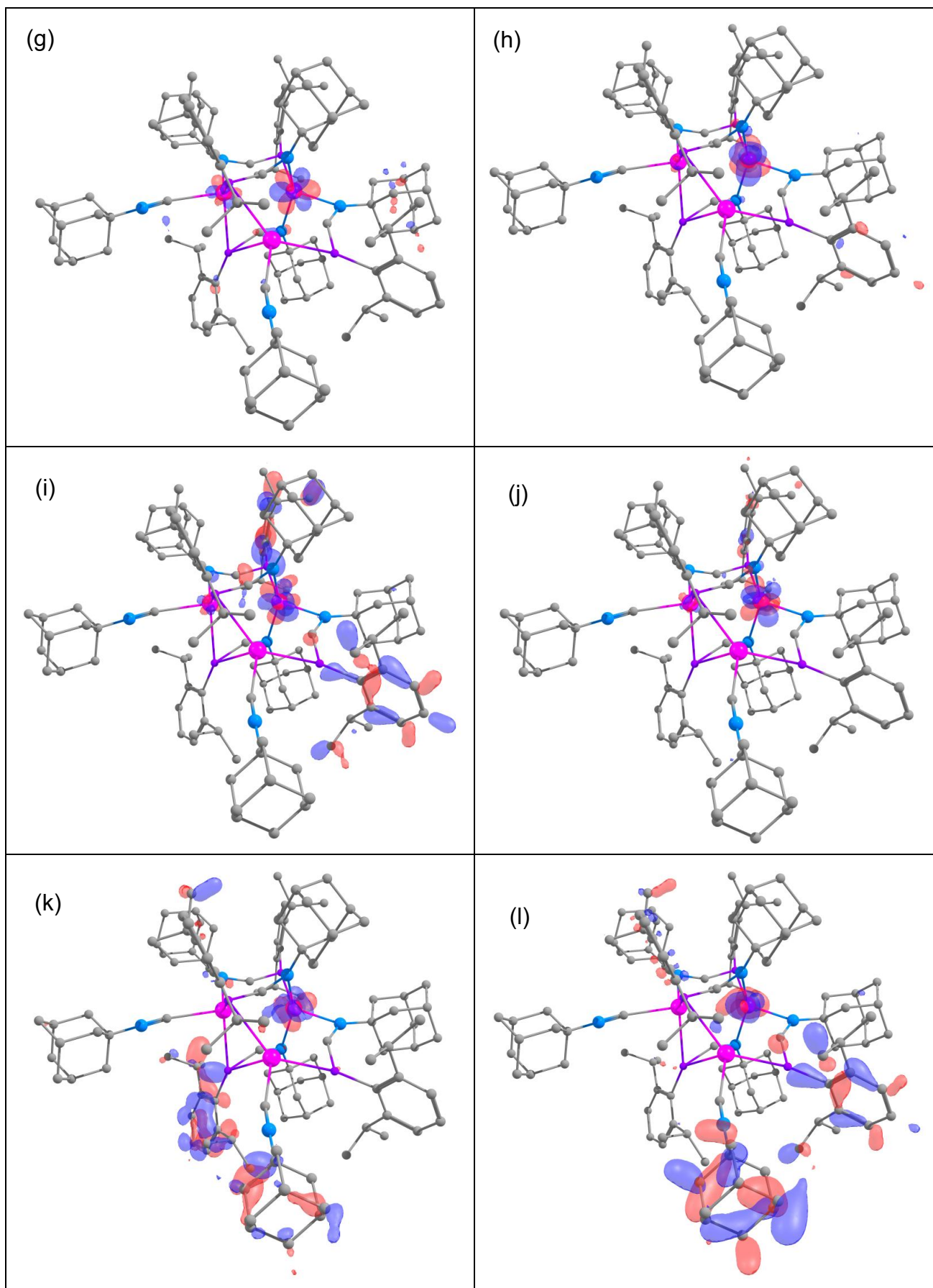
(0.74780) LP (1) C 30 s(40.14%)p 1.49(59.85%)d 0.00(0.02%)	(0.08329) BD*(1)Yb 2- C 41 (87.91%) 0.9376*Yb 2 s(35.70%)p 0.00(0.12%)d 1.79(64.05%)f 0.00(0.12%)g 0.00(0.02%) (12.09%) -0.3477* C 41 s(65.11%)p 0.54(34.88%)d 0.00(0.01%)	11.96
(0.97244) BD (1) P 6- C 18 (36.16%) 0.6014* P 6 s(23.37%)p 3.25(75.94%)d 0.03(0.69%) (63.84%) 0.7990* C 18 s(34.06%)p 1.93(65.88%)d 0.00(0.06%)	(0.07509) LV (2)Yb 1 s(17.64%)p 0.03(0.54%)d 4.62(81.48%)f 0.02(0.31%)g 0.00(0.03%)	5.81
(0.97299) BD (1) P 7- C 30 (34.63%) 0.5884* P 7 s(22.41%)p 3.43(76.81%)d 0.03(0.78%) (65.37%) 0.8085* C 30 s(33.93%)p 1.95(66.02%)d 0.00(0.05%)	(0.11979) LV (2)Yb 3 s(0.06%)p 1.75(0.11%)d99.99(99.68%)f 2.17(0.13%)g 0.20(0.01%)	8.08
(0.98648) BD (1) N 10- C 18 (60.71%) 0.7791* N 10 s(35.70%)p 1.80(64.18%)d 0.00(0.12%) (39.29%) 0.6268* C 18 s(27.04%)p 2.69(72.84%)d 0.00(0.12%)	(0.11979) LV (2)Yb 3 s(0.06%)p 1.75(0.11%)d99.99(99.68%)f 2.17(0.13%)g 0.20(0.01%)	9.18
(0.98595) BD (1) N 11- C 30 (60.47%) 0.7776* N 11 s(34.69%)p 1.88(65.19%)d 0.00(0.12%) (39.53%) 0.6288* C 30 s(25.60%)p 2.90(74.28%)d 0.00(0.12%)	(0.10856) LV (4)Yb 2 s(13.33%)p 0.02(0.33%)d 6.47(86.22%)f 0.01(0.11%)g 0.00(0.02%)	6.60
(0.80245) LP (1) P 4 s(42.17%)p 1.37(57.75%)d 0.00(0.08%)	(0.16225) LV (1)Yb 2 s(0.06%)p 2.08(0.12%)d99.99(99.74%)f 1.38(0.08%)g 0.25(0.01%)	17.58
(0.80245) LP (1) P 4 s(42.17%)p 1.37(57.75%)d 0.00(0.08%)	(0.14701) LV (2)Yb 2 s(23.61%)p 0.01(0.32%)d 3.21(75.82%)f 0.01(0.24%)g 0.00(0.01%)	9.66
(0.80245) LP (1) P 4 s(42.17%)p 1.37(57.75%)d 0.00(0.08%)	(0.12034) LV (1)Yb 1 s(0.01%)p 1.00(0.12%)d99.99(99.81%)f 0.48(0.06%)g 0.10(0.01%)	11.73
(0.72566) LP (2) P 4 s(1.17%)p84.56(98.65%)d 0.16(0.18%)	(0.16225) LV (1)Yb 2	8.88

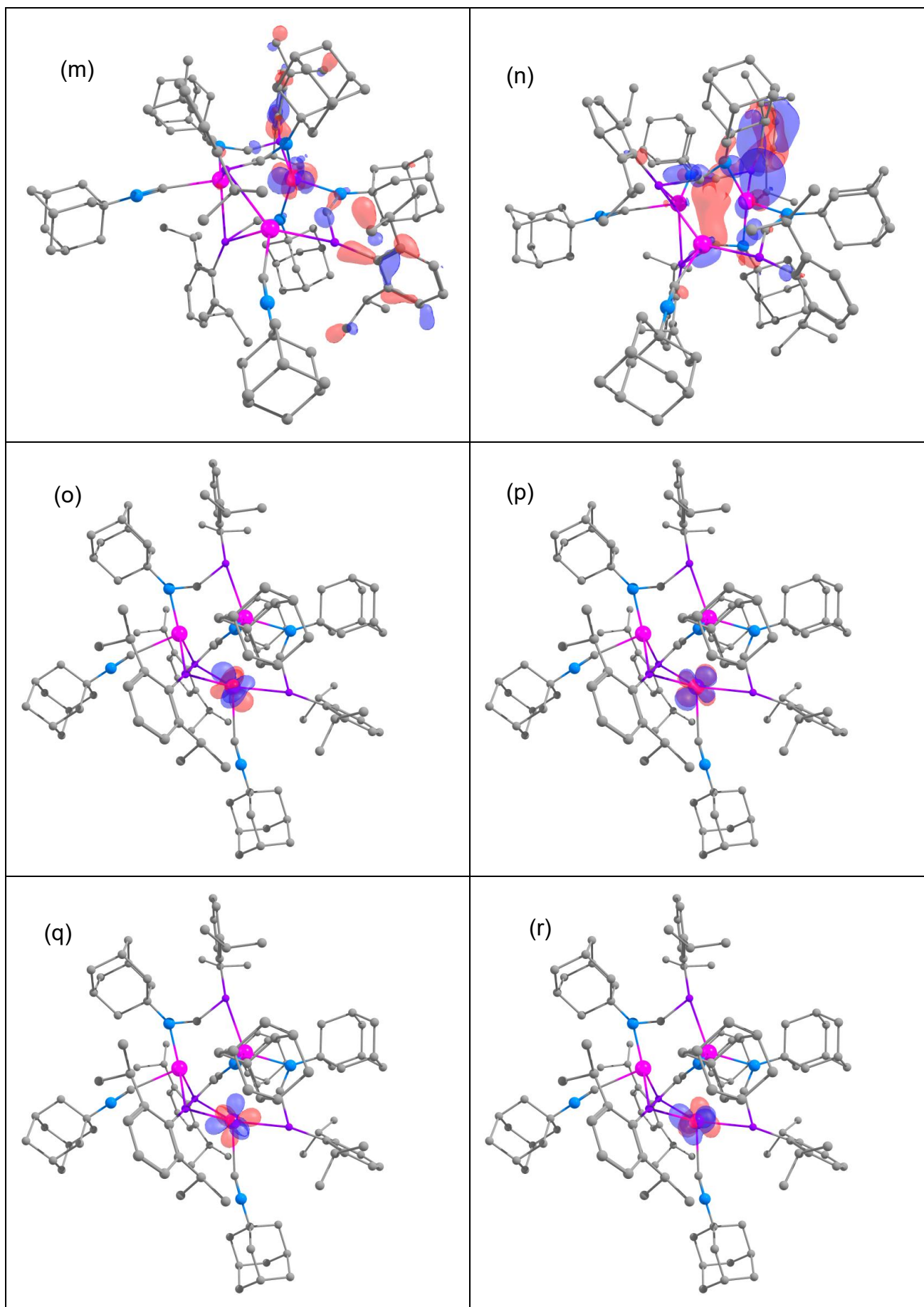
	s(0.06%)p 2.08(0.12%)d99.99(99.74%)f 1.38(0.08%)g 0.25(0.01%)	
(0.72566) LP (2) P 4 s(1.17%)p84.56(98.65%)d 0.16(0.18%)	(0.14701) LV (2)Yb 2 s(23.61%)p 0.01(0.32%)d 3.21(75.82%)f 0.01(0.24%)g 0.00(0.01%)	8.15
(0.72566) LP (2) P 4 s(1.17%)p84.56(98.65%)d 0.16(0.18%)	(0.10856) LV (4)Yb 2 s(13.33%)p 0.02(0.33%)d 6.47(86.22%)f 0.01(0.11%)g 0.00(0.02%)	8.00
(0.88952) LP (1) N 8 s(32.09%)p 2.12(67.88%)d 0.00(0.03%)	(0.13509) LV (1)Yb 3 s(21.67%)p 0.02(0.53%)d 3.58(77.48%)f 0.01(0.24%)g 0.00(0.07%)	32.72
(0.71793) LP (1) C 16 s(46.08%)p 1.17(53.92%)d 0.00(0.01%)	(0.10352) LV (3)Yb 3 s(0.22%)p 2.83(0.62%)d99.99(99.00%)f 0.68(0.15%)g 0.05(0.01%)	19.80
(0.71793) LP (1) C 16 s(46.08%)p 1.17(53.92%)d 0.00(0.01%)	(0.12161) LV (3)Yb 2 s(0.85%)p 0.60(0.51%)d99.99(98.50%)f 0.15(0.13%)g 0.01(0.01%)	20.00
(0.71793) LP (1) C 16 s(46.08%)p 1.17(53.92%)d 0.00(0.01%)	(0.05598) BD*(1)Yb 1- C114 (90.72%) 0.9525*Yb 1 s(38.24%)p 0.00(0.16%)d 1.60(61.36%)f 0.01(0.23%)g 0.00(0.01%) (9.28%) -0.3046* C114 s(65.15%)p 0.53(34.83%)d 0.00(0.01%)	7.65
(0.96244) BD (1) P 4- C 16 (36.59%) 0.6049* P 4 s(17.08%)p 4.82(82.26%)d 0.04(0.67%) (63.41%) 0.7963* C 16 s(28.42%)p 2.52(71.52%)d 0.00(0.06%)	(0.12161) LV (3)Yb 2 s(0.85%)p 0.60(0.51%)d99.99(98.50%)f 0.15(0.13%)g 0.01(0.01%)	8.21
(0.98575) BD (1) N 8- C 16 (59.94%) 0.7742* N 8 s(33.97%)p 1.94(65.88%)d 0.00(0.15%) (40.06%) 0.6329* C 16 s(25.10%)p 2.98(74.78%)d 0.00(0.12%)	(0.13509) LV (1)Yb 3 s(21.67%)p 0.02(0.53%)d 3.58(77.48%)f 0.01(0.24%)g 0.00(0.07%)	6.19
(0.98575) BD (1) N 8- C 16	(0.10352) LV (3)Yb 3	6.62

(59.94%) 0.7742* N 8 s(33.97%)p 1.94(65.88%)d 0.00(0.15%) (40.06%) 0.6329* C 16 s(25.10%)p 2.98(74.78%)d 0.00(0.12%)	s(0.22%)p 2.83(0.62%)d99.99(99.00%)f 0.68(0.15%)g 0.05(0.01%)	
(0.80497) LP (1) P 5 s(42.26%)p 1.36(57.66%)d 0.00(0.08%)	(0.16225) LV (1)Yb 2 s(0.06%)p 2.08(0.12%)d99.99(99.74%)f 1.38(0.08%)g 0.25(0.01%)	13.88
(0.80497) LP (1) P 5 s(42.26%)p 1.36(57.66%)d 0.00(0.08%)	(0.14701) LV (2)Yb 2 s(23.61%)p 0.01(0.32%)d 3.21(75.82%)f 0.01(0.24%)g 0.00(0.01%)	13.66
(0.80497) LP (1) P 5 s(42.26%)p 1.36(57.66%)d 0.00(0.08%)	(0.12034) LV (1)Yb 1 s(0.01%)p 1.00(0.12%)d99.99(99.81%)f 0.48(0.06%)g 0.10(0.01%)	11.04
(0.72997) LP (2) P 5 s(1.15%)p85.54(98.67%)d 0.16(0.18%)	(0.16225) LV (1)Yb 2 s(0.06%)p 2.08(0.12%)d99.99(99.74%)f 1.38(0.08%)g 0.25(0.01%)	9.19
(0.72997) LP (2) P 5 s(1.15%)p85.54(98.67%)d 0.16(0.18%)	(0.14701) LV (2)Yb 2 s(23.61%)p 0.01(0.32%)d 3.21(75.82%)f 0.01(0.24%)g 0.00(0.01%)	9.40
(0.72997) LP (2) P 5 s(1.15%)p85.54(98.67%)d 0.16(0.18%)	(0.10856) LV (4)Yb 2 s(13.33%)p 0.02(0.33%)d 6.47(86.22%)f 0.01(0.11%)g 0.00(0.02%)	7.02
(0.85624) LP (1) N 9 s(42.26%)p 1.37(57.71%)d 0.00(0.03%)	(0.13509) LV (1)Yb 3 s(21.67%)p 0.02(0.53%)d 3.58(77.48%)f 0.01(0.24%)g 0.00(0.07%)	34.74
(0.71624) LP (1) C 13 s(46.16%)p 1.17(53.83%)d 0.00(0.01%)	(0.11979) LV (2)Yb 3 s(0.06%)p 1.75(0.11%)d99.99(99.68%)f 2.17(0.13%)g 0.20(0.01%)	10.54
(0.71624) LP (1) C 13 s(46.16%)p 1.17(53.83%)d 0.00(0.01%)	(0.10352) LV (3)Yb 3 s(0.22%)p 2.83(0.62%)d99.99(99.00%)f 0.68(0.15%)g 0.05(0.01%)	14.05
(0.71624) LP (1) C 13 s(46.16%)p 1.17(53.83%)d 0.00(0.01%)	(0.12161) LV (3)Yb 2	18.48

	s(0.85%)p 0.60(0.51%)d99.99(98.50%)f 0.15(0.13%)g 0.01(0.01%)	
(0.71624) LP (1) C 13 s(46.16%)p 1.17(53.83%)d 0.00(0.01%)	(0.10856) LV (4)Yb 2 s(13.33%)p 0.02(0.33%)d 6.47(86.22%)f 0.01(0.11%)g 0.00(0.02%)	8.79
(0.71624) LP (1) C 13 s(46.16%)p 1.17(53.83%)d 0.00(0.01%)	(0.08329) BD*(1)Yb 2- C 41 (87.91%) 0.9376*Yb 2 s(35.70%)p 0.00(0.12%)d 1.79(64.05%)f 0.00(0.12%)g 0.00(0.02%) (12.09%) -0.3477* C 41 s(65.11%)p 0.54(34.88%)d 0.00(0.01%)	6.79
(0.71624) LP (1) C 13 s(46.16%)p 1.17(53.83%)d 0.00(0.01%)	(0.05598) BD*(1)Yb 1- C114 (90.72%) 0.9525*Yb 1 s(38.24%)p 0.00(0.16%)d 1.60(61.36%)f 0.01(0.23%)g 0.00(0.01%) (9.28%) -0.3046* C114 s(65.15%)p 0.53(34.83%)d 0.00(0.01%)	7.93
(0.96311) BD (1) P 5- C 13 (36.58%) 0.6048* P 5 s(17.82%)p 4.57(81.51%)d 0.04(0.67%) (63.42%) 0.7964* C 13 s(28.34%)p 2.53(71.60%)d 0.00(0.05%)	(0.12161) LV (3)Yb 2 s(0.85%)p 0.60(0.51%)d99.99(98.50%)f 0.15(0.13%)g 0.01(0.01%)	6.95
(0.98803) BD (1) N 9- C 13 (61.88%) 0.7866* N 9 s(21.62%)p 3.62(78.23%)d 0.01(0.15%) (38.12%) 0.6174* C 13 s(25.10%)p 2.98(74.77%)d 0.00(0.12%)	(0.13509) LV (1)Yb 3 s(21.67%)p 0.02(0.53%)d 3.58(77.48%)f 0.01(0.24%)g 0.00(0.07%)	5.83







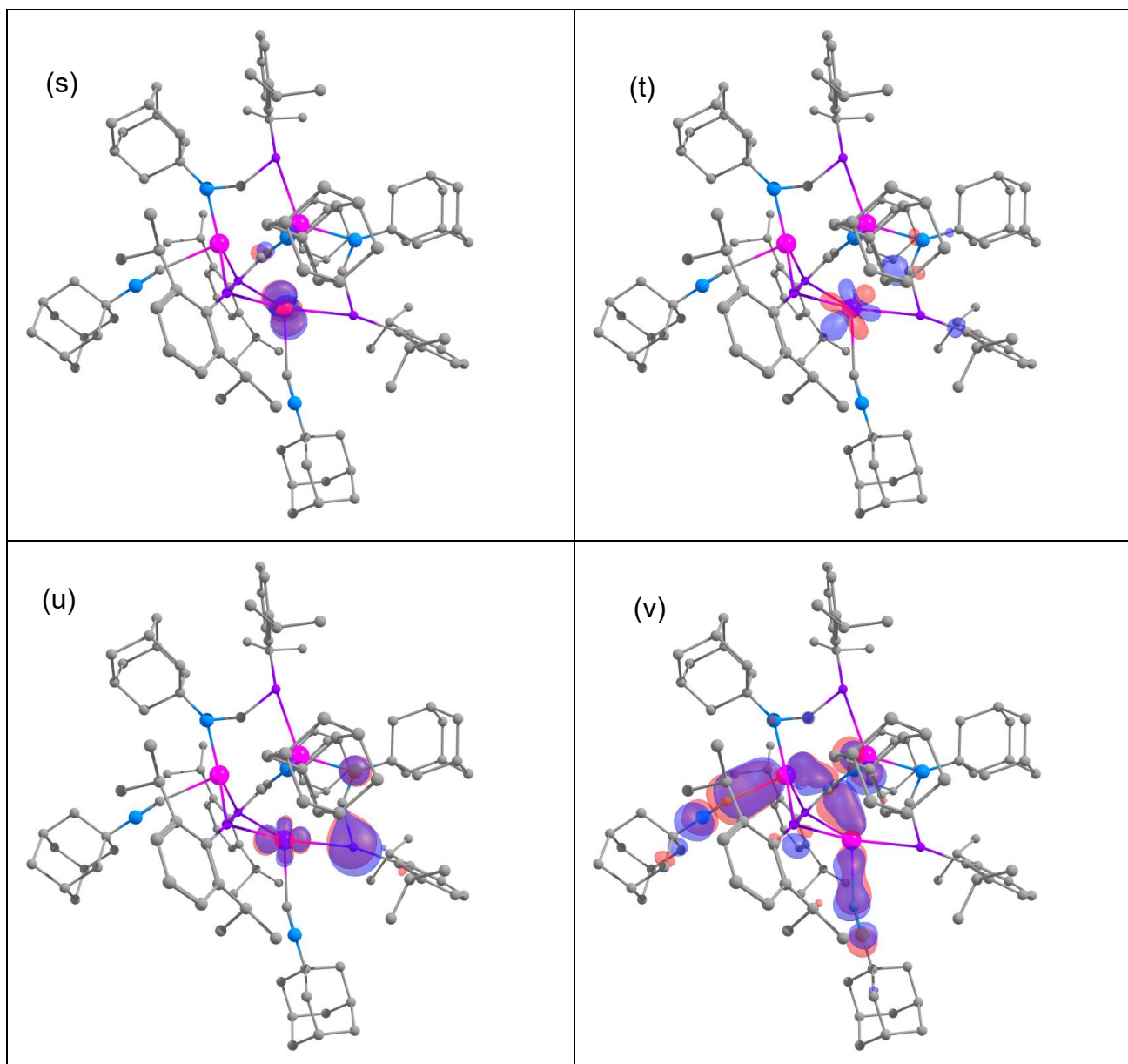


Fig. S56 Computed MOs (AMOs) for complex **7**, $S=1$. (a)HOMO-139 (b)HOMO-135 (c)HOMO-134 (d)HOMO-133 (e)HOMO-127 (f)HOMO-125 (g)HOMO-120 (h)HOMO-119 (i)HOMO-118 (j)HOMO-113 (k)HOMO-112 (l)HOMO-109 (m)HOMO-105 (n)HOMO-16 (o)HOMO-6 (p)HOMO-5 (q)HOMO-4 (r)HOMO-3 (s)HOMO-2 (t)HOMO-1 (u)HOMO (v)LUMO.

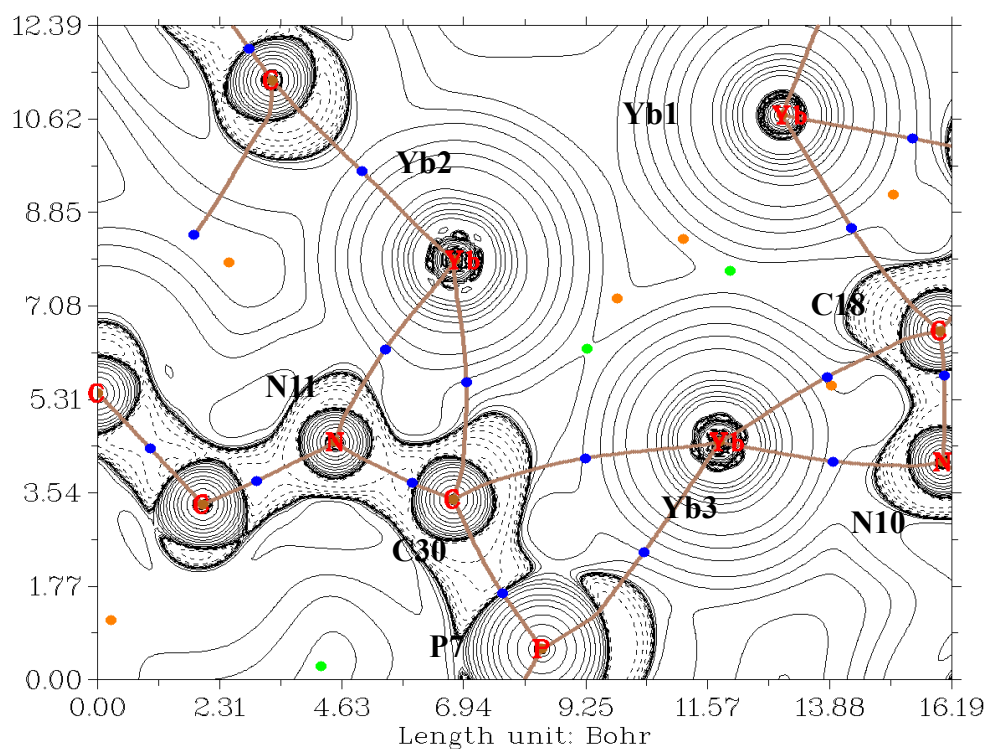


Fig. S57 Computed Laplacian distribution for complex **7** ($S=1$).

Table S23 Computed BCP descriptors for complex **7**, $S=1$.

Atom labels	$\rho(r)$	$\nabla^2\rho(r)$	$G(r)$	$V(r)$	$H(r)$	ϵ
Yb3-P7	0.04	0.08	0.03	-0.03	-0.006	0.09
Yb3-N8	0.06	0.22	0.06	-0.07	-0.005	0.06
Yb3-N9	0.06	0.23	0.06	-0.07	-0.005	0.06
Yb3-N10	0.07	0.27	0.08	-0.09	-0.01	0.01
Yb3-C13	0.04	0.15	0.04	-0.04	-0.002	3.65
Yb3-C18	0.05	0.16	0.04	-0.05	-0.004	3.36
Yb3-C30	0.03	0.09	0.02	-0.03	-0.002	0.68
Yb2-P4	0.04	0.09	0.03	-0.03	-0.005	0.57
Yb2-P5	0.03	0.09	0.03	-0.03	-0.006	0.34
Yb2-N11	0.08	0.30	0.09	-0.11	-0.02	0.06
Yb2-C13	0.04	0.12	0.04	-0.04	-0.005	0.34
Yb2-C16	0.05	0.13	0.04	-0.04	-0.006	0.22
Yb2-C30	0.06	0.17	0.05	-0.06	-0.009	0.98
Yb2-C41	0.04	0.13	0.03	-0.04	-0.002	0.07
Yb1-P4	0.02	0.05	0.02	-0.02	-0.002	0.39
Yb1-P5	0.04	0.10	0.03	-0.04	-0.005	0.17
Yb1-C13	0.02	0.07	0.02	-0.02	0.0003	1.02
Yb1-C16	0.02	0.07	0.02	-0.02	0.0004	1.40
Yb1-C18	0.03	0.10	0.03	-0.03	-0.002	0.47

Yb1-C114	0.03	0.11	0.03	-0.03	-0.0001	0.04
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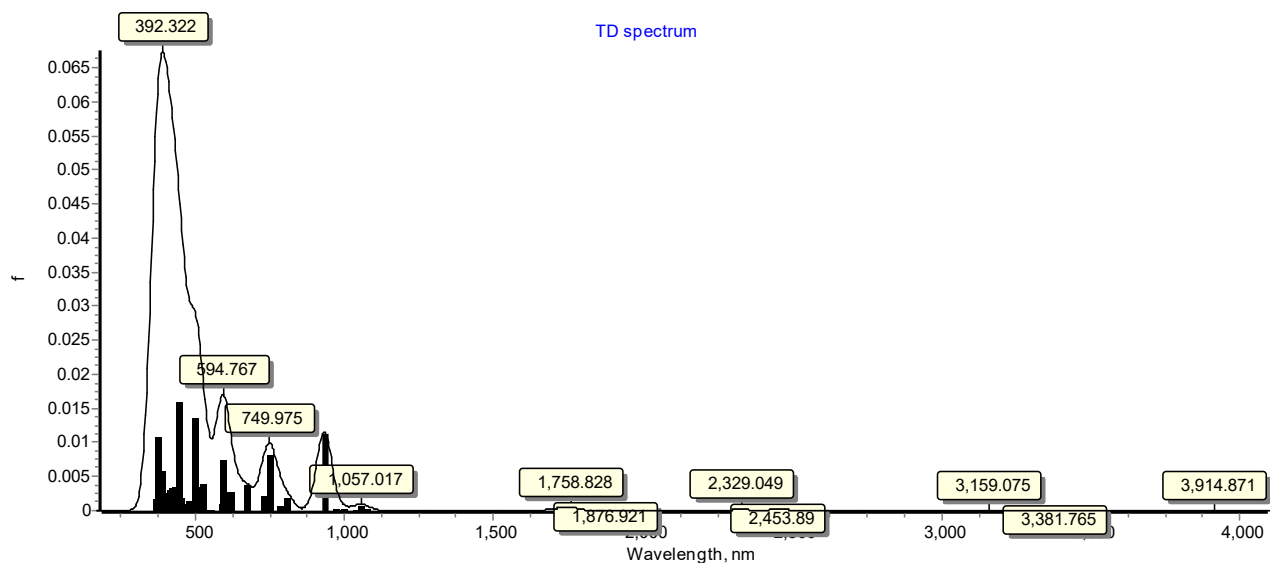
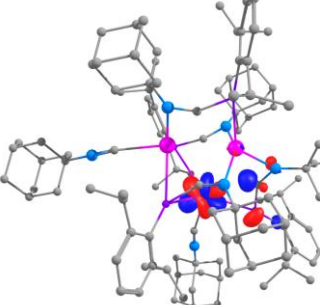
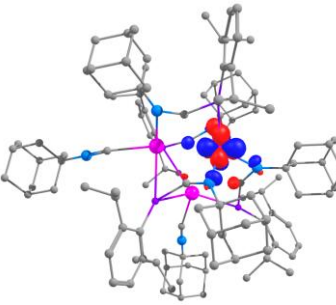
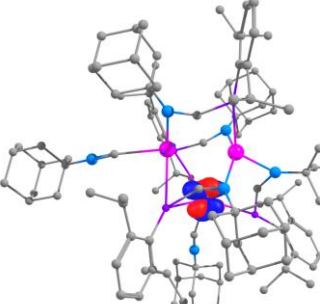
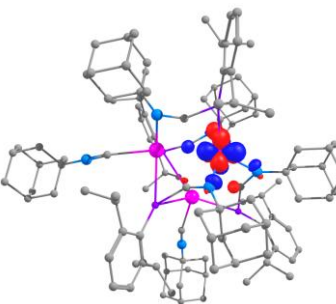
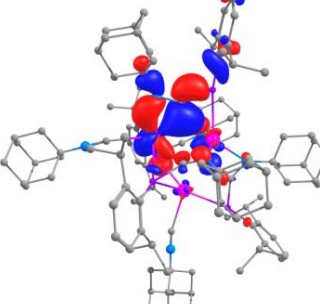
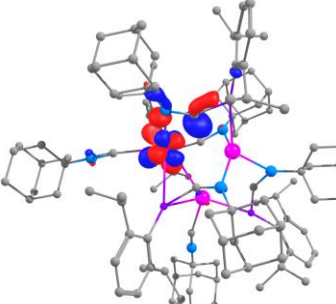
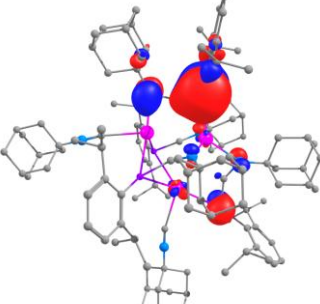
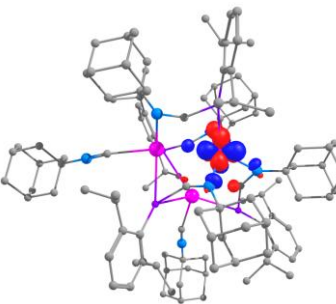


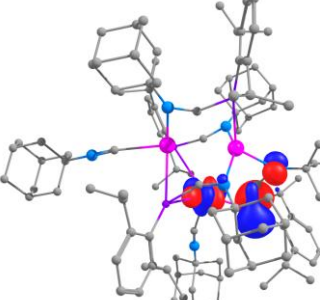
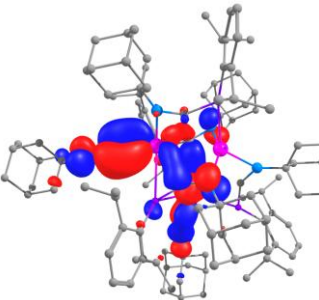
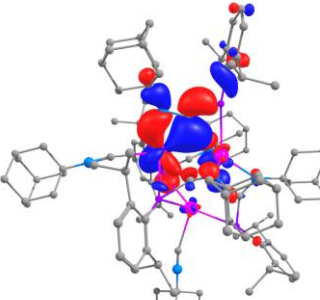
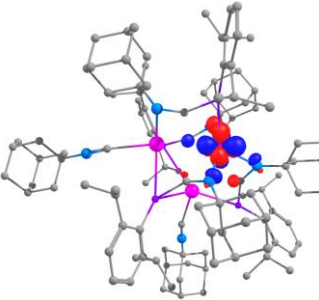
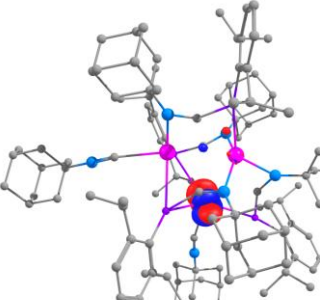
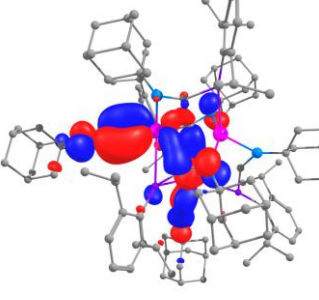
Fig. S58 Computed TDDFT spectrum for complex **7**, nstates=200 (no solvent).

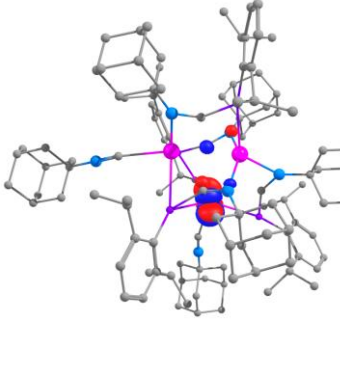
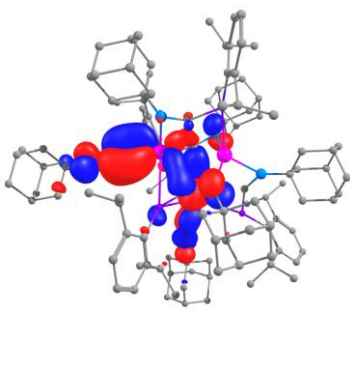
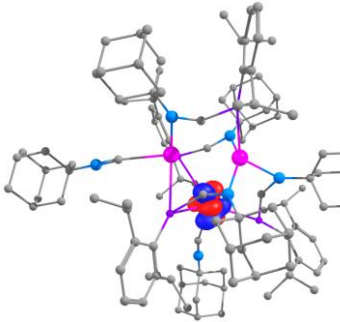
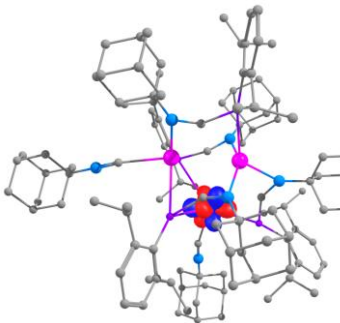
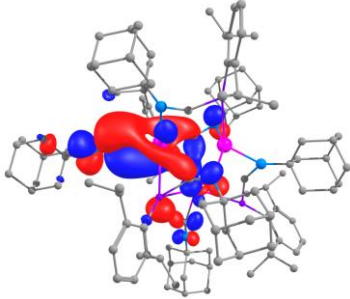
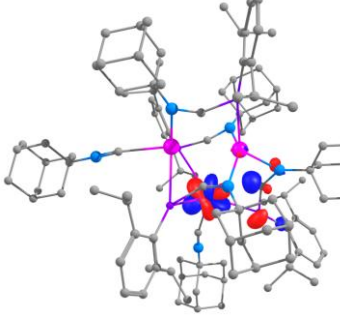
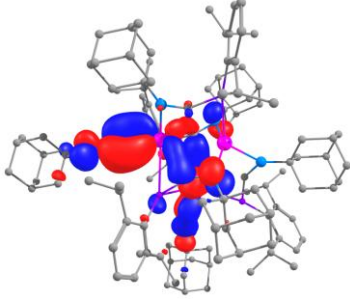
Table S23 AMO-HOMO=516, BMO-HOMO=514.

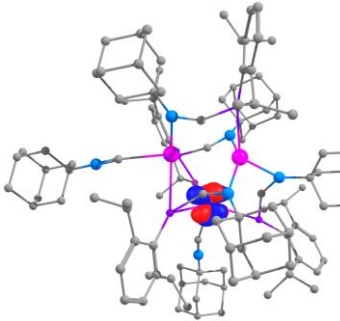
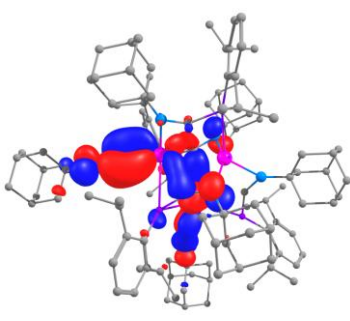
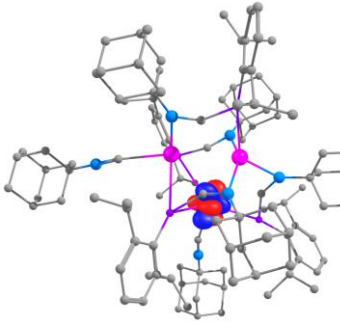
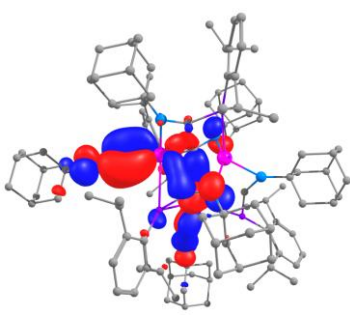
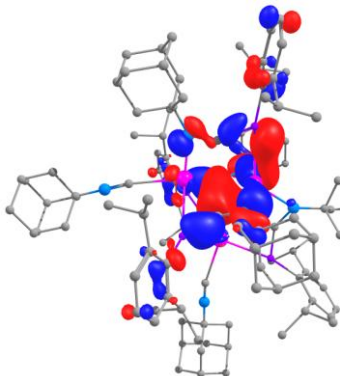
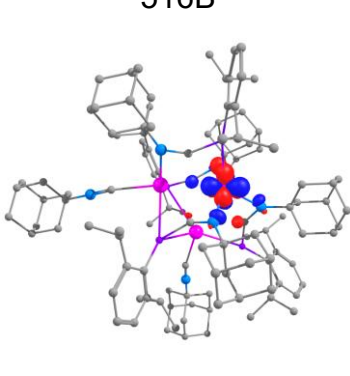
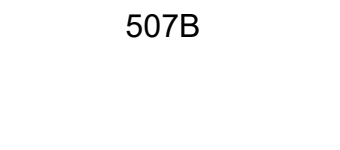
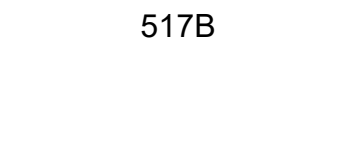
<p>Excited State 20: 3.009-A 0.9648 eV 1285.08 nm f=0.0000 <S**2>=2.014</p> <p>394B -> 515B -0.10861 402B -> 515B 0.12276 425B -> 515B 0.10772 506B -> 515B 0.84821 507B -> 515B -0.41709</p>	<p style="text-align: center;">506B</p>	<p style="text-align: center;">515B</p>
<p>Excited State 21: 3.012-A 1.1568 eV 1071.74 nm f=0.0003 <S**2>=2.019</p> <p>402B -> 515B 0.10915 419B -> 515B -0.10124 423B -> 515B 0.10203 503B -> 515B -0.13471 504B -> 515B -0.36771 505B -> 515B 0.51420 506B -> 515B 0.33361 507B -> 515B 0.60192 514B -> 515B -0.12745</p>	<p style="text-align: center;">507B</p>	<p style="text-align: center;">515B</p>
<p>Excited State 22: 3.008-A 1.1770 eV 1053.35 nm f=0.0006 <S**2>=2.012</p>	<p style="text-align: center;">513B</p>	<p style="text-align: center;">516B</p>

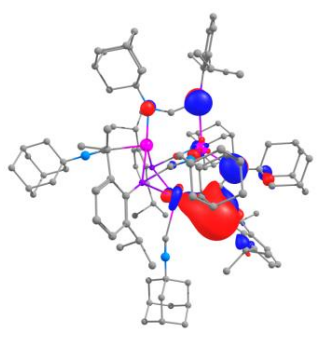
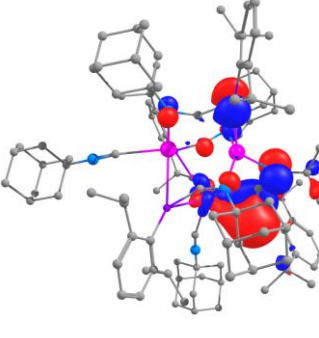
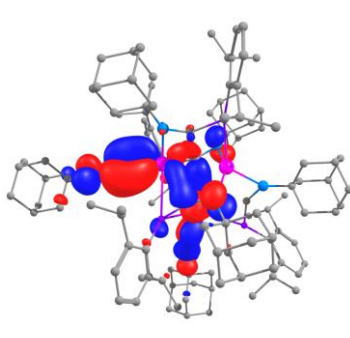
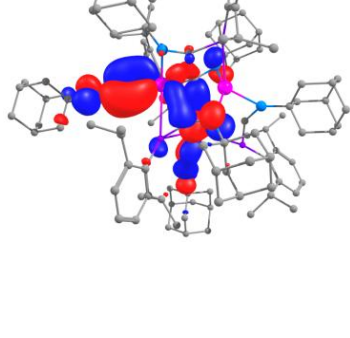
<p>513B -> 516B 0.90510 514B -> 516B 0.37040</p>		
<p>Excited State 24: 3.008-A 1.2434 eV 997.14 nm f=0.0002 <S**2>=2.013 510B -> 516B -0.23888 512B -> 516B 0.96325</p>	<p style="text-align: center;">512B</p> 	<p style="text-align: center;">516B</p> 
<p>Excited State 30: 3.006-A 1.3296 eV 932.53 nm f=0.0113 <S**2>=2.009 419B -> 515B -0.14179 423B -> 515B 0.25369 424B -> 515B 0.10623 501B -> 515B 0.21296 503B -> 515B 0.84473 504B -> 515B -0.27248</p>	<p style="text-align: center;">503B</p> 	<p style="text-align: center;">515B</p> 
<p>Excited State 32: 3.010-A 1.5395 eV 805.34 nm f=0.0019 <S**2>=2.015 442B -> 516B -0.14055 502B -> 515B 0.14299 505B -> 516B 0.16946 506B -> 516B 0.85236 507B -> 516B -0.39546</p>	<p style="text-align: center;">506B</p> 	<p style="text-align: center;">516B</p> 
<p>Excited State 35: 3.006-A 1.6512 eV 750.87 nm f=0.0081 <S**2>=2.010 437B -> 516B 0.12404 438B -> 516B 0.10186 439B -> 516B 0.12905 442B -> 516B 0.13046 503B -> 516B 0.10514</p>	<p style="text-align: center;">505B</p>	<p style="text-align: center;">516B</p>

504B -> 516B 0.46618 505B -> 516B 0.78675 506B -> 516B -0.10118		
Excited State 36: 3.016-A 1.7012 eV 728.82 nm f=0.0020 <S**2>=2.024 499B -> 515B -0.13068 501B -> 515B 0.91273 502B -> 515B 0.12444 503B -> 515B -0.18540 504B -> 515B 0.12737 505B -> 515B 0.12310	501B 	515B
Excited State 37: 3.012-A 1.8564 eV 667.86 nm f=0.0036 <S**2>=2.017 437B -> 516B -0.14600 438B -> 516B -0.13001 439B -> 516B -0.14897 504B -> 516B 0.84444 505B -> 516B -0.39638 507B -> 516B -0.12162	504B 	516B
Excited State 41: 3.143-A 2.0129 eV 615.94 nm f=0.0028 <S**2>=2.219 511A -> 517A 0.13951 498B -> 515B 0.23337 500B -> 515B 0.88802 501B -> 515B 0.10751 509B -> 517B -0.13087 513B -> 517B 0.13499	500B 	515B
Excited State 47: 3.030-A 2.0697 eV 599.05 nm f=0.0027 <S**2>=2.046 509A -> 517A 0.15495 514A -> 517A -0.15096 516A -> 517A 0.48047	514B	517B

<p>516A -> 519A -0.22309 507B -> 517B 0.20373 507B -> 519B -0.10985 511B -> 517B -0.20691 512B -> 517B -0.10672 513B -> 517B -0.19616 514B -> 517B 0.59371 514B -> 519B -0.27778</p>	 <p style="text-align: center;">516A</p>	 <p style="text-align: center;">517A</p>
<p>Excited State 49: 3.013-A 2.0886 eV 593.61 nm f=0.0026 <S**2>=2.019 442B -> 516B -0.11275 501B -> 516B 0.22188 503B -> 516B 0.92647</p>	 <p style="text-align: center;">503B</p>	 <p style="text-align: center;">516B</p>
<p>Excited State 51: 3.008-A 2.1025 eV 589.69 nm f=0.0073 <S**2>=2.012 514A -> 517A 0.54355 514A -> 519A -0.24517 516A -> 517A 0.21213 511B -> 517B 0.57164 511B -> 519B -0.26598 512B -> 517B 0.21259 514B -> 517B 0.18990</p>	 <p style="text-align: center;">511B</p>	 <p style="text-align: center;">517B</p>

		
<p>Excited State 60: 3.692-A 2.3627 eV 524.75 nm f=0.0015 $\langle S^{*2} \rangle = 3.158$</p> <p>510A -> 518A 0.42963 510A -> 520A 0.17139 510A -> 521A -0.19966 512A -> 518A 0.42225 512A -> 520A 0.18508 512A -> 521A -0.19189 514A -> 518A -0.13542 515A -> 518A -0.39194 515A -> 520A -0.14280 515A -> 521A 0.15516 508B -> 518B -0.16372 510B -> 518B -0.16486 513B -> 518B -0.21857 514B -> 518B -0.19399</p>	<p>510A</p>  <p>512A</p> 	<p>518A</p> 
<p>Excited State 63: 3.436-A 2.3750 eV 522.04 nm f=0.0039 $\langle S^{*2} \rangle = 2.702$</p> <p>510A -> 518A 0.14040 511A -> 518A 0.12424 512A -> 518A 0.20687 512A -> 521A -0.10317 513A -> 518A -0.14091 515A -> 518A 0.31721 515A -> 520A 0.10321 516A -> 518A -0.10428 508B -> 518B -0.33417 508B -> 520B -0.13244 508B -> 521B 0.15956 513B -> 518B 0.59196</p>	<p>513B</p> 	<p>518B</p> 

513B -> 520B	0.22637		
513B -> 521B	-0.24765		
Excited State 64:	3.056-A		
	2.4049 eV	515.54 nm	
	f=0.0014	<S**2>=2.085	
510A -> 518A	0.17304		
512A -> 518A	-0.12809		
513A -> 518A	0.43500		
513A -> 520A	0.19216		
513A -> 521A	-0.19693		
510B -> 518B	-0.12849		
511B -> 518B	-0.20204		
512B -> 518B	0.60704		
512B -> 520B	0.25563		
512B -> 521B	-0.28588		
		512B	518B
			
Excited State 69:	3.030-A		
	2.4494 eV	506.19 nm	
	f=0.0035	<S**2>=2.046	
510A -> 518A	0.46483		
510A -> 520A	0.17396		
510A -> 521A	-0.19350		
515A -> 518A	0.16019		
501B -> 516B	-0.21636		
508B -> 518B	0.61111		
508B -> 520B	0.23591		
508B -> 521B	-0.27633		
513B -> 518B	0.13681		
		508B	518B
			
Excited State 70:	3.017-A		
	2.4835 eV	499.23 nm	
	f=0.0136	<S**2>=2.025	
498B -> 516B	0.21114		
500B -> 516B	0.93247		
		500B	516B
			
Excited State 101:	3.075-A		
	2.7729 eV	447.13 nm	
	f=0.0159	<S**2>=2.113	
509A -> 517A	0.36562		
510A -> 518A	0.10944		
514A -> 519A	0.13777		
		507B	517B
			

515A -> 520A	0.24360	 <p>509A</p>  <p>498B</p>	 <p>517A</p>  <p>516B</p>
515A -> 523A	-0.13174		
515A -> 530A	-0.10526		
516A -> 519A	0.15143		
505B -> 517B	0.11966		
507B -> 517B	0.39579		
510B -> 518B	-0.13559		
510B -> 520B	0.15143		
510B -> 521B	-0.12507		
510B -> 523B	-0.12635		
511B -> 519B	0.15053		
512B -> 518B	0.10373		
512B -> 520B	-0.12125		
512B -> 521B	0.10546		
513B -> 518B	-0.10335		
513B -> 520B	0.27194		
513B -> 521B	-0.12143		
513B -> 523B	-0.13035		
513B -> 530B	-0.11607		
514B -> 519B	0.15480		
Excited State 110: 3.034-A 2.8831 eV 430.04 nm f=0.0034 <S**2>=2.051			
490B -> 516B	0.13048		
491B -> 516B	-0.12210		
498B -> 516B	0.67391		
499B -> 516B	-0.65771		
500B -> 516B	-0.16902		

optimized geometries

complex 3 (dispersion)

Yb	-2.544716000	-0.904193000	-0.346558000
Yb	2.429076000	0.947221000	-0.484699000
Yb	0.435778000	-2.565389000	-0.243622000
Yb	-0.440800000	2.721673000	-0.195972000
P	-0.028332000	0.072886000	0.825025000
P	3.079450000	-1.817602000	-1.088957000
P	-3.117919000	1.899075000	-0.779697000
P	-1.702722000	-2.858194000	1.582706000

P	1.820025000	2.981135000	1.523377000
Si	-2.230640000	-1.809377000	-3.616785000
Si	1.638072000	2.927526000	-3.292536000
O	-4.851738000	-1.391037000	0.276589000
O	4.836468000	1.202664000	-0.174180000
O	1.104353000	-4.869987000	-0.167701000
O	-1.303105000	4.930939000	0.261456000
C	-0.785389000	0.569159000	3.552167000
C	0.139891000	-0.065277000	2.681208000
C	1.179513000	-0.821760000	3.287543000
C	5.373627000	-3.370691000	-1.895678000
C	-1.901220000	1.440912000	3.024985000
H	-1.691922000	1.573254000	1.955878000
C	4.123798000	-2.795438000	-2.250029000
C	1.241764000	-0.967319000	4.675696000
H	2.043062000	-1.561647000	5.108808000
C	3.293506000	3.785396000	2.277713000
C	3.798215000	3.414675000	3.555927000
C	-0.704170000	0.388497000	4.934187000
H	-1.443143000	0.864914000	5.573743000
C	2.244730000	-1.524646000	2.477151000
C	0.706145000	1.714851000	-2.250303000
H	0.982259000	0.684348000	-2.540619000
C	-2.623211000	-4.361022000	2.111204000
C	6.077189000	-4.107742000	-2.851851000
H	7.030867000	-4.550795000	-2.583050000
C	0.299288000	-0.380861000	5.509894000
H	0.350212000	-0.513239000	6.586745000
C	-2.617162000	-4.833516000	3.450777000
C	-4.555431000	2.836035000	-1.461324000
C	-1.926699000	2.819648000	3.680751000
H	-2.154745000	2.763342000	4.750354000
H	-2.691051000	3.447704000	3.214336000
H	-0.954955000	3.310091000	3.570684000
C	3.620443000	-2.997720000	-3.561594000
C	5.587278000	-4.291875000	-4.139370000
H	6.155305000	-4.866308000	-4.865458000
C	3.052078000	2.443478000	4.453514000
H	2.647726000	1.646560000	3.820342000
C	-1.074040000	-2.074877000	-2.175249000
C	4.010771000	4.730244000	1.501729000
C	5.924444000	-3.270971000	-0.485052000
H	5.660895000	-2.278563000	-0.099876000

C	2.149880000	-3.044302000	2.619942000
H	2.411026000	-3.363779000	3.634754000
H	2.828032000	-3.546393000	1.922558000
H	1.122221000	-3.383229000	2.435253000
C	4.997747000	3.978840000	3.997155000
H	5.391630000	3.689957000	4.966325000
C	-4.579058000	3.057017000	-2.863205000
C	-6.315428000	-1.138081000	2.069500000
H	-6.962441000	-1.638903000	2.793790000
H	-5.825259000	-0.295120000	2.565785000
C	-3.372442000	-5.961431000	3.779118000
H	-3.376672000	-6.319145000	4.804459000
C	-5.659211000	3.156950000	0.837614000
H	-5.232901000	2.170539000	1.057817000
C	-5.622983000	3.336815000	-0.668787000
C	1.753053000	-5.462692000	-1.317682000
H	2.584447000	-4.816831000	-1.611908000
H	1.022053000	-5.504225000	-2.135438000
C	-5.963355000	-0.627181000	-0.253489000
H	-6.279229000	-1.076510000	-1.199478000
H	-5.594471000	0.382784000	-0.455038000
C	-3.246912000	0.723509000	3.124356000
H	-3.204276000	-0.235141000	2.594042000
H	-4.051877000	1.329838000	2.694777000
H	-3.502362000	0.506829000	4.167594000
C	5.198038000	5.276661000	1.990109000
H	5.740385000	6.001428000	1.389822000
C	5.247039000	-4.320168000	0.408477000
H	4.158218000	-4.259073000	0.328335000
H	5.522491000	-4.189316000	1.460894000
H	5.552618000	-5.325474000	0.097154000
C	2.294326000	-2.390169000	-3.965444000
H	1.676609000	-2.350384000	-3.057244000
C	-5.272892000	-2.066106000	1.479391000
H	-4.380565000	-2.229285000	2.085260000
H	-5.697306000	-3.043481000	1.219370000
C	4.359686000	-3.738758000	-4.483105000
H	3.967106000	-3.887214000	-5.484505000
C	-4.779878000	4.214535000	1.516190000
H	-3.752991000	4.171989000	1.142958000
H	-4.759869000	4.074608000	2.602272000
H	-5.178870000	5.214260000	1.310586000
C	-3.371856000	-5.069768000	1.133821000

C	5.702187000	4.900790000	3.229782000
H	6.632068000	5.324992000	3.597994000
C	-1.832821000	-4.111114000	4.531671000
H	-0.938928000	-3.691475000	4.055785000
C	-4.103937000	-6.198315000	1.506293000
H	-4.673423000	-6.739110000	0.755515000
C	3.472379000	5.175284000	0.156262000
H	2.873610000	4.342451000	-0.240685000
C	1.859270000	3.144592000	5.115865000
H	1.231688000	2.421460000	5.644957000
H	1.240022000	3.647052000	4.367786000
H	2.211987000	3.900265000	5.827234000
C	-3.439819000	2.571449000	-3.742080000
H	-3.044017000	1.648996000	-3.295630000
C	3.649789000	-1.013054000	2.789085000
H	3.711698000	0.065547000	2.616698000
H	4.392302000	-1.510051000	2.155022000
H	3.923042000	-1.195046000	3.833567000
C	7.445029000	-3.396492000	-0.385835000
H	7.787558000	-4.416390000	-0.590745000
H	7.774662000	-3.145961000	0.627749000
H	7.952317000	-2.727112000	-1.087731000
C	-2.647403000	-2.940143000	5.098873000
H	-2.991231000	-2.273804000	4.303352000
H	-2.044255000	-2.342677000	5.789998000
H	-3.527675000	-3.316611000	5.632503000
C	-4.116015000	-6.644651000	2.822652000
H	-4.694523000	-7.521286000	3.100515000
C	-3.958215000	-1.236900000	-3.031903000
H	-4.418169000	-1.987473000	-2.376940000
H	-4.622048000	-1.116166000	-3.894448000
H	-3.960471000	-0.267594000	-2.513111000
C	2.166491000	-6.854532000	-0.864351000
H	2.224078000	-7.559666000	-1.696839000
H	3.147476000	-6.816335000	-0.379107000
C	-7.060282000	-0.671922000	0.815345000
H	-7.831482000	-1.399327000	0.542134000
H	-7.544286000	0.297980000	0.942710000
C	5.538578000	1.712358000	0.972599000
H	4.832681000	1.761689000	1.799763000
H	5.889836000	2.730786000	0.768709000
C	-1.554546000	-0.493944000	-4.798715000
H	-2.291080000	-0.223153000	-5.559993000

H	-0.661458000	-0.862882000	-5.311970000
H	-1.267097000	0.410289000	-4.252074000
C	-3.340187000	-4.653936000	-0.326481000
H	-3.092800000	-3.583761000	-0.349096000
C	2.529647000	6.369788000	0.340758000
H	1.746891000	6.124998000	1.062678000
H	2.056970000	6.655141000	-0.605533000
H	3.083058000	7.234552000	0.722763000
C	0.879012000	-5.863553000	0.858103000
H	-0.121026000	-5.701857000	1.269356000
H	1.618854000	-5.710981000	1.651903000
C	5.808369000	0.679774000	-1.105629000
H	5.939026000	1.400277000	-1.920183000
H	5.388012000	-0.245465000	-1.510259000
C	-2.107775000	5.705556000	-0.660461000
H	-2.995201000	5.121667000	-0.920349000
H	-1.508537000	5.869691000	-1.562296000
C	3.913526000	1.746700000	5.504386000
H	4.258619000	2.434403000	6.284701000
H	4.792710000	1.272761000	5.055169000
H	3.320320000	0.967539000	5.992572000
C	-1.081555000	5.681270000	1.473922000
H	-0.091749000	5.403271000	1.844178000
H	-1.834327000	5.387703000	2.214817000
C	-6.651305000	4.055392000	-1.285010000
H	-7.464150000	4.443916000	-0.679664000
C	-5.630538000	3.774595000	-3.433600000
H	-5.643347000	3.942582000	-4.505516000
C	1.076791000	-7.196228000	0.154880000
H	1.361990000	-7.991877000	0.847332000
H	0.154786000	-7.496239000	-0.354210000
C	-1.255334000	7.128330000	1.055280000
H	-1.472822000	7.785350000	1.900893000
H	-0.349318000	7.489307000	0.557644000
C	-6.663881000	4.280907000	-2.654986000
H	-7.475033000	4.839850000	-3.112675000
C	1.137590000	4.692834000	-2.785380000
H	0.124074000	4.924532000	-3.128403000
H	1.809695000	5.440814000	-3.218234000
H	1.172913000	4.820662000	-1.696976000
C	-1.343518000	-5.015506000	5.663068000
H	-2.164856000	-5.369214000	6.296057000
H	-0.657226000	-4.458674000	6.309247000

H	-0.813568000	-5.891637000	5.275741000
C	-2.414478000	7.014568000	0.061418000
H	-3.365978000	6.938352000	0.597051000
H	-2.480178000	7.857944000	-0.630055000
C	3.493141000	2.704804000	-2.904642000
H	3.751120000	2.933371000	-1.863598000
H	4.103325000	3.370021000	-3.523649000
H	3.815209000	1.680435000	-3.130159000
C	4.548626000	5.485468000	-0.882286000
H	5.114196000	6.388382000	-0.629026000
H	4.088318000	5.654471000	-1.860702000
H	5.258936000	4.658691000	-0.980243000
C	-3.856753000	2.236697000	-5.172723000
H	-4.673089000	1.508458000	-5.191780000
H	-3.007528000	1.818411000	-5.718301000
H	-4.181301000	3.126874000	-5.721469000
C	1.509304000	-3.210065000	-4.985874000
H	0.503111000	-2.797380000	-5.095168000
H	1.416198000	-4.254232000	-4.670834000
H	1.977738000	-3.195206000	-5.975741000
C	-2.300743000	3.595258000	-3.748339000
H	-2.628921000	4.535921000	-4.203876000
H	-1.439117000	3.219572000	-4.307803000
H	-1.975897000	3.808046000	-2.726439000
C	-2.564777000	-3.405107000	-4.589787000
H	-1.636796000	-3.844099000	-4.968762000
H	-3.223730000	-3.213591000	-5.443605000
H	-3.053830000	-4.152926000	-3.957083000
C	2.479663000	-0.946489000	-4.443748000
H	3.042339000	-0.922543000	-5.383538000
H	3.034824000	-0.364197000	-3.702822000
H	1.514090000	-0.457347000	-4.602880000
C	-4.667153000	-4.820428000	-1.064856000
H	-4.937266000	-5.873442000	-1.194400000
H	-4.595995000	-4.382363000	-2.065722000
H	-5.485820000	-4.324485000	-0.536472000
C	-7.062996000	3.179767000	1.444017000
H	-7.493628000	4.186939000	1.446601000
H	-7.023553000	2.845316000	2.485668000
H	-7.750144000	2.526256000	0.898247000
C	7.104468000	0.473724000	-0.304960000
H	7.864702000	1.196102000	-0.617012000
H	7.515903000	-0.526965000	-0.447837000

C	1.486891000	2.795290000	-5.182484000
H	2.055107000	3.585175000	-5.686717000
H	0.445097000	2.869241000	-5.509285000
H	1.872070000	1.830001000	-5.526027000
C	6.683161000	0.734343000	1.147156000
H	6.314843000	-0.184104000	1.614487000
H	7.489694000	1.138018000	1.763771000
C	-2.215800000	-5.384932000	-1.067157000
H	-2.164528000	-5.074657000	-2.115219000
H	-2.381574000	-6.467660000	-1.036668000
H	-1.247052000	-5.177275000	-0.606538000
H	2.038036000	-1.262488000	1.429085000
H	1.459891000	2.077671000	2.549687000
H	-1.382116000	-2.249441000	2.816397000
H	-3.383251000	2.029438000	0.614160000
H	3.796716000	-2.017735000	0.119014000
H	-0.372778000	1.752152000	-2.485561000
H	-0.179500000	-1.472811000	-2.428223000
H	-0.773136000	-3.135848000	-2.282005000

complex **3** (no dispersion)

Yb	-2.196216000	1.696518000	-0.322261000
Yb	2.161730000	-1.616907000	-0.432572000
Yb	-2.133758000	-1.772197000	-0.202741000
Yb	2.133035000	1.801172000	-0.091546000
P	-0.014518000	-0.018416000	0.928137000
P	0.014726000	-3.583155000	-1.208330000
P	-0.013770000	3.743628000	-0.848563000
P	-3.808655000	-0.050395000	1.500795000
P	3.776459000	-0.067281000	1.524004000
Si	-3.037341000	0.757889000	-3.725267000
Si	3.367456000	0.003584000	-3.579916000
O	-3.735493000	3.599063000	0.183982000
O	3.775823000	-3.518088000	-0.198123000
O	-3.767531000	-3.629636000	-0.120196000
O	3.720834000	3.690110000	0.145132000
C	-0.051433000	1.029219000	3.644986000
C	-0.050978000	-0.135506000	2.824326000
C	-0.081530000	-1.391737000	3.498776000
C	0.147232000	-6.473550000	-1.606546000
C	0.010628000	2.436573000	3.080513000
H	-0.079289000	2.334752000	1.991627000
C	-0.017229000	-5.178415000	-2.181441000

C	-0.117734000	-1.453321000	4.896162000
H	-0.150498000	-2.426641000	5.381251000
C	5.433413000	-0.386072000	2.320981000
C	5.571505000	-0.821140000	3.673507000
C	-0.081765000	0.922855000	5.039561000
H	-0.074198000	1.831245000	5.637878000
C	-0.113759000	-2.722403000	2.768138000
C	2.098244000	0.286506000	-2.226855000
H	1.225543000	-0.359006000	-2.466950000
C	-5.564240000	-0.187065000	2.111921000
C	0.065679000	-7.601747000	-2.430623000
H	0.183841000	-8.587676000	-1.990930000
C	-0.118165000	-0.307749000	5.679118000
H	-0.145757000	-0.372755000	6.763630000
C	-5.886842000	-0.516933000	3.461428000
C	0.067324000	5.494823000	-1.506742000
C	1.366455000	3.089179000	3.378934000
H	1.514607000	3.223363000	4.456604000
H	1.442258000	4.075054000	2.907519000
H	2.191898000	2.460741000	3.020979000
C	-0.223982000	-5.082659000	-3.583339000
C	-0.160187000	-7.501421000	-3.797406000
H	-0.221242000	-8.394473000	-4.413442000
C	4.382049000	-1.011580000	4.605486000
H	3.520558000	-1.289803000	3.989826000
C	-2.668446000	-0.187652000	-2.141463000
C	6.611101000	-0.226601000	1.542607000
C	0.370979000	-6.698405000	-0.116016000
H	0.907060000	-5.823563000	0.269831000
C	-1.477705000	-3.406130000	2.926224000
H	-1.661135000	-3.683460000	3.970662000
H	-1.534797000	-4.320372000	2.324260000
H	-2.293532000	-2.731367000	2.634340000
C	6.850269000	-1.047432000	4.192082000
H	6.950418000	-1.366391000	5.225368000
C	0.250529000	5.660666000	-2.906410000
C	-4.762570000	5.090628000	1.670339000
H	-5.671960000	5.322961000	2.230960000
H	-3.898511000	5.365584000	2.284691000
C	-7.228803000	-0.568040000	3.851962000
H	-7.468969000	-0.802544000	4.885044000
C	-0.232940000	6.625016000	0.813007000
H	-0.755507000	5.692203000	1.051846000

C	-0.030613000	6.665211000	-0.696609000
C	-3.939042000	-4.568452000	-1.211593000
H	-2.951177000	-4.926653000	-1.514039000
H	-4.399933000	-4.034286000	-2.051903000
C	-3.733491000	4.888426000	-0.483146000
H	-4.041582000	4.746789000	-1.522882000
H	-2.704509000	5.258371000	-0.475346000
C	-1.148297000	3.320027000	3.555504000
H	-2.112153000	2.847185000	3.339914000
H	-1.121193000	4.294699000	3.054305000
H	-1.107479000	3.507164000	4.634312000
C	7.865662000	-0.480878000	2.105320000
H	8.755782000	-0.358468000	1.492619000
C	-0.971326000	-6.788999000	0.625087000
H	-1.579337000	-5.896710000	0.448296000
H	-0.822908000	-6.893688000	1.706260000
H	-1.538108000	-7.660165000	0.276281000
C	-0.394839000	-3.747156000	-4.293311000
H	-0.189649000	-2.949244000	-3.568602000
C	-4.682114000	3.626886000	1.275203000
H	-4.315153000	2.950631000	2.048531000
H	-5.651118000	3.249945000	0.925227000
C	-0.296512000	-6.241077000	-4.361367000
H	-0.465019000	-6.150665000	-5.431732000
C	1.121372000	6.603516000	1.536047000
H	1.733035000	5.760263000	1.201154000
H	0.992526000	6.525674000	2.621858000
H	1.675181000	7.526957000	1.329066000
C	-6.631368000	0.022885000	1.193725000
C	7.997999000	-0.883624000	3.426049000
H	8.979309000	-1.071791000	3.853511000
C	-4.823396000	-0.793376000	4.516290000
H	-3.936815000	-1.168390000	3.994582000
C	-7.956318000	-0.056465000	1.632116000
H	-8.762688000	0.105990000	0.921878000
C	6.574041000	0.194373000	0.080707000
H	5.543965000	0.496252000	-0.150897000
C	4.037826000	0.306102000	5.316749000
H	3.124581000	0.202808000	5.912036000
H	3.881107000	1.114741000	4.597390000
H	4.856185000	0.603163000	5.983425000
C	0.339669000	4.480803000	-3.863552000
H	0.057087000	3.575248000	-3.311492000

C	1.021773000	-3.663238000	3.184600000
H	1.994407000	-3.172469000	3.077415000
H	1.019686000	-4.569137000	2.566873000
H	0.928124000	-3.980977000	4.228906000
C	1.236862000	-7.920074000	0.216345000
H	0.716658000	-8.865123000	0.026120000
H	1.497765000	-7.912116000	1.280257000
H	2.165592000	-7.928653000	-0.363122000
C	-4.423595000	0.499385000	5.243776000
H	-4.110339000	1.271853000	4.535441000
H	-3.592032000	0.321080000	5.933932000
H	-5.270649000	0.893892000	5.817504000
C	-8.265136000	-0.337544000	2.956060000
H	-9.300026000	-0.386321000	3.284451000
C	-3.598175000	2.542973000	-3.339400000
H	-4.448320000	2.554057000	-2.646272000
H	-3.914929000	3.060786000	-4.251544000
H	-2.784899000	3.139708000	-2.904876000
C	-4.859291000	-5.657333000	-0.673728000
H	-5.444548000	-6.130021000	-1.466781000
H	-4.276166000	-6.436138000	-0.170885000
C	-4.700153000	5.777384000	0.303688000
H	-5.691096000	5.776147000	-0.163218000
H	-4.355910000	6.813386000	0.353474000
C	4.575902000	-3.781341000	0.980734000
H	4.050800000	-3.369349000	1.843748000
H	5.533986000	-3.258380000	0.886682000
C	-1.475899000	0.850423000	-4.801928000
H	-1.649770000	1.433527000	-5.712331000
H	-1.157939000	-0.152711000	-5.105180000
H	-0.642499000	1.305975000	-4.257665000
C	-6.378582000	0.278628000	-0.284988000
H	-5.352795000	0.662227000	-0.376211000
C	7.477295000	1.401719000	-0.206096000
H	7.265913000	2.227237000	0.480000000
H	7.332824000	1.757388000	-1.232454000
H	8.537674000	1.149681000	-0.097187000
C	-4.690270000	-3.942369000	0.954253000
H	-5.102048000	-3.001374000	1.326933000
H	-4.129056000	-4.429336000	1.760689000
C	3.838317000	-4.653596000	-1.099114000
H	4.134548000	-4.292878000	-2.087587000
H	2.833427000	-5.081642000	-1.170628000

C	3.886063000	4.746811000	-0.833691000
H	2.893927000	5.115321000	-1.106874000
H	4.368239000	4.317093000	-1.720421000
C	4.557661000	-2.136790000	5.632719000
H	5.291244000	-1.886551000	6.407203000
H	4.874708000	-3.072294000	5.159858000
H	3.605662000	-2.318734000	6.142371000
C	4.616664000	3.905126000	1.263649000
H	5.041228000	2.938012000	1.543365000
H	4.031170000	4.289888000	2.107601000
C	0.103738000	7.924652000	-1.292132000
H	0.040121000	8.811931000	-0.668962000
C	0.378881000	6.941298000	-3.450734000
H	0.532506000	7.048443000	-4.521597000
C	-5.711324000	-4.887940000	0.338766000
H	-6.182032000	-5.530527000	1.087485000
H	-6.499465000	-4.322384000	-0.169594000
C	5.625746000	4.934225000	0.775817000
H	6.066181000	5.502707000	1.599193000
H	6.436810000	4.446767000	0.224658000
C	0.316213000	8.076659000	-2.655581000
H	0.421657000	9.066372000	-3.091656000
C	4.784222000	1.266105000	-3.428442000
H	4.417962000	2.279574000	-3.628422000
H	5.582980000	1.059712000	-4.149174000
H	5.222479000	1.254217000	-2.425620000
C	-5.216444000	-1.874483000	5.530937000
H	-6.002192000	-1.541098000	6.218062000
H	-4.348342000	-2.137456000	6.145050000
H	-5.569367000	-2.784417000	5.034571000
C	4.775694000	5.789173000	-0.166844000
H	4.169014000	6.501794000	0.401412000
H	5.365652000	6.351774000	-0.895125000
C	4.090510000	-1.755979000	-3.429245000
H	4.595852000	-1.916911000	-2.470410000
H	4.825990000	-1.948421000	-4.218148000
H	3.297822000	-2.506834000	-3.538585000
C	6.938182000	-0.975927000	-0.842835000
H	7.956995000	-1.327939000	-0.644279000
H	6.885137000	-0.680445000	-1.896367000
H	6.258928000	-1.820460000	-0.692676000
C	-0.631143000	4.612744000	-5.044424000
H	-1.657566000	4.769735000	-4.700480000

H	-0.611427000	3.706208000	-5.657364000
H	-0.365850000	5.452600000	-5.695632000
C	-1.837837000	-3.562448000	-4.781579000
H	-1.965278000	-2.590386000	-5.269996000
H	-2.545136000	-3.618310000	-3.948664000
H	-2.110922000	-4.338597000	-5.505452000
C	1.776705000	4.285355000	-4.364132000
H	2.122764000	5.166761000	-4.915803000
H	1.845063000	3.422243000	-5.034566000
H	2.465883000	4.123268000	-3.529916000
C	-4.427196000	-0.014381000	-4.777707000
H	-4.193208000	-1.051553000	-5.039570000
H	-4.573556000	0.543117000	-5.710061000
H	-5.381648000	-0.014672000	-4.239970000
C	0.598037000	-3.571772000	-5.449556000
H	0.421199000	-4.297332000	-6.250897000
H	1.630932000	-3.698285000	-5.111589000
H	0.501984000	-2.573386000	-5.889497000
C	-7.312383000	1.323775000	-0.908224000
H	-8.340897000	0.956537000	-0.993884000
H	-6.979182000	1.573499000	-1.921530000
H	-7.340120000	2.246873000	-0.320916000
C	-1.102116000	7.764227000	1.361505000
H	-0.589300000	8.731782000	1.334175000
H	-1.353594000	7.569366000	2.409760000
H	-2.035651000	7.867287000	0.799495000
C	4.848886000	-5.618344000	-0.484648000
H	5.858482000	-5.406505000	-0.853732000
H	4.615977000	-6.660330000	-0.718341000
C	2.696430000	0.137706000	-5.359207000
H	3.487016000	-0.037064000	-6.098307000
H	2.272308000	1.128513000	-5.551032000
H	1.904743000	-0.597285000	-5.535404000
C	4.752193000	-5.290760000	1.006829000
H	3.874086000	-5.772064000	1.451001000
H	5.634672000	-5.594489000	1.576106000
C	-6.457460000	-1.033614000	-1.079532000
H	-6.251388000	-0.867840000	-2.142925000
H	-7.458956000	-1.471893000	-0.995363000
H	-5.736380000	-1.766301000	-0.705367000
H	0.027667000	-2.488901000	1.704383000
H	2.933495000	-0.087011000	2.666375000
H	-3.107235000	0.055700000	2.731282000

H	-0.029222000	4.042059000	0.551122000
H	0.071604000	-4.130715000	0.112065000
H	1.678233000	1.288880000	-2.458843000
H	-1.932784000	-0.938248000	-2.501197000
H	-3.608373000	-0.746610000	-1.947677000

complex 4 (dispersion)

Yb	0.223189000	2.309556000	0.388672000
Yb	3.056467000	0.161495000	-0.338152000
Yb	0.301293000	-2.325259000	-0.485061000
Yb	-2.407461000	0.440026000	-1.642543000
Yb	-2.039916000	-0.428667000	2.050005000
P	0.812225000	-0.275052000	1.473032000
P	0.540560000	0.355047000	-1.706625000
P	-2.502202000	1.991097000	0.829246000
P	-2.469770000	-1.959190000	-0.267799000
P	2.949923000	3.074384000	-0.129488000
P	3.231031000	-2.681287000	-0.693195000
O	-2.366735000	-0.217836000	4.429270000
O	-3.020409000	-0.065516000	-3.964930000
O	-0.106165000	-4.712528000	-0.316338000
O	4.262955000	0.384189000	-2.414661000
O	-4.575697000	1.484749000	-2.006737000
C	1.716462000	0.522285000	4.069246000
C	1.316243000	-0.392756000	-4.369493000
C	0.759277000	0.623669000	-3.533465000
C	2.169904000	1.813199000	3.417878000
H	2.490225000	1.541766000	2.401269000
C	1.105167000	-0.508557000	3.290791000
C	-3.760975000	-3.271746000	-0.279985000
C	1.881258000	0.359675000	5.446484000
H	2.351406000	1.148937000	6.025113000
C	0.693665000	-1.698068000	3.964864000
C	1.003757000	2.798066000	3.265402000
H	1.290845000	3.637679000	2.617151000
H	0.717632000	3.219360000	4.235280000
C	-3.684399000	3.393725000	1.024207000
C	-4.374680000	-3.717781000	0.927238000
C	4.061915000	4.410554000	0.534545000
C	-4.109448000	-3.942255000	-1.485394000
C	-3.495815000	-3.552021000	-2.816099000
H	-3.023872000	-2.574491000	-2.662093000
C	4.541429000	-3.440988000	1.692521000

C	0.353728000	1.834524000	-4.160412000
C	1.423112000	-0.191147000	-5.746990000
H	1.839849000	-0.977614000	-6.368693000
C	3.338509000	2.505716000	4.111383000
H	3.053983000	2.917485000	5.086140000
H	3.691351000	3.340614000	3.498483000
H	4.172704000	1.815929000	4.267485000
C	4.193072000	-3.841604000	0.375839000
C	1.779071000	-1.708988000	-3.782584000
H	2.177538000	-1.464516000	-2.790878000
C	0.604695000	-2.669908000	-3.574427000
H	0.924529000	-3.557980000	-3.012918000
H	0.207093000	-3.017540000	-4.533678000
C	3.753077000	5.775614000	0.314593000
C	-0.238154000	2.987130000	-3.376265000
H	-0.267641000	2.652324000	-2.329051000
C	4.269463000	-2.025669000	2.178942000
H	3.264693000	-1.733279000	1.835721000
C	0.863883000	-1.810045000	5.347799000
H	0.542996000	-2.715707000	5.853650000
C	5.214315000	4.079359000	1.291983000
C	5.186894000	-4.344696000	2.537900000
H	5.441271000	-4.042144000	3.548037000
C	5.278055000	-1.048538000	1.564120000
H	5.336840000	-1.176684000	0.475848000
H	6.282419000	-1.221312000	1.964124000
H	5.009766000	-0.012872000	1.810520000
C	-4.912540000	3.249074000	1.733384000
C	1.013553000	0.996790000	-6.344877000
H	1.107145000	1.136699000	-7.418002000
C	0.488799000	2.000664000	-5.541552000
H	0.173777000	2.938391000	-5.994504000
C	0.121146000	-2.884809000	3.203868000
H	-0.476027000	-2.488845000	2.362752000
C	-2.941444000	-0.861922000	5.578668000
H	-2.733303000	-1.932109000	5.517812000
H	-4.027681000	-0.709955000	5.553768000
C	-2.059839000	4.928233000	-0.210718000
H	-1.828621000	4.010633000	-0.778121000
C	1.449964000	-0.793399000	6.094858000
H	1.581685000	-0.904871000	7.167420000
C	-2.090829000	-0.724012000	-4.850627000
H	-2.214651000	-1.808497000	-4.751856000

H	-1.086164000	-0.444132000	-4.542798000
C	-2.384724000	-4.531450000	-3.204533000
H	-1.596759000	-4.532255000	-2.444896000
H	-1.930221000	-4.256628000	-4.163433000
H	-2.773705000	-5.552268000	-3.297451000
C	-3.397776000	4.672382000	0.456935000
C	4.542237000	-5.145792000	-0.061521000
C	-1.601505000	0.946660000	4.848185000
H	-1.818248000	1.749135000	4.136784000
H	-0.542705000	0.691593000	4.800271000
C	5.653601000	2.635181000	1.476648000
H	4.741317000	2.047096000	1.645941000
C	2.579197000	6.195771000	-0.546088000
H	1.897537000	5.337031000	-0.581619000
C	-1.672733000	3.288179000	-3.812916000
H	-1.704079000	3.667655000	-4.840387000
H	-2.132157000	4.039322000	-3.164494000
H	-2.289816000	2.382473000	-3.794519000
C	-4.092371000	-3.010246000	2.239823000
H	-2.999519000	-2.834346000	2.245250000
C	5.518944000	-5.625243000	2.109609000
H	6.023290000	-6.314398000	2.781217000
C	-6.691567000	1.536051000	2.432668000
H	-6.809288000	0.559960000	2.914696000
H	-7.049327000	1.446700000	1.403656000
H	-7.353339000	2.235025000	2.955966000
C	-5.803819000	4.320179000	1.827465000
H	-6.731272000	4.190995000	2.379189000
C	4.581021000	6.766300000	0.849705000
H	4.344692000	7.811457000	0.671024000
C	2.887521000	-2.403108000	-4.568117000
H	3.256300000	-3.265435000	-4.004615000
H	3.730417000	-1.728950000	-4.747508000
H	2.539209000	-2.777132000	-5.537517000
C	4.269553000	-1.854800000	3.695067000
H	5.266010000	-2.019373000	4.120627000
H	3.567579000	-2.535331000	4.181930000
H	3.962082000	-0.839325000	3.952315000
C	-5.256772000	-4.799788000	0.910701000
H	-5.711259000	-5.138111000	1.836684000
C	-5.229927000	1.975088000	2.486898000
H	-4.613644000	1.193688000	2.023760000
C	3.957962000	1.375119000	-3.409629000

H	3.074839000	1.912592000	-3.067156000
H	3.715912000	0.873221000	-4.353738000
C	-0.970669000	5.097978000	0.859113000
H	-1.056377000	4.305458000	1.614250000
H	-1.088690000	6.052185000	1.381837000
H	0.038310000	5.098060000	0.421993000
C	5.204680000	-6.010920000	0.813198000
H	5.473957000	-7.007166000	0.474962000
C	6.005210000	5.101298000	1.823019000
H	6.884689000	4.850148000	2.406316000
C	-4.221441000	0.276412000	-4.689472000
H	-4.350020000	1.360506000	-4.626986000
H	-5.074061000	-0.204112000	-4.204209000
C	6.311586000	2.120776000	0.191274000
H	7.179344000	2.738751000	-0.062562000
H	5.600493000	2.165922000	-0.637943000
H	6.654745000	1.086928000	0.310935000
C	0.645571000	4.231056000	-3.442638000
H	1.661257000	4.000671000	-3.112913000
H	0.256617000	5.021194000	-2.793900000
H	0.703669000	4.631655000	-4.460583000
C	-5.598909000	0.943742000	-1.149738000
H	-5.286500000	1.074860000	-0.107508000
H	-5.679428000	-0.124196000	-1.370812000
C	-4.832780000	2.887858000	-2.226042000
H	-4.788599000	3.057140000	-3.307602000
H	-4.054173000	3.474639000	-1.734253000
C	-5.566104000	-5.464447000	-0.270912000
H	-6.247909000	-6.310189000	-0.265457000
C	5.696223000	6.439292000	1.607531000
H	6.325627000	7.220268000	2.025250000
C	-4.992659000	-5.023470000	-1.457382000
H	-5.229576000	-5.539250000	-2.384943000
C	4.256807000	-5.598394000	-1.480371000
H	3.360202000	-5.057093000	-1.805122000
C	3.053521000	6.469072000	-1.977827000
H	2.212239000	6.718491000	-2.633392000
H	3.564592000	5.595651000	-2.394563000
H	3.759902000	7.306717000	-1.994341000
C	1.801239000	7.388474000	0.011652000
H	2.380799000	8.316950000	-0.030564000
H	1.510987000	7.220264000	1.053047000
H	0.889399000	7.551049000	-0.572699000

C	-4.817084000	-1.657015000	2.268187000
H	-5.899740000	-1.814842000	2.255127000
H	-4.567323000	-1.064461000	1.377125000
H	-4.587156000	-1.078723000	3.173517000
C	-2.299452000	-0.195963000	6.787316000
H	-2.942108000	-0.231726000	7.670417000
H	-1.348527000	-0.685331000	7.018849000
C	-1.275099000	-5.264422000	0.338136000
H	-2.082442000	-5.347875000	-0.393633000
H	-1.593546000	-4.552305000	1.101209000
C	-3.997271000	-0.188776000	-6.127209000
H	-4.416322000	-1.189028000	-6.275094000
H	-4.464776000	0.483652000	-6.851105000
C	-4.770806000	2.125205000	3.939614000
H	-5.376588000	2.877034000	4.458065000
H	-3.729550000	2.452911000	3.970623000
H	-4.858915000	1.178459000	4.484323000
C	-5.532147000	5.545217000	1.229940000
H	-6.241102000	6.365246000	1.299661000
C	-2.040391000	1.220679000	6.272807000
H	-1.266365000	1.745183000	6.837670000
H	-2.957723000	1.817582000	6.293368000
C	-0.789936000	-3.796569000	4.020736000
H	-0.233921000	-4.365923000	4.773124000
H	-1.275109000	-4.522400000	3.361693000
H	-1.574710000	-3.235804000	4.534091000
C	-4.326521000	5.709737000	0.554843000
H	-4.102675000	6.672421000	0.105766000
C	5.406894000	-5.186794000	-2.409278000
H	5.605233000	-4.113435000	-2.337996000
H	5.177631000	-5.426154000	-3.454123000
H	6.325860000	-5.714834000	-2.131444000
C	0.863673000	-5.752473000	-0.564666000
H	1.740529000	-5.567829000	0.066032000
H	1.170978000	-5.690913000	-1.611512000
C	-4.536226000	-3.412371000	-3.927396000
H	-5.031534000	-4.361679000	-4.157925000
H	-4.064733000	-3.066588000	-4.853883000
H	-5.312969000	-2.693360000	-3.647489000
C	5.598886000	-0.064399000	-2.672839000
H	6.020280000	-0.405519000	-1.724727000
H	5.558537000	-0.919752000	-3.357290000
C	3.970400000	-7.094238000	-1.618581000

H	4.867941000	-7.702301000	-1.462512000
H	3.605603000	-7.315799000	-2.627163000
H	3.214837000	-7.427729000	-0.900718000
C	6.584004000	2.399740000	2.665480000
H	6.710366000	1.325600000	2.832414000
H	6.195240000	2.844202000	3.585140000
H	7.581143000	2.815267000	2.483249000
C	-0.829844000	-6.618477000	0.861115000
H	-1.671574000	-7.303948000	0.985283000
H	-0.323019000	-6.516441000	1.827229000
C	-2.471962000	-0.231954000	-6.231925000
H	-2.106686000	-0.888009000	-7.025273000
H	-2.053454000	0.766309000	-6.390912000
C	-4.430718000	-3.814499000	3.491642000
H	-4.098822000	-3.279242000	4.385690000
H	-3.946181000	-4.795158000	3.484303000
H	-5.510197000	-3.968511000	3.594379000
C	1.243321000	-3.706341000	2.565651000
H	1.811472000	-3.103861000	1.852860000
H	0.842147000	-4.571582000	2.033746000
H	1.946178000	-4.066160000	3.322075000
C	-2.034229000	6.109867000	-1.175217000
H	-2.815340000	6.028884000	-1.938239000
H	-1.066990000	6.161521000	-1.683396000
H	-2.171284000	7.063889000	-0.654518000
C	-6.825240000	1.770384000	-1.490251000
H	-7.262053000	1.424883000	-2.434006000
H	-7.595396000	1.722705000	-0.717065000
C	0.160980000	-7.059534000	-0.217423000
H	0.862472000	-7.826091000	0.120781000
H	-0.378012000	-7.447902000	-1.088081000
C	5.232052000	2.196358000	-3.495299000
H	5.322242000	2.726454000	-4.446539000
H	5.244307000	2.933795000	-2.687376000
C	-6.216523000	3.168048000	-1.637244000
H	-6.113492000	3.638970000	-0.657872000
H	-6.809030000	3.827252000	-2.276437000
C	6.337280000	1.139243000	-3.291279000
H	6.799296000	0.855576000	-4.240751000
H	7.127865000	1.508135000	-2.634266000
H	3.752829000	-3.016681000	-1.969444000
H	0.103552000	2.300798000	2.874891000
H	-0.227622000	-2.179589000	-3.050706000

H	2.892497000	3.498173000	-1.490997000
complex 4 (no dispersion)			
Yb	0.315108000	2.311182000	0.396785000
Yb	3.074009000	0.105166000	-0.341375000
Yb	0.168342000	-2.330416000	-0.364674000
Yb	-2.568264000	0.482712000	-1.673612000
Yb	-2.166494000	-0.221838000	2.072956000
P	0.757813000	-0.274036000	1.643727000
P	0.547697000	0.323720000	-1.800021000
P	-2.496747000	2.234503000	0.718713000
P	-2.712489000	-1.940037000	-0.158791000
P	3.178794000	3.117812000	0.062100000
P	3.249007000	-2.836638000	-0.456674000
O	-2.740941000	-0.136520000	4.488871000
O	-2.970379000	0.349607000	-4.195889000
O	-0.171325000	-4.793569000	-0.249434000
O	4.735027000	0.305097000	-2.163638000
O	-4.984020000	1.117646000	-1.964105000
C	1.599913000	0.582127000	4.274778000
C	1.530850000	-0.528336000	-4.398027000
C	1.019102000	0.557565000	-3.614174000
C	1.989910000	1.914686000	3.652552000
H	2.277299000	1.693137000	2.614977000
C	1.037982000	-0.480786000	3.495292000
C	-4.036670000	-3.253700000	-0.368862000
C	1.804634000	0.416532000	5.648454000
H	2.233318000	1.232403000	6.223275000
C	0.712660000	-1.693684000	4.178672000
C	0.804125000	2.889682000	3.598756000
H	1.083131000	3.811121000	3.070313000
H	0.490557000	3.180249000	4.608524000
C	-3.687731000	3.675451000	0.830457000
C	-4.773338000	-3.758559000	0.748772000
C	4.383701000	4.445526000	0.648964000
C	-4.331381000	-3.827013000	-1.643097000
C	-3.657435000	-3.384181000	-2.933116000
H	-3.025168000	-2.525157000	-2.674387000
C	4.861851000	-3.574871000	1.768230000
C	0.852255000	1.811452000	-4.278249000
C	1.815238000	-0.346400000	-5.756025000
H	2.193646000	-1.183044000	-6.335563000
C	3.183171000	2.601553000	4.323172000

H	2.927796000	3.012445000	5.307085000
H	3.524921000	3.438226000	3.705739000
H	4.020878000	1.910639000	4.456367000
C	4.420801000	-3.959356000	0.471666000
C	1.762694000	-1.911134000	-3.807566000
H	2.082083000	-1.749158000	-2.768542000
C	0.467114000	-2.730795000	-3.759361000
H	0.631643000	-3.696755000	-3.264234000
H	0.102617000	-2.943449000	-4.770998000
C	4.147228000	5.819709000	0.376241000
C	0.311843000	3.051099000	-3.584837000
H	0.246929000	2.801481000	-2.517729000
C	4.473550000	-2.231157000	2.372306000
H	3.447435000	-1.995707000	2.053693000
C	0.945509000	-1.811361000	5.555012000
H	0.710188000	-2.749044000	6.052852000
C	5.549765000	4.093308000	1.382181000
C	5.724694000	-4.407920000	2.484899000
H	6.054001000	-4.109174000	3.475307000
C	5.395303000	-1.131804000	1.825488000
H	5.424450000	-1.157534000	0.728661000
H	6.422767000	-1.278544000	2.177200000
H	5.070840000	-0.139937000	2.164257000
C	-4.918821000	3.587397000	1.549033000
C	1.628022000	0.876424000	-6.389356000
H	1.854705000	0.994805000	-7.445708000
C	1.154586000	1.942891000	-5.639380000
H	1.011700000	2.907780000	-6.120787000
C	0.135531000	-2.917255000	3.476880000
H	-0.211530000	-2.575128000	2.490999000
C	-3.661286000	-0.800005000	5.380462000
H	-3.719130000	-1.851956000	5.091960000
H	-4.654501000	-0.347319000	5.267731000
C	-2.058619000	5.157747000	-0.491196000
H	-1.784488000	4.208754000	-0.977178000
C	1.482795000	-0.770071000	6.298831000
H	1.659658000	-0.882967000	7.365273000
C	-2.061197000	-0.329613000	-5.099895000
H	-2.211728000	-1.409720000	-4.990134000
H	-1.041643000	-0.076074000	-4.808960000
C	-2.747238000	-4.481056000	-3.500165000
H	-1.963623000	-4.746712000	-2.783760000
H	-2.259229000	-4.150548000	-4.424589000

H	-3.313146000	-5.390787000	-3.732234000
C	-3.402805000	4.915343000	0.175496000
C	4.879690000	-5.196132000	-0.062499000
C	-1.912046000	0.793142000	5.249361000
H	-1.939619000	1.759211000	4.739580000
H	-0.889504000	0.408378000	5.251075000
C	5.944514000	2.645810000	1.642593000
H	5.015997000	2.065711000	1.706937000
C	2.954872000	6.318545000	-0.424380000
H	2.257367000	5.478159000	-0.514532000
C	-1.103136000	3.382644000	-4.076131000
H	-1.094860000	3.653864000	-5.138853000
H	-1.528568000	4.224988000	-3.521394000
H	-1.769692000	2.520491000	-3.966818000
C	-4.613230000	-3.174705000	2.142698000
H	-3.567188000	-2.835596000	2.205955000
C	6.179820000	-5.608584000	1.954192000
H	6.855290000	-6.242194000	2.523015000
C	-6.713689000	1.978762000	2.460529000
H	-6.832046000	1.048525000	3.027357000
H	-7.100162000	1.806073000	1.451327000
H	-7.357926000	2.725492000	2.938278000
C	-5.824326000	4.654201000	1.534706000
H	-6.755683000	4.567028000	2.088868000
C	5.061180000	6.782674000	0.819728000
H	4.877902000	7.829835000	0.593145000
C	2.853934000	-2.726509000	-4.506484000
H	3.072245000	-3.628909000	-3.926710000
H	3.783849000	-2.158542000	-4.608884000
H	2.549991000	-3.057583000	-5.506403000
C	4.478422000	-2.190069000	3.903089000
H	5.495878000	-2.233109000	4.308940000
H	3.907144000	-3.017743000	4.331317000
H	4.024776000	-1.258649000	4.253702000
C	-5.714841000	-4.778306000	0.579897000
H	-6.264797000	-5.144396000	1.442194000
C	-5.242243000	2.404080000	2.445069000
H	-4.644551000	1.562328000	2.068255000
C	4.673156000	1.347658000	-3.170079000
H	4.984713000	2.290282000	-2.705234000
H	3.636136000	1.433313000	-3.502406000
C	-0.995647000	5.457743000	0.577743000
H	-1.032006000	4.706795000	1.377027000

H	-1.179038000	6.432815000	1.042851000
H	0.014319000	5.486157000	0.148603000
C	5.757730000	-5.986797000	0.687536000
H	6.114128000	-6.924744000	0.270336000
C	6.423326000	5.094141000	1.820811000
H	7.311017000	4.817825000	2.381326000
C	-4.073888000	0.905241000	-4.946104000
H	-3.969985000	1.998132000	-4.948045000
H	-5.000445000	0.638744000	-4.434634000
C	6.748392000	2.106204000	0.450415000
H	7.655109000	2.703472000	0.301413000
H	6.152559000	2.150402000	-0.466174000
H	7.053485000	1.066769000	0.619991000
C	1.232919000	4.265420000	-3.736324000
H	2.246898000	4.040097000	-3.394739000
H	0.859138000	5.106907000	-3.143582000
H	1.297637000	4.604830000	-4.776250000
C	-5.957537000	0.354970000	-1.224862000
H	-5.779583000	0.488110000	-0.150725000
H	-5.815763000	-0.699089000	-1.474401000
C	-5.469901000	2.476675000	-2.099563000
H	-5.313458000	2.768411000	-3.142678000
H	-4.886139000	3.131108000	-1.446482000
C	-5.969746000	-5.341483000	-0.663667000
H	-6.699543000	-6.139197000	-0.774228000
C	6.190552000	6.434324000	1.543912000
H	6.884469000	7.197101000	1.887708000
C	-5.275112000	-4.854164000	-1.760280000
H	-5.469782000	-5.282574000	-2.741434000
C	4.492707000	-5.683477000	-1.451943000
H	3.546977000	-5.194182000	-1.709452000
C	3.388654000	6.727658000	-1.839425000
H	2.529179000	7.051674000	-2.437335000
H	3.873417000	5.897137000	-2.361968000
H	4.103544000	7.557989000	-1.804366000
C	2.210811000	7.467084000	0.268911000
H	2.820988000	8.374406000	0.335922000
H	1.911665000	7.191480000	1.284968000
H	1.306665000	7.728725000	-0.291803000
C	-5.525275000	-1.948130000	2.291442000
H	-6.575043000	-2.238146000	2.169115000
H	-5.290273000	-1.203453000	1.523125000
H	-5.425459000	-1.478724000	3.277379000

C	-3.103473000	-0.576731000	6.777529000
H	-3.874185000	-0.655156000	7.548917000
H	-2.317589000	-1.307898000	6.994095000
C	-1.368361000	-5.392442000	0.312711000
H	-2.160076000	-5.374647000	-0.442068000
H	-1.691527000	-4.772616000	1.151481000
C	-3.952664000	0.342686000	-6.356840000
H	-4.472579000	-0.618212000	-6.432958000
H	-4.375152000	1.017935000	-7.106010000
C	-4.767202000	2.721978000	3.869912000
H	-5.320437000	3.576517000	4.276395000
H	-3.704590000	2.982370000	3.867043000
H	-4.921095000	1.870230000	4.542709000
C	-5.557469000	5.829620000	0.845863000
H	-6.275654000	6.645365000	0.839913000
C	-2.506076000	0.825685000	6.650881000
H	-1.745358000	1.039772000	7.405480000
H	-3.290644000	1.586112000	6.726510000
C	-1.073129000	-3.516128000	4.205421000
H	-0.796297000	-3.969180000	5.163886000
H	-1.534724000	-4.302698000	3.599513000
H	-1.832833000	-2.755370000	4.408200000
C	-4.340466000	5.952264000	0.186615000
H	-4.112902000	6.882216000	-0.325400000
C	5.541293000	-5.250281000	-2.488094000
H	5.687440000	-4.165895000	-2.474115000
H	5.243619000	-5.542903000	-3.502112000
H	6.508813000	-5.717810000	-2.271846000
C	0.790252000	-5.828069000	-0.567846000
H	1.634400000	-5.743810000	0.124531000
H	1.160654000	-5.651808000	-1.580965000
C	-4.680403000	-2.931367000	-3.983014000
H	-5.355139000	-3.743653000	-4.274376000
H	-4.177086000	-2.590266000	-4.894775000
H	-5.298976000	-2.109961000	-3.606889000
C	5.887390000	-0.537510000	-2.391973000
H	6.419176000	-0.663223000	-1.444828000
H	5.534376000	-1.519283000	-2.724638000
C	4.256526000	-7.196708000	-1.540061000
H	5.185270000	-7.769463000	-1.443427000
H	3.825829000	-7.453900000	-2.514393000
H	3.570662000	-7.544216000	-0.760766000
C	6.721728000	2.427974000	2.945381000

H	6.809347000	1.356914000	3.154995000
H	6.229067000	2.903061000	3.798527000
H	7.742608000	2.821448000	2.884583000
C	-0.969191000	-6.812274000	0.684896000
H	-1.828783000	-7.487437000	0.705452000
H	-0.489570000	-6.838629000	1.670044000
C	-2.441787000	0.147584000	-6.492763000
H	-2.163415000	-0.573292000	-7.265759000
H	-1.943286000	1.096095000	-6.716845000
C	-4.855428000	-4.171018000	3.280798000
H	-4.560046000	-3.735930000	4.241904000
H	-4.281178000	-5.092171000	3.140294000
H	-5.911917000	-4.446104000	3.374907000
C	1.198075000	-3.997676000	3.242509000
H	2.019780000	-3.628625000	2.624499000
H	0.762702000	-4.865703000	2.734790000
H	1.618903000	-4.344637000	4.193192000
C	-2.050726000	6.255758000	-1.557451000
H	-2.827923000	6.097525000	-2.312815000
H	-1.082142000	6.278130000	-2.068343000
H	-2.202230000	7.251916000	-1.125968000
C	-7.288984000	0.951477000	-1.649951000
H	-7.577157000	0.569660000	-2.635800000
H	-8.094574000	0.720361000	-0.947735000
C	0.043563000	-7.148014000	-0.410658000
H	0.714009000	-7.970984000	-0.149244000
H	-0.474939000	-7.412886000	-1.338907000
C	5.633153000	0.903986000	-4.263647000
H	5.129280000	0.220966000	-4.955403000
H	6.020516000	1.748531000	-4.839640000
C	-6.956011000	2.448171000	-1.710813000
H	-7.089224000	2.914679000	-0.731008000
H	-7.578845000	2.991707000	-2.426275000
C	6.710703000	0.171810000	-3.461309000
H	7.299835000	-0.529084000	-4.058811000
H	7.398457000	0.890198000	-3.002047000
H	3.644452000	-3.165512000	-1.785114000
H	-0.075870000	2.447315000	3.109226000
H	-0.326724000	-2.189680000	-3.229444000
H	3.102477000	3.507941000	-1.313422000
complex 5 (dispersion)			
Yb	12.227244000	5.930220000	8.833135000

Yb	15.954481000	4.899189000	8.057667000
Yb	13.134328000	9.753755000	8.262443000
P	14.551650000	7.320099000	7.948418000
P	13.675761000	3.476015000	8.774010000
P	15.736482000	4.727347000	5.252789000
N	18.829589000	5.759652000	9.995798000
N	17.767737000	4.189779000	10.966785000
C	16.100423000	8.187153000	10.214827000
C	17.777588000	4.922870000	9.823499000
C	16.937131000	3.645856000	4.351784000
C	18.083355000	3.112570000	5.007686000
C	13.683338000	2.273400000	10.171465000
C	13.284196000	2.670064000	11.482041000
N	14.148326000	12.953947000	9.533647000
C	17.069915000	8.969164000	10.846496000
H	17.218454000	8.864449000	11.917165000
N	12.043278000	12.724967000	9.748487000
C	16.722598000	9.219368000	8.080592000
C	15.288250000	7.214383000	11.046695000
H	15.077191000	6.349965000	10.397944000
C	15.884921000	8.310036000	8.804401000
C	16.002516000	6.711327000	12.299920000
H	17.028804000	6.405019000	12.089372000
H	15.461821000	5.853469000	12.709586000
H	16.030282000	7.475353000	13.085613000
C	19.861189000	3.534204000	6.812772000
H	19.971648000	3.916438000	7.833250000
H	20.393255000	4.202327000	6.129092000
H	20.352833000	2.555637000	6.780377000
C	16.628215000	9.341890000	6.572685000
H	15.581395000	9.128043000	6.313298000
C	19.459406000	5.574911000	11.220294000
C	12.831819000	4.094447000	11.752354000
H	13.510234000	4.732306000	11.159690000
C	18.378125000	3.446910000	6.457774000
H	17.952194000	4.456598000	6.600413000
C	16.729174000	3.288345000	2.987012000
C	18.930566000	2.225132000	4.339789000
H	19.792317000	1.815864000	4.860011000
C	17.683533000	9.976188000	8.758069000
H	18.306866000	10.664360000	8.194072000
C	18.780578000	4.563409000	11.841268000
C	17.858216000	9.870693000	10.134698000

H	18.605054000	10.473892000	10.644458000
C	14.128996000	0.933666000	9.985214000
C	13.942715000	7.822875000	11.438313000
H	14.095174000	8.688024000	12.089629000
H	13.326546000	7.103318000	11.987311000
H	13.360243000	8.142081000	10.565422000
C	17.663977000	2.459915000	7.387644000
H	16.576738000	2.485609000	7.229508000
H	17.871321000	2.671993000	8.442647000
H	17.989652000	1.435682000	7.180321000
C	17.596267000	2.396403000	2.355372000
H	17.419361000	2.128626000	1.317277000
C	19.227377000	6.746415000	9.012535000
H	20.254301000	6.567796000	8.681344000
H	19.133374000	7.755420000	9.417989000
H	18.563200000	6.662778000	8.153545000
C	16.765896000	3.178441000	11.252080000
H	16.222238000	3.416857000	12.168985000
H	17.220144000	2.189417000	11.352879000
H	16.039372000	3.154387000	10.436563000
C	15.596068000	3.918304000	2.206334000
H	14.777900000	4.040869000	2.925382000
C	16.012612000	5.320466000	1.748450000
H	16.328500000	5.915853000	2.611316000
H	15.184434000	5.836631000	1.248862000
H	16.850800000	5.263283000	1.044710000
C	13.160243000	12.031775000	9.404986000
C	18.689752000	1.847281000	3.022763000
H	19.355020000	1.152989000	2.516603000
C	14.145192000	0.045311000	11.061228000
H	14.482596000	-0.975742000	10.905593000
C	20.606273000	6.407563000	11.663395000
H	20.332710000	7.468335000	11.697731000
H	21.467202000	6.309726000	10.992296000
H	20.928212000	6.111570000	12.663874000
C	18.957860000	3.939758000	13.177339000
H	19.824797000	4.366766000	13.685710000
H	19.112244000	2.857735000	13.102755000
H	18.081302000	4.103518000	13.814601000
C	13.673269000	14.190031000	9.942783000
C	14.563963000	0.457997000	8.614217000
H	14.973595000	1.345891000	8.113733000
C	11.404704000	4.319786000	11.232570000

H	11.112456000	5.382077000	11.260827000
H	10.677952000	3.780674000	11.848341000
H	11.313285000	3.920682000	10.213449000
C	12.920013000	4.525702000	13.213921000
H	12.698234000	5.592826000	13.311409000
H	13.916436000	4.345332000	13.629140000
H	12.195144000	3.992727000	13.838813000
C	12.321859000	14.043312000	10.081589000
C	13.315967000	1.747652000	12.530253000
H	13.007624000	2.054570000	13.525061000
C	10.710261000	12.152239000	9.738229000
H	10.068822000	12.680117000	9.029290000
H	10.253976000	12.185267000	10.730154000
H	10.778639000	11.104507000	9.437615000
C	15.084642000	3.096399000	1.027327000
H	15.815319000	3.039088000	0.211658000
H	14.182950000	3.561613000	0.614033000
H	14.833820000	2.076714000	1.331442000
C	15.646005000	-0.618421000	8.636259000
H	16.493960000	-0.315561000	9.258961000
H	16.020534000	-0.801316000	7.623823000
H	15.273894000	-1.576590000	9.016321000
C	13.738041000	0.437704000	12.331522000
H	13.753062000	-0.266975000	13.158431000
C	17.521671000	8.300743000	5.889490000
H	18.575063000	8.459287000	6.150176000
H	17.438887000	8.367847000	4.797615000
H	17.239581000	7.278640000	6.169727000
C	14.563756000	15.349391000	10.196970000
H	15.167882000	15.597892000	9.317520000
H	15.241178000	15.143474000	11.032752000
H	13.973483000	16.230653000	10.456260000
C	15.536437000	12.678816000	9.240699000
H	15.659630000	11.607116000	9.086881000
H	16.166307000	12.975641000	10.081600000
H	15.852607000	13.206623000	8.336048000
C	16.904363000	10.741843000	6.030803000
H	16.294230000	11.490283000	6.543886000
H	16.638842000	10.782403000	4.970351000
H	17.958000000	11.031856000	6.118886000
C	13.344465000	0.011778000	7.800788000
H	12.876535000	-0.870237000	8.252449000
H	13.612229000	-0.232851000	6.766311000

H	12.600030000	0.814794000	7.786247000
C	11.274327000	14.998776000	10.521225000
H	10.776509000	14.656543000	11.435800000
H	10.500149000	15.134180000	9.757595000
H	11.715546000	15.976035000	10.727206000
Yb	14.240237000	7.105401000	5.126722000
Yb	10.690296000	8.330460000	6.034940000
Yb	13.385486000	3.321532000	5.982012000
P	11.872303000	5.749324000	5.993930000
P	13.079245000	9.690345000	5.478617000
P	10.761906000	8.325803000	8.869897000
N	7.810247000	7.294907000	4.383402000
N	8.533192000	8.903841000	3.192438000
C	10.233838000	4.929717000	3.775509000
C	8.783556000	8.239653000	4.349604000
C	9.350808000	9.134144000	9.756939000
C	8.258401000	9.713408000	9.049248000
C	12.598731000	10.833109000	4.110341000
C	12.785585000	10.461109000	2.742984000
N	12.694733000	1.118481000	3.188716000
C	9.204793000	4.195689000	3.183721000
H	8.957632000	4.373232000	2.141803000
N	14.602451000	0.693518000	4.025700000
C	9.825800000	3.728996000	5.869633000
C	11.017430000	5.914330000	2.932469000
H	11.219940000	6.784836000	3.573846000
C	10.559843000	4.727019000	5.153776000
C	10.285708000	6.402031000	1.685569000
H	9.268846000	6.728762000	1.915029000
H	10.827605000	7.242743000	1.246223000
H	10.227651000	5.622570000	0.916618000
C	6.728374000	9.569517000	6.994832000
H	6.745128000	9.319855000	5.929475000
H	6.110466000	8.834490000	7.519501000
H	6.241813000	10.546352000	7.089785000
C	10.051874000	3.493607000	7.350829000
H	11.105337000	3.737430000	7.565145000
C	6.977591000	7.347783000	3.274468000
C	13.411746000	9.124645000	2.376865000
H	12.899460000	8.380068000	3.013866000
C	8.154506000	9.585571000	7.541735000
H	8.595052000	8.597292000	7.319470000
C	9.353973000	9.253606000	11.172894000

C	7.275607000	10.431032000	9.734231000
H	6.457969000	10.881365000	9.178388000
C	8.821916000	2.997377000	5.225820000
H	8.277048000	2.242685000	5.785506000
C	7.439832000	8.382175000	2.509707000
C	8.496327000	3.226870000	3.892965000
H	7.709448000	2.654026000	3.409692000
C	12.031432000	12.115471000	4.378986000
C	12.373895000	5.316725000	2.553066000
H	12.248243000	4.447181000	1.899780000
H	12.992570000	6.044861000	2.019266000
H	12.924871000	4.996693000	3.444505000
C	8.973084000	10.677054000	6.845615000
H	10.016052000	10.664644000	7.188082000
H	8.950064000	10.573808000	5.753040000
H	8.566324000	11.662887000	7.089653000
C	8.349120000	9.972608000	11.822765000
H	8.381527000	10.065036000	12.906472000
C	7.633967000	6.369246000	5.483141000
H	6.736475000	6.619462000	6.056185000
H	7.573049000	5.344426000	5.115159000
H	8.500317000	6.436947000	6.140004000
C	9.357033000	9.989274000	2.696017000
H	9.869962000	9.698646000	1.776815000
H	8.752259000	10.878058000	2.501282000
H	10.115018000	10.238245000	3.438311000
C	10.466435000	8.658640000	12.010349000
H	11.066448000	8.051550000	11.322077000
C	9.949633000	7.748090000	13.124477000
H	9.313272000	6.957306000	12.715009000
H	10.785494000	7.274739000	13.652663000
H	9.361328000	8.295759000	13.869456000
C	13.484402000	1.431274000	4.248679000
C	7.316479000	10.578774000	11.116583000
H	6.546126000	11.143342000	11.634711000
C	11.613772000	12.931918000	3.327355000
H	11.169016000	13.898694000	3.546120000
C	5.871590000	6.380151000	3.063127000
H	6.254134000	5.353274000	3.043166000
H	5.120212000	6.438655000	3.858652000
H	5.369050000	6.574038000	2.113328000
C	6.986634000	8.904703000	1.195380000
H	6.121580000	8.340310000	0.840988000

H	6.695965000	9.959668000	1.253684000
H	7.774095000	8.821844000	0.437480000
C	13.299883000	0.216368000	2.321941000
C	11.957245000	12.644880000	5.797678000
H	11.794919000	11.770994000	6.444173000
C	14.910637000	9.087575000	2.711940000
H	15.331725000	8.084374000	2.553441000
H	15.463826000	9.771527000	2.060275000
H	15.076588000	9.408638000	3.747576000
C	13.222078000	8.712446000	0.919067000
H	13.590248000	7.694155000	0.761016000
H	12.171840000	8.744799000	0.615352000
H	13.785803000	9.364615000	0.242978000
C	14.526207000	-0.053520000	2.859493000
C	12.373716000	11.322307000	1.723230000
H	12.516451000	11.035925000	0.686102000
C	15.740810000	0.657893000	4.919256000
H	15.785473000	-0.302565000	5.440521000
H	16.666180000	0.828468000	4.368459000
H	15.634767000	1.458417000	5.649494000
C	11.368645000	9.766956000	12.553301000
H	10.797358000	10.477482000	13.162413000
H	12.172698000	9.363822000	13.177505000
H	11.824004000	10.319002000	11.724045000
C	10.834229000	13.645640000	6.056014000
H	9.863660000	13.260058000	5.730036000
H	10.776392000	13.864069000	7.127888000
H	11.006418000	14.601195000	5.547429000
C	11.771572000	12.545068000	2.000799000
H	11.447121000	13.195180000	1.192872000
C	9.185352000	4.454099000	8.176498000
H	8.125751000	4.323342000	7.928882000
H	9.295448000	4.263921000	9.249537000
H	9.449376000	5.503011000	7.988204000
C	12.659763000	-0.247432000	1.064656000
H	11.696251000	-0.734935000	1.251606000
H	12.481377000	0.585199000	0.374098000
H	13.303542000	-0.967682000	0.555649000
C	11.370281000	1.666609000	2.993431000
H	11.148733000	2.351143000	3.810334000
H	11.311663000	2.219571000	2.053167000
H	10.617180000	0.874024000	2.989194000
C	9.850747000	2.049436000	7.805250000

H	10.364665000	1.346408000	7.141533000
H	10.266990000	1.921713000	8.809304000
H	8.792944000	1.764861000	7.843900000
C	13.312055000	13.250996000	6.182576000
H	13.577608000	14.056057000	5.488239000
H	13.282781000	13.664478000	7.195664000
H	14.090984000	12.483216000	6.135520000
C	15.650215000	-0.894852000	2.376564000
H	16.552061000	-0.288431000	2.235894000
H	15.894461000	-1.695613000	3.083770000
H	15.397061000	-1.357566000	1.420456000
C	15.801826000	12.056231000	12.567564000
H	16.548577000	11.359209000	12.200662000
C	14.449429000	11.750208000	12.422947000
H	14.152009000	10.825608000	11.941936000
C	16.184571000	13.257464000	13.164306000
H	17.238493000	13.496220000	13.279406000
C	15.213661000	14.151853000	13.617216000
H	15.511117000	15.086488000	14.084815000
C	13.479802000	12.642234000	12.876129000
H	12.429287000	12.400433000	12.755268000
C	13.861325000	13.843420000	13.471347000
H	13.104798000	14.540056000	13.821725

Complex 7 (S=1)

Yb	-1.651043000	0.716334000	0.020382000
Yb	1.933476000	0.940148000	-0.002144000
Yb	0.423697000	-1.902302000	-0.024980000
P	0.337475000	1.657782000	2.162575000
P	0.327034000	1.664039000	-2.144023000
P	-3.635700000	-1.126114000	0.021718000
P	2.959059000	-2.924544000	-0.168776000
N	0.376471000	-1.302478000	2.234975000
N	0.304329000	-1.292883000	-2.275348000
N	-1.473944000	-3.111318000	-0.020645000
N	3.838987000	-0.127618000	0.064646000
N	2.898654000	4.535668000	0.006851000
C	0.398640000	-0.094549000	-1.784839000
C	-5.292937000	-2.037780000	0.016332000
C	-2.097296000	-4.444682000	-0.029834000
C	0.455019000	-0.091258000	1.770156000
C	0.086517000	-1.715907000	3.616215000
C	-2.060880000	-1.931874000	0.003907000

C	0.009554000	-1.688725000	-3.659938000
C	0.323533000	2.301997000	3.944007000
C	-2.964403000	-4.680782000	1.221319000
H	-3.775812000	-3.947341000	1.240457000
H	-2.355332000	-4.520666000	2.119493000
C	1.038346000	-1.141208000	-4.661710000
H	2.040715000	-1.476178000	-4.365031000
H	1.027856000	-0.049110000	-4.630845000
C	-1.394622000	-1.203038000	-4.063947000
H	-1.426115000	-0.107415000	-4.018497000
H	-2.123751000	-1.582218000	-3.337307000
C	3.049668000	-1.184207000	-0.037506000
C	5.033387000	-4.480880000	1.069428000
N	-4.741774000	2.910288000	0.048705000
C	-2.974505000	-4.669207000	-1.275453000
H	-2.374419000	-4.499082000	-2.177632000
H	-3.787350000	-3.937524000	-1.279108000
C	4.542548000	-3.948122000	-0.150203000
C	-5.965106000	-2.295724000	1.239558000
C	0.099211000	-3.251532000	3.660359000
H	1.086258000	-3.608650000	3.341247000
H	-0.629565000	-3.634183000	2.936702000
C	2.725586000	3.380273000	0.018717000
C	0.044940000	-3.223177000	-3.724337000
H	1.041806000	-3.567911000	-3.422833000
H	-0.666516000	-3.624558000	-2.993976000
C	-0.893661000	2.766205000	4.507560000
C	-5.346030000	-1.962181000	2.590110000
H	-4.263676000	-1.884621000	2.433230000
C	1.541433000	2.441076000	-4.657862000
C	-3.538523000	-6.107078000	1.220091000
H	-4.150199000	-6.250460000	2.121178000
C	-5.323695000	-1.991847000	-2.559121000
H	-4.240570000	-1.939700000	-2.397307000
C	0.340294000	2.363802000	-3.902526000
C	-1.303862000	-1.216557000	4.047965000
H	-2.049415000	-1.576353000	3.327620000
H	-1.321395000	-0.120812000	4.018206000
C	-1.731750000	-1.685240000	-5.484080000
H	-2.734676000	-1.330376000	-5.757611000
C	-0.963598000	-5.485203000	-0.038654000
H	-0.326731000	-5.329268000	0.842664000
H	-0.332190000	-5.321191000	-0.922320000

C	6.181870000	-5.281095000	1.050486000
H	6.565364000	-5.688268000	1.982134000
C	-1.528177000	-6.913849000	-0.042682000
H	-0.698332000	-7.632713000	-0.048892000
C	5.814711000	-0.837897000	1.388830000
H	5.519167000	-1.887511000	1.305308000
H	5.333314000	-0.432960000	2.289127000
C	4.307701000	-4.281731000	2.392615000
H	3.650681000	-3.411949000	2.268696000
C	-0.850005000	2.925371000	-4.432296000
C	-5.955246000	-2.308750000	-1.209908000
C	-3.547496000	-6.096064000	-1.283578000
H	-4.165470000	-6.231628000	-2.181594000
C	-4.409271000	-6.306581000	-0.029546000
H	-5.246478000	-5.597243000	-0.023426000
H	-4.839889000	-7.317483000	-0.032318000
C	-1.698479000	-3.221063000	-5.526843000
H	-1.959100000	-3.576171000	-6.533278000
H	-2.445685000	-3.634065000	-4.836975000
C	5.181900000	-4.288037000	-1.370635000
C	-2.148598000	2.966964000	-3.640687000
H	-2.104601000	2.148711000	-2.910613000
C	1.141893000	-1.197671000	4.606888000
H	1.152863000	-0.105093000	4.585548000
H	2.132867000	-1.547901000	4.289422000
C	0.702693000	-1.621151000	-6.084819000
H	1.443018000	-1.214123000	-6.786794000
C	-2.397235000	-7.113602000	-1.294257000
H	-1.788490000	-6.986107000	-2.199605000
H	-2.796828000	-8.136704000	-1.318414000
C	3.116951000	5.950250000	-0.033580000
C	-0.295601000	-3.714139000	-5.139360000
H	-0.271384000	-4.811501000	-5.158702000
C	-2.388503000	-7.124855000	1.213311000
H	-2.787985000	-8.148150000	1.230773000
H	-1.773267000	-7.005940000	2.115454000
C	2.880543000	1.927597000	-4.143356000
H	2.668200000	1.204311000	-3.347802000
C	6.835892000	-5.574811000	-0.139263000
H	7.729275000	-6.194395000	-0.133993000
C	1.520603000	2.403357000	4.702248000
C	3.415208000	-5.499992000	2.676444000
H	2.685097000	-5.649740000	1.875117000

H	2.868187000	-5.373762000	3.617655000
H	4.017275000	-6.412634000	2.756842000
C	6.328373000	-5.090448000	-1.338506000
H	6.826404000	-5.349723000	-2.268735000
C	5.302965000	-0.068795000	0.158277000
C	-5.593422000	-3.028658000	3.662789000
H	-6.645263000	-3.077520000	3.967103000
H	-5.011913000	-2.797247000	4.561646000
H	-5.299160000	-4.023788000	3.315973000
C	-3.691974000	2.393260000	0.042169000
C	-0.698399000	-1.122311000	-6.472307000
H	-0.941598000	-1.441133000	-7.495091000
H	-0.723075000	-0.025140000	-6.461742000
C	-5.771889000	-0.607840000	-3.048892000
H	-6.860502000	-0.571068000	-3.176031000
H	-5.309675000	-0.367903000	-4.013283000
H	-5.482196000	0.165166000	-2.330848000
C	0.732168000	-3.155403000	-6.134519000
H	1.737127000	-3.522054000	-5.886072000
H	0.506359000	-3.506241000	-7.150884000
C	0.827997000	-3.224251000	6.058914000
H	1.823041000	-3.602879000	5.788555000
H	0.614120000	-3.584727000	7.074460000
C	-6.016730000	4.791701000	-0.797592000
H	-5.693161000	4.553861000	-1.817754000
H	-5.280933000	5.484169000	-0.371174000
C	5.237462000	-4.007808000	3.579960000
H	5.837210000	-4.884850000	3.848883000
H	4.646468000	-3.743114000	4.463463000
H	5.924652000	-3.181731000	3.374283000
C	-5.592310000	-3.053030000	-3.631902000
H	-5.330768000	-4.056201000	-3.282122000
H	-4.996722000	-2.839461000	-4.525826000
H	-6.642361000	-3.070816000	-3.945728000
C	-6.470125000	3.830263000	1.486904000
H	-5.740158000	4.517091000	1.931587000
H	-6.466967000	2.911188000	2.083966000
C	-0.224964000	-3.755712000	5.074839000
H	-0.216284000	-4.853527000	5.079795000
C	2.892344000	2.051603000	4.141134000
H	2.736688000	1.394514000	3.278100000
C	-6.048221000	3.498799000	0.041024000
C	5.970557000	-0.634740000	-1.107728000

H	5.599946000	-0.084522000	-1.983368000
H	5.677936000	-1.681400000	-1.229890000
C	3.723525000	1.211583000	-5.206278000
H	4.118111000	1.906498000	-5.956074000
H	3.151589000	0.441122000	-5.729555000
H	4.585685000	0.729549000	-4.733450000
C	0.820296000	-1.688752000	6.029194000
H	1.577594000	-1.301519000	6.724089000
C	1.517490000	3.056598000	-5.914302000
H	2.433930000	3.115990000	-6.494601000
C	5.715848000	1.405451000	0.302254000
H	5.232292000	1.829368000	1.193034000
H	5.344788000	1.969824000	-0.564526000
C	4.613247000	-3.885949000	-2.724684000
H	3.946546000	-3.031906000	-2.553506000
C	-2.187854000	2.817736000	3.709730000
H	-2.120520000	2.039480000	2.938645000
C	-1.624944000	-1.711487000	5.467609000
H	-2.617867000	-1.345542000	5.762117000
C	3.685643000	3.080905000	-3.528682000
H	4.635595000	2.718902000	-3.118824000
H	3.125396000	3.562869000	-2.723747000
H	3.912310000	3.839361000	-4.287519000
C	-0.823474000	3.528194000	-5.695039000
H	-1.734411000	3.957118000	-6.102486000
C	7.343356000	-0.722012000	1.492716000
H	7.690348000	-1.283460000	2.370249000
C	-2.231767000	4.282090000	-2.852356000
H	-2.228951000	5.141452000	-3.532989000
H	-1.378869000	4.384797000	-2.173672000
H	-3.147254000	4.323828000	-2.253027000
C	-7.418580000	5.421329000	-0.806657000
H	-7.387434000	6.339406000	-1.406063000
C	-3.447023000	2.537838000	4.535065000
H	-3.679619000	3.353738000	5.228658000
H	-3.348877000	1.616972000	5.117545000
H	-4.309875000	2.425059000	3.871338000
C	2.368704000	6.622232000	1.135133000
H	2.725003000	6.205603000	2.084162000
H	1.298748000	6.395841000	1.059089000
C	-7.259903000	-2.826973000	1.212796000
H	-7.775861000	-3.026285000	2.148252000
C	-0.899635000	3.270398000	5.812877000

H	-1.831655000	3.619352000	6.247397000
C	-0.567179000	-1.174878000	6.444911000
H	-0.797895000	-1.502960000	7.467691000
H	-0.576486000	-0.077549000	6.447890000
C	3.806517000	1.314133000	5.126875000
H	4.132349000	1.959249000	5.950506000
H	4.711279000	0.975826000	4.610866000
H	3.317516000	0.437329000	5.558865000
C	-7.249843000	-2.840200000	-1.187136000
H	-7.758326000	-3.050524000	-2.124128000
C	7.987540000	-1.302946000	0.223964000
H	9.082127000	-1.244921000	0.297535000
H	7.725662000	-2.363076000	0.120451000
C	4.119020000	8.420982000	1.201001000
H	4.499657000	8.047554000	2.160518000
H	4.300258000	9.503151000	1.185580000
C	3.579270000	3.329880000	3.639066000
H	2.966488000	3.827132000	2.882656000
H	4.556550000	3.102840000	3.198170000
H	3.736239000	4.032821000	4.465670000
C	1.463401000	2.915891000	6.003350000
H	2.376950000	2.988404000	6.586673000
C	-3.406036000	2.754073000	-4.489165000
H	-4.278299000	2.631794000	-3.838586000
H	-3.323536000	1.857582000	-5.110843000
H	-3.613377000	3.604428000	-5.148522000
C	-2.293206000	4.171098000	2.990713000
H	-3.206341000	4.224798000	2.388628000
H	-1.439070000	4.329595000	2.324446000
H	-2.312781000	4.991984000	3.716967000
C	-7.839148000	5.753698000	0.633741000
H	-7.140269000	6.475855000	1.075989000
H	-8.829788000	6.225605000	0.635813000
C	-7.870415000	4.464579000	1.469196000
H	-8.161458000	4.697654000	2.500647000
C	2.613179000	8.139310000	1.080576000
H	2.079482000	8.609497000	1.915303000
C	-8.873567000	3.475313000	0.855868000
H	-8.920102000	2.559379000	1.458583000
H	-9.880412000	3.911983000	0.860317000
C	-1.613693000	-3.247892000	5.491717000
H	-2.378412000	-3.641883000	4.809932000
H	-1.862062000	-3.611716000	6.498117000

C	7.499892000	-0.517590000	-1.003875000
H	7.957304000	-0.933282000	-1.911505000
C	4.628399000	6.229730000	0.087441000
H	5.156087000	5.726583000	-0.731339000
H	5.000840000	5.808557000	1.028594000
C	-5.830842000	-0.587757000	3.072938000
H	-5.557607000	0.190586000	2.353168000
H	-5.379363000	-0.332256000	4.038275000
H	-6.920603000	-0.577444000	3.195113000
C	0.348305000	3.593831000	-6.436567000
H	0.351376000	4.063972000	-7.416667000
C	0.265846000	3.337939000	6.564323000
H	0.242339000	3.726471000	7.579247000
C	-7.901114000	-3.102129000	0.011774000
H	-8.906122000	-3.517068000	0.009785000
C	-8.450492000	3.143317000	-0.583609000
H	-9.157508000	2.429802000	-1.023175000
C	5.670326000	-3.462371000	-3.750676000
H	6.332137000	-2.685158000	-3.357079000
H	5.180833000	-3.067163000	-4.647429000
H	6.295162000	-4.302839000	-4.073856000
C	7.737236000	0.755478000	1.637307000
H	8.827402000	0.851347000	1.731385000
H	7.299194000	1.175934000	2.552986000
C	3.758717000	-5.035763000	-3.280239000
H	4.368593000	-5.933676000	-3.433958000
H	3.313556000	-4.761860000	-4.243437000
H	2.949301000	-5.294377000	-2.590855000
C	-8.420733000	4.431230000	-1.421393000
H	-9.420651000	4.881982000	-1.453531000
H	-8.140010000	4.202236000	-2.457649000
C	7.242833000	1.536186000	0.409199000
H	7.510760000	2.596459000	0.512786000
C	-7.052789000	2.504094000	-0.574916000
H	-7.049065000	1.574674000	0.005511000
H	-6.736000000	2.252646000	-1.593316000
C	2.089994000	8.696414000	-0.252761000
H	1.010035000	8.519997000	-0.339919000
H	2.240465000	9.782751000	-0.290369000
C	4.862331000	7.748006000	0.036490000
H	5.938714000	7.939804000	0.122523000
C	2.590603000	6.505622000	-1.372432000
H	1.522455000	6.277250000	-1.465022000

H	3.104790000	6.006455000	-2.201290000
C	7.892818000	0.960089000	-0.858423000
H	7.566222000	1.527193000	-1.741032000
H	8.985306000	1.059161000	-0.801081000
C	2.833335000	8.022421000	-1.416437000
H	2.457616000	8.408951000	-2.371495000
C	4.339631000	8.303245000	-1.297868000
H	4.525159000	9.383360000	-1.352668000
H	4.878123000	7.843669000	-2.136792000

Yb1 (S=0, open shell singlet)

Yb	-1.647093000	0.627629000	-0.007922000
Yb	1.910390000	1.024070000	0.027689000
Yb	0.542920000	-1.891531000	-0.017333000
P	0.261589000	1.609851000	2.189878000
P	0.299428000	1.709831000	-2.128233000
P	-3.546590000	-1.297557000	-0.069201000
P	3.131333000	-2.778719000	-0.179929000
N	0.469304000	-1.343198000	2.255830000
N	0.404380000	-1.244618000	-2.257421000
N	-1.300234000	-3.185053000	0.037393000
N	3.867690000	0.059206000	0.045148000
N	2.546397000	4.684138000	0.096026000
C	0.454338000	-0.041787000	-1.768600000
C	-5.164379000	-2.277886000	-0.055788000
C	-1.870927000	-4.541757000	0.063831000
C	0.470736000	-0.130291000	1.790403000
C	0.203895000	-1.772186000	3.637023000
C	-1.938022000	-2.033209000	-0.007313000
C	0.135370000	-1.642943000	-3.646898000
C	0.235408000	2.250413000	3.972370000
C	-2.758878000	-4.772143000	1.300796000
H	-3.595401000	-4.067801000	1.278382000
H	-2.178609000	-4.563841000	2.207799000
C	1.181438000	-1.082051000	-4.624253000
H	2.179966000	-1.409682000	-4.306764000
H	1.161778000	0.009948000	-4.587159000
C	-1.265215000	-1.174212000	-4.079635000
H	-1.313924000	-0.079901000	-4.032055000
H	-2.004763000	-1.567060000	-3.370800000
C	3.134134000	-1.037478000	-0.038059000
C	5.316094000	-4.170901000	1.069707000
N	-4.835350000	2.672218000	0.016043000

C	-2.708522000	-4.833676000	-1.195324000
H	-2.089204000	-4.672510000	-2.086294000
H	-3.543256000	-4.128688000	-1.242759000
C	4.770151000	-3.709517000	-0.155358000
C	-5.837001000	-2.525248000	1.169559000
C	0.285183000	-3.305417000	3.682346000
H	1.287070000	-3.619274000	3.363544000
H	-0.424989000	-3.719384000	2.958074000
C	2.503147000	3.516635000	0.080571000
C	0.188459000	-3.176994000	-3.713135000
H	1.181323000	-3.512837000	-3.388156000
H	-0.537792000	-3.587654000	-3.002180000
C	-0.997033000	2.656123000	4.548417000
C	-5.249268000	-2.118091000	2.513902000
H	-4.169575000	-1.997300000	2.367157000
C	1.456594000	2.540545000	-4.650129000
C	-3.282921000	-6.217335000	1.328912000
H	-3.909465000	-6.357065000	2.220309000
C	-5.170984000	-2.310261000	-2.630178000
H	-4.092375000	-2.214903000	-2.458396000
C	0.264723000	2.400123000	-3.889941000
C	-1.208608000	-1.337336000	4.067525000
H	-1.935685000	-1.735678000	3.348398000
H	-1.279463000	-0.244093000	4.032881000
C	-1.565622000	-1.655235000	-5.508423000
H	-2.566525000	-1.311486000	-5.802811000
C	-0.701932000	-5.541151000	0.108261000
H	-0.089029000	-5.339891000	0.997141000
H	-0.059177000	-5.379191000	-0.767797000
C	6.513990000	-4.895185000	1.051972000
H	6.939515000	-5.247234000	1.987825000
C	-1.217730000	-6.988415000	0.132874000
H	-0.363654000	-7.677594000	0.165946000
C	5.985373000	-0.510722000	1.225226000
H	5.762585000	-1.579663000	1.162744000
H	5.546570000	-0.137466000	2.160379000
C	4.602541000	-3.983365000	2.401559000
H	3.869952000	-3.178790000	2.264258000
C	-0.961718000	2.869393000	-4.427805000
C	-5.803589000	-2.612551000	-1.278414000
C	-3.234937000	-6.277885000	-1.173659000
H	-3.827769000	-6.459262000	-2.080489000
C	-4.117349000	-6.482510000	0.066857000

H	-4.978826000	-5.803661000	0.033521000
H	-4.512840000	-7.507565000	0.083874000
C	-1.513225000	-3.190253000	-5.554941000
H	-1.746888000	-3.545523000	-6.567921000
H	-2.269941000	-3.614701000	-4.882682000
C	5.406430000	-4.048492000	-1.377971000
C	-2.251336000	2.862976000	-3.620523000
H	-2.171506000	2.042101000	-2.895928000
C	1.235079000	-1.207371000	4.627454000
H	1.198795000	-0.115384000	4.604367000
H	2.240374000	-1.515032000	4.310679000
C	0.880462000	-1.560277000	-6.055837000
H	1.631007000	-1.142891000	-6.740631000
C	-2.051417000	-7.255117000	-1.130407000
H	-1.427688000	-7.133503000	-2.026351000
H	-2.414978000	-8.291872000	-1.131838000
C	2.569955000	6.115543000	0.110584000
C	-0.113814000	-3.667781000	-5.137509000
H	-0.075984000	-4.764721000	-5.159220000
C	-2.098084000	-7.193635000	1.375974000
H	-2.461933000	-8.229518000	1.415078000
H	-1.507766000	-7.026959000	2.287119000
C	2.831079000	2.158057000	-4.115175000
H	2.678845000	1.434066000	-3.306985000
C	7.163993000	-5.183776000	-0.141072000
H	8.096212000	-5.743215000	-0.134868000
C	1.434637000	2.411924000	4.717361000
C	3.824561000	-5.262410000	2.747561000
H	3.099068000	-5.504867000	1.965038000
H	3.282116000	-5.147176000	3.692808000
H	4.504619000	-6.116028000	2.851580000
C	6.603147000	-4.773767000	-1.344424000
H	7.099216000	-5.031380000	-2.276057000
C	5.327635000	0.214166000	0.037818000
C	-5.463988000	-3.153878000	3.623033000
H	-6.516271000	-3.236130000	3.918261000
H	-4.903452000	-2.864577000	4.518467000
H	-5.123626000	-4.147719000	3.317374000
C	-3.759594000	2.211599000	0.028650000
C	-0.517707000	-1.076447000	-6.471803000
H	-0.734472000	-1.395039000	-7.500625000
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C	-5.661292000	-0.956518000	-3.162697000

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H	-5.401267000	-0.153253000	-2.466674000
C	0.928788000	-3.094028000	-6.108576000
H	1.932397000	-3.449939000	-5.839997000
H	0.728298000	-3.444619000	-7.130333000
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H	2.020313000	-3.579999000	5.812852000
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C	-6.221697000	4.460474000	-0.863546000
H	-5.855865000	4.247329000	-1.874886000
H	-5.550230000	5.205717000	-0.420008000
C	5.529550000	-3.588837000	3.556969000
H	6.216663000	-4.397231000	3.831698000
H	4.936537000	-3.357879000	4.448645000
H	6.129533000	-2.707068000	3.313505000
C	-5.391071000	-3.409839000	-3.674708000
H	-5.097199000	-4.392747000	-3.294265000
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H	-6.436777000	-3.473829000	-3.996887000
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H	-6.604674000	2.552987000	2.009589000
C	-0.018622000	-3.822194000	5.097513000
H	0.038461000	-4.918565000	5.103118000
C	2.817846000	2.123911000	4.146975000
H	2.688119000	1.462843000	3.282879000
C	-6.178961000	3.168616000	-0.023387000
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H	5.707091000	-1.379008000	-1.368916000
C	3.748929000	1.503793000	-5.155050000
H	4.081122000	2.216179000	-5.918534000
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H	4.649614000	1.119542000	-4.664920000
C	0.934992000	-1.711054000	6.050276000
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H	5.202609000	2.106841000	1.077098000
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C	4.786089000	-3.728824000	-2.731627000

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H	4.353276000	8.319101000	-1.645141000

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