ELECTRONIC SUPPLEMENTARY INFORMATION

Phosphorescent biaryl Pt(IV) complexes obtained through double metalation of dibenzoiodolium ions

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1. Experimental details

1.1. General considerations and materials

Unless otherwise noted, all reactions were carried out at room temperature using extra-dry MeCN and flame-dried glassware under an N_2 atmosphere. Synthesis grade Et_2O and CH_2Cl_2 were degassed and dried using a Pure Solv MD-5 solvent purification system from Innovative Technologies, Inc. Other solvents were used as received. Complexes *cis*-[Pt(C^N)$_2$] [C^N = ppy (**1a**), tpy (**1b**) or thpy (**1c**)][1,2] and the dibenzoiodolium triflates[3,4] were prepared following published procedures. All other reagents were obtained from commercial sources. Irradiations were performed using a previously described setup.[1]

1.2. Spectroscopic and analytical methods

NMR spectra were registered on Bruker Avance 600, 400 or 300 MHz spectrometers at 298 K. Chemical shifts are referred to residual signals of non-deuterated solvents and are given in ppm downfield from tetramethylsilane. Elemental analyses were carried out with a LECO CHNS-932 microanalyzer. High-resolution electrospray ionization mass spectra (ESI-MS) were recorded on an Agilent 6220 Accurate-Mass time-of-flight (TOF) LC/MS.

1.3. Synthesis and characterization data of new complexes

General procedure for the synthesis of [Pt(C^N)$_2$(C^C)] complexes [C^N = cyclometalated 2-phenylpyridine (ppy), 2-(*p*-tolyl)pyridine (tpy) or 2-(2-thienyl)pyridine, and C^C = dimetalated 4,4'-di-*tert*-butylbiphenyl (dbbph), biphenyl (bph) or 4,4'-difluorobiphenyl (dFbph)] (2). To a suspension of the appropriate complex **1** (0.20 mmol) in MeCN (20 mL) was added the dibenzoiodolium triflate (0.1 mmol) and the mixture was stirred at 60 °C for 24 h. The resulting pale yellow solution was cooled to room temperature and the solvent was evaporated under reduced pressure. The residue was chromatographed on silica gel using a hexane/AcOEt (4:1) mixture as the eluent. The corresponding complex **2** was isolated after partial evaporation of the solvents and addition of pentane.

[Pt(ppy)$_2$(dbbph)] (2aa). White solid. Yield: 68%. ^{1}H NMR (400.9 MHz, CD_2Cl_2): δ 8.05 (d, J = 9.1 Hz, 1H), 8.01 (d, J = 9.1 Hz, 1H), 7.96 (ddd with satellites, J_{PtH} = 13.7 Hz, J_{HH} = 0.8, 1.7, 5.5 Hz, 1H), 7.90-7.80 (m, 3H), 7.74 (dd with satellites, J_{PtH} = 14.0 Hz, J = 7.8, 1.5 Hz, 1H), 7.62 (ddd with satellites, J_{PtH} = 9.1 Hz, J_{HH} = 5.5, 1.7, 0.8 Hz, 1H), 7.40 (d, J = 8.4 Hz, 1H), 7.35-7.28 (m, 1H), 7.19-6.95 (m, 8H), 6.89 (dd with satellites, J_{PtH} = 48.5 Hz, J_{HH} = 7.8, 1.2 Hz, 1H), 6.77 (dd with satellites, J_{PtH} = 25.1 Hz, J_{HH} = 7.3, 1.5 Hz, 1H), 6.64 (d with satellites, J_{PtH} = 50.1 Hz, J_{HH} = 2.1 Hz, 1H), 6.27 (d with satellites, J_{PtH} = 20.1 Hz, J_{HH} = 2.1 Hz, 1H), 1.06 (s, 9H), 1.01 (s, 9H). ^{13}C NMR (151 MHz, CD_2Cl_2): δ 169.8 (J_{PtC} = 589.8 Hz, C), 167.4 (C), 163.4 (J_{PtC} = 53.3 Hz, C), 161.6 (J_{PtC} = 561.3 Hz, C), 150.1 (J_{PtC} = 36.7 Hz, C), 149.5 (C), 149.4 (C), 149.20 (CH), 146.4 (CH), 144.9 (J_{PtC} = 891.3 Hz, C), 144.6 (C), 143.1 (J_{PtC} = 891.3 Hz, C), 140.8 (C), 139.3 (CH), 138.4 (CH), 135.0 (J_{PtC} = 38.3 Hz, CH), 132.3 (J_{PtC} = 57.1 Hz, CH), 131.6 (J_{PtC} = 53.1 Hz, CH), 131.3 (J_{PtC} = 40.0 Hz, CH), 131.3 (J_{PtC} = 36.7 Hz, C), 130.3 (J_{PtC} = 36.3 Hz, CH), 127.4 (CH), 125.2 (CH), 125.1 (CH), 124.1 (CH), 123.9 (CH), 123.4 (CH), 123.3 (CH), 121.5 (CH), 121.0 (CH), 120.8 (CH), 120.73 (CH), 120.67 (CH), 120.59 (CH), 34.8 (C), 34.7 (C), 31.7 (CH_3), 31.6 (CH_3). Elemental analysis calcd (%) for $C_{42}H_{40}N_2Pt$: C 65.70, H 5.25, N 3.65; found: C 65.74, H 5.23, N 3.66.

[Pt(ppy)$_2$(bph)] (2ab). White solid. Yield: 58%. ^{1}H NMR (400.9 MHz, CD_2Cl_2): δ 8.09-7.96 (m, 3H), 7.89-7.79 (m, 3H), 7.75 (dd, J = 7.7, 1.4 Hz, 1H), 7.61-7.54 (m, 2H), 7.51 (dd with satellites, J_{PtH} = 7.1

Hz, J_{HH} = 1.3 Hz, 1H), 7.19-6.93 (m, 8H), 6.87-6.73 (m, 3H), 6.73-6.50 (m, 2H), 6.35 (dd with satellites, J_{PtH} = 26.9 Hz, J_{HH} = 7.2, 1.1 Hz, 1H). ^{13}C NMR (151 MHz, CD_2Cl_2): δ 169.3 (J_{PtC} = 589.1 Hz, C), 167.1 (J_{PtC} = 23.1 Hz, C), 163.1 (J_{PtC} = 47.1 Hz, C), 162.1 (J_{PtC} = 561.9 Hz, C), 152.9 (J_{PtC} = 39.4 Hz, C), 152.9 (J_{PtC} = 60.9 Hz, C), 149.4 (CH), 146.3 (CH), 144.5 (J_{PtC} =884.0 Hz, C), 144.5 (C), 143.7 (J_{PtC} = 889.6 Hz, C), 140.7 (C), 139.4 (CH), 138.6 (CH), 134.7 (J_{PtC} = 39.4 Hz, CH), 133.1 (J_{PtC} = 33.4 Hz, CH), 132.2 (J_{PtC} = 57.0 Hz, CH), 131.6 (J_{PtC} = 62.0 Hz, CH), 131.5 (J_{PtC} = 36.0 Hz, CH), 131.2 (CH), 127.3 (J_{PtC} = 23.6 Hz, CH), 127.2 (J_{PtC} = 60.0 Hz, CH), 125.4 (J_{PtC} = 19.7 Hz, CH), 125.2 (J_{PtC} = 33.4 Hz, CH), 124.7 (CH), 124.6 (CH), 124.2 (CH), 124.0 (CH), 123.6 (CH), 123.5 (CH), 121.7 (J_{PtC} = 45.4 Hz, CH), 121.5 (J_{PtC} = 29.5 Hz, CH), 120.9 (CH), 120.8 (CH). Elemental analysis calcd (%) for $C_{34}H_{24}N_2Pt$: C 66.40, H 5.57, N 3.52; found: C 66.66, H 5.52, N 3.57.

[Pt(ppy)$_2$(dFbph)] (2ac). White solid. Yield: 60%. ^{1}H NMR (400.9 MHz, CD_2Cl_2): δ 8.09-7.93 (m, 3H), 7.93-7.79 (m, 3H), 7.76 (dd, J = 7.8, 1.6 Hz, 1H), 7.55 (dd with satellites, J_{PtH} = 10.0 Hz, J_{HH} = 5.7, 1.6 Hz, 1H), 7.51-7.44 (m, 1H), 7.44-7.35 (m, 1H), 7.22-6.95 (m, 6H), 6.86-6.61 (m, 4H), 6.27 (dd with satellites, J_{PtH} = 54.1 Hz, J_{FH} = 10.0, J_{HH} = 2.8 Hz, 1H), 6.05 (dd with satellites, J_{PtH} = 22.6 Hz, J_{FH} = 8.5, J_{HH} = 2.8 Hz, 1H). ^{19}F NMR (282.4 MHz, CD_2Cl_2): δ –116.9 (m, 1F), –117.3 (m, 1F). ^{13}C NMR (151 MHz, CD_2Cl_2): δ 167.2 (J_{PtC} = 589.5 Hz, C), 166.9 (J_{PtC} = 25.2 Hz, C), 164.3 (J_{PtC} = 561.9 Hz, C), 163.1 (J_{PtC} = 52.1 Hz, C), 162.6 (d, J_{CF} = 250.3 Hz, C), 161.3 (J_{CF} = 147.3 Hz, C), 149.3 (CH), 148.2 (J_{PtC} = 35.3 Hz, C), 147.2 (J_{PtC} = 60.5 Hz, C), 146.2 (CH), 144.3 (C), 144.2 (C), 143.7 (J_{PtC} = 869.1 Hz, C), 140.6 (C), 139.7 (CH), 139.0 (CH), 134.5 (J_{PtC} = 38.3 Hz, CH), 132.1 (J_{PtC} = 54.5 Hz, CH), 131.9 (CH), 131.8 (J_{PtC} = 38.4 Hz, CH), 125.6 (J_{PtC} = 16.2 Hz, CH), 125.3 (J_{PtC} = 33.0 Hz, CH), 124.6 (CH), 124.1 (CH), 123.8 (CH), 122.7-122.1 (m, CH), 121.1 (CH), 121.0 (CH), 119.6 (J_{PtC} = 32.3 Hz, CH), 119.4 (J_{PtC} = 39.5 Hz, CH), 117.6 (CH), 117.5 (CH), 111.0 (CH). Elemental analysis calcd (%) for $C_{34}H_{22}F_2N_2Pt$: C 59.04, H 3.21, N 4.05; found: C 59.10, H 3.29, N 4.00.

[Pt(tpy)$_2$(dbbph)] (2ba). White solid. Yield: 52%. ^{1}H NMR (400.9 MHz, CD_2Cl_2): δ 7.99 (d, J = 8.2 Hz, 1H), 7.94 (d, J = 8.1, Hz, 1H), 7.90 (ddd with satellites, J_{PtH} = 13.0 Hz, J_{HH} = 5.6, 1.7, 0.8 Hz, 1H), 7.86-7.74 (m, 2H), 7.70 (d, J = 8.0 Hz, 1H), 7.66-7.59 (m, 1H), 7.57 (ddd with satellites, J_{PtH} = 8.8 Hz, J_{HH} = 5.6, 1.7, 0.8 Hz, 1H), 7.40 (d, J = 8.0, 1H), 7.34-7.29 (m, 1H), 7.11-6.88 (m, 6H), 6.76 (s with satellites, J_{PtH} = 25.5 Hz, 1H), 6.71 (d with satellites, J_{PtH} = 50.7 Hz, J_{HH} = 2.2 Hz, 1H), 6.57 (s with satellites, J_{PtH} = 50.0 Hz, 1H), 6.26 (d with satellites, J_{PtH} = 20.1 Hz, J_{HH} = 2.1 Hz, 1H), 2.18 (s, 3H), 2.15 (s, 3H), 1.07 (s, 9H), 1.04 (s, 9H). ^{13}C NMR (151 MHz, CD_2Cl_2): δ 170.0 (J_{PtC} = 597.5 Hz, C), 167.6 (J_{PtC} = 27.1 Hz, C), 163.6 (J_{PtC} = 45.4 Hz, C), 161.8 (J_{PtC} = 563.4 Hz, C), 150.1 (J_{PtC} = 38.5 Hz, C), 149.4 (J_{PtC} = 64.0 Hz, C), 149.3 (2 C), 149.0 (J_{PtC} = 13.5 Hz, CH), 146.2 (CH), 145.0 (J_{PtC} = 887.0 Hz, C), 143.2 (J_{PtC} = 887.0 Hz, C), 142.0 (C), 141.9 (J_{PtC} = 63.4 Hz, C), 141.3 (J_{PtC} = 34.1 Hz, C), 139.1 (CH), 138.3 (CH), 138.2 (C), 135.7 (J_{PtC} = 38.5 Hz, CH), 133.0 (J_{PtC} = 59.2 Hz, CH), 130.5 (J_{PtC} = 36.0 Hz, CH), 127.4 (J_{PtC} = 15.8 Hz, CH), 125.1 (J_{PtC} = 19.8 Hz, CH), 125.0 (CH), 124.9 (J_{PtC} = 35.7 Hz, CH), 124.2 (CH), 123.2 (J_{PtC} = 15.8 Hz, CH), 122.8 (CH), 121.3 (CH), 120.8 (CH), 120.58 (CH), 120.51 (CH), 120.4 (CH), 120.3 (CH), 34.74 (C), 34.71 (C), 31.7 ($3CH_3$), 31.6 ($3CH_3$), 22.2 (CH_3), 22.0 (CH_3). Elemental analysis calcd (%) for $C_{44}H_{44}N_2Pt$: C 66.40, H 5.57, N 3.52; found: C 66.66, H 5.52, N 3.57.

[Pt(tpy)$_2$(bph)] (2bb). White solid. Yield: 80%. ^{1}H NMR (400.9 MHz, CD_2Cl_2): δ 8.06-7.88 (m, 3H), 7.84-7.76 (m, 2H), 7.70 (d, J = 7.9 Hz, 1H), 7.67-7.60 (m, 1H), 7.56 (dd, J = 7.6, 1.4 Hz, 1H), 7.53-7.43 (m, 2H), 7.10-6.87 (m, 6H), 6.81-6.73 (m, 1H), 6.68 (s with satellites, J_{PtH} = 12.8 Hz, 1H), 6.66-6.61 (m, 2H), 6.57 (s with satellites, J_{PtH} = 24.8 Hz, 1H), 6.32 (d with satellites, J_{PtH} = 27.2, J_{HH} = 7.3, 1 Hz 1H), 2.15 (s, 3H), 2.15 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2): δ 169.5 (J_{PtC} = 588.4 Hz, C), 167.2 (C), 163.2 (C), 162.4 (J_{PtC} = 555.0 Hz, C), 152.9 (J_{PtC} = 34.0 Hz, C), 152.2 (J_{PtC}= 60.8 Hz, C), 149.1 (J_{PtC} =

35.3 Hz, CH), 152.6 (J_{PtC} = 60.9 Hz, CH), 149.1 (J_{PtC} = 12.5 Hz, CH), 146.1 (CH), 144.5 (J_{PtC} = 873.0 Hz, C), 143.7 (J_{PtC} = 893.0 Hz, C), 142.0 (J_{PtC} = 63.7 Hz, C), 141.8 (C), 141.5(J_{PtC} = 34.6 Hz, C) 139.3 (CH), 138.4 (CH), 138.0 (C), 135.4 (J_{PtC} = 38.1 Hz, CH), 133.0 (J_{PtC} = 31.8 Hz, CH), 132.7 (J_{PtC} = 56.6 Hz, CH), 131.2 (J_{PtC} = 13.2 Hz, CH), 127.3 (J_{PtC} = 25.4 Hz, CH), 127.1 (J_{PtC} = 58.4 Hz, CH), 125.3 (CH), 125.2 (CH), 125.0 (J_{PtC} = 35.1 Hz, CH), 124.6 (CH), 124.5 (CH), 123.4 (CH), 123.0 (CH), 121.7 (J_{PtC} = 43.2 Hz, CH), 121.5 (J_{PtC} = 27.6 Hz, CH), 120.5 (CH), 120.4 (CH), 22.2 (CH_3), 22.1 (CH_3). Elemental analysis calcd (%) for $C_{36}H_{28}N_2Pt$: C 63.24, H 4.13, N 4.10; found: C 63.22, H 4.14, N 4.01.

[Pt(tpy)$_2$(dFbph)] (2bc). White solid. Yield: 72%. ^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.02 (d, J_{HH} = 8.1 Hz, 1H), 8.00 (d, J_{HH} = 8.1 Hz, 1H), 7.93 (d with satellites, J_{PtH} = 12.7, J_{HH} = 6.1 Hz, 1H), 7.89-7.82 (m, 2H), 7.71 (dd, J_{HH} = 8.0, 2.3 Hz, 1H), 7.68-7.61 (m, 1H), 7.55-7.48 (m, 2H), 7.42 (dd, J_{HH} = 8.5 Hz, J_{FH} = 5.8 Hz, 1H), 7.11-7.03 (m, 2H), 7.03-6.97 (m, 2H), 6.77-6.70 (m, 2H), 6.66 (s with satellites, J_{PtH} = 28.0 Hz, 1H), 6.58 (s with satellites, J_{PtH} = 48.0 Hz, 1H), 6.30 (dd with satellites, J_{PtH} = 54.4 Hz, J_{FH} = 9.9, J_{HH} = 2.8 Hz, 1H), 6.02 (dd with satellites, J_{PtH} = 22.5 Hz, J_{FH} = 8.4, J_{HH} = 2.6 Hz, 1H), 2.18 (s, 3H), 2.16 (s, 3H). ^{19}F NMR (282.4 MHz, CD_2Cl_2): δ –117.1 (m, 1F), –117.4 (m, 1F). ^{13}C NMR (151 MHz, CD_2Cl_2): δ 166.7 (C), 166.4 (J_{PtC} = 28.4 Hz, C), 164.1 (C), 162.7 (C), 162.3 (d, J_{CF} = 248.7 Hz, C), 160.8 (d, J_{CF} = 248.7 Hz, C), 148.5 (CH), 147.6 (C), 146.7 (C), 145.4 (CH), 143.74 (C), 143.72 (C), 143.2 (C), 141.7 (J_{PtC} = 64.6 Hz, C), 141.3 (C), 141.1 (C), 138.9 (CH), 138.2 (CH), 137.4 (C), 134.7 (J_{PtC} = 40.2 Hz, CH), 132.0 (J_{PtC} = 57.5 Hz, CH), 125.0 (CH), 124.9 (J_{PtC} = 18.1 Hz, CH), 124.5 (J_{PtC} = 33.1 Hz, CH), 124.3 (CH), 122.9 (CH), 122.6 (CH), 122.5 - 121.1 (m, CH), 120.1 (CH), 120.06 (CH), 118.9 (CH), 118.8 (CH), 116.9 (CH), 116.8 (CH), 110.2 (t, J_{CF} = 21.7 Hz, CH), 21.6 (CH_3), 21.5 (CH_3). Elemental analysis calcd (%) for $C_{36}H_{26}F_2N_2Pt$: C 60.08, H 3.64, N 3.89; found: C 60.21, H 3.59, N 3.66.

[Pt(thpy)$_2$(dbbph)] (2ca). White solid. Yield: 66%. ^{1}H NMR (400.9 MHz, CD_2Cl_2): δ 7.82-7.56 (m, 6H), 7.41-7.34 (m, 2H), 7.34-7.24 (m, 2H), 7.06 (dd, J = 8.03, 2.1 Hz, 1H), 7.03-6.95 (m, 2H), 6.91-6.85 (m, 1H), 6.64 (d with satellites, J_{PtH} = 52.5 Hz, J_{HH} = 2.3 Hz, 1H), 6.59 (d with satellites, J_{PtH} = 13.7 Hz, J_{HH} = 4.8 Hz, 1H), 6.45 (d with satellites, J_{PtH} = 22.0 Hz, J_{HH} = 2.3 Hz, 1H), 6.35 (d with satellites, J_{PtH} = 22.0 Hz, J_{HH} = 4.8 Hz, 1H), 1.10 (s, 9H), 1.09 (s, 9H). ^{13}C NMR (151 MHz, CD_2Cl_2): δ 174.2 (J_{PtC} = 581.7 Hz, C), 162.7 (J_{PtC} = 18.4 Hz, C), 159.1 (J_{PtC} = 40.0 Hz, C), 158.4 (J_{PtC} = 589.2 Hz, C), 150.4 (J_{PtC} = 44.6 Hz, C), 149.7 (J_{PtC} = 26.3 Hz, C), 149.3 (C), 149.2 (J_{PtC} = 63.3 Hz, C) 149.11 (CH), 147.0 (CH), 142.0 (J_{PtC} = 913.2 Hz, C), 141.8 (C), 139.8 (CH), 138.8 (CH), 138.1 (J_{PtC} = 861.8 Hz, C), 134.1 (C), 134.0 (J_{PtC} = 54.7 Hz, CH), 131.4 (J_{PtC} = 72.8 Hz, CH), 131.2 (J_{PtC} = 39.6 Hz, CH), 129.9 (J_{PtC} = 37.8 Hz, CH), 128.6 (J_{PtC} = 74.5 Hz, CH), 127.7 (CH), 127.7 (CH), 121.4 (J_{PtC} = 14.8 Hz, CH), 121.3 (CH), 121.0 (CH), 120.43 (CH), 120.39 (CH), 119.6 (J_{PtC} = 13.3 Hz, CH), 119.5 (J_{PtC} = 12.0 Hz, CH), 34.9 (C), 34.8 (C), 31.73 (CH_3), 31.63 (CH_3). Elemental analysis calcd (%) for $C_{38}H_{36}N_2PtS_2$: C 58.82, H 4.65, N 3.59, S 8.22; found: C 58.72, H 4.77, N 3.47, S 8.12.

[Pt(thpy)$_2$(bph)] (2cb). Pale yellow solid. Yield: 40%. ^{1}H NMR (400.9 MHz, CD_2Cl_2): δ 7.82 (ddd with satellites, J_{PtH} = 16.0 Hz, J_{HH} = 5.6, 1.6, 0.8 Hz, 1H), 7.78-7.69 (m, 2H), 7.67-7.57 (m, 3H), 7.54 (dd, J = 7.6, 1.4 Hz, 1H), 7.48 (dd with satellites, J_{PtH} = 6.8 Hz, J_{HH} = 1.5 Hz, 1H), 7.34 (d with satellites, J_{PtH} = 14.6 Hz, J_{HH} = 4.7 Hz, 1H), 7.27 (d with satellites, J_{PtH} = 11.3 Hz, J_{HH} = 4.7 Hz, 1H), 7.10-6.92 (m, 3H), 6.91-6.77 (m, 2H), 6.72-6.58 (m, 2H), 6.52 (d with satellites, J_{PtH} = 8.9, J_{HH} = 4.5 Hz, 1H), 6.49 (dd with satellites, J_{PtH} = 8.9, J_{HH} = 7.3, 1.3 Hz, 1H), 6.35 (d with satellites, J_{PtH} = 20.2 Hz, J_{HH} = 4.7 Hz, 1H). ^{13}C NMR (151 MHz, CD_2Cl_2): δ 173.8 (J_{PtC} = 583.2 Hz, C), 162.5 (J_{PtC} = 17.8 Hz, C), 159.0 (J_{PtC} = 583.2 Hz, C), 158.8 (J_{PtC} = 38.8 Hz, C), 153.3 (J_{PtC} = 44.0 Hz, C), 152.0 (J_{PtC} = 62.3 Hz, C), 149.3 (CH), 146.8 (CH), 141.8 (C), 141.6 (J_{PtC} = 903.0 Hz, C), 140.0 (CH), 139.0 (CH), 138.6 (C),

133.9 (J_{PtC} = 32.8 Hz, CH), 133.8 (J_{PtC} = 55.1 Hz, CH), 131.4 (C), 131.2 (J_{PtC} = 92.0 Hz, CH), 130.1 (J_{PtC} = 36.8 Hz, CH), 128.8 (J_{PtC} = 73.5 Hz, CH), 127.5 (J_{PtC} = 24.0 Hz, CH), 126.9 (J_{PtC} = 55.2 Hz, CH), 125.0 (CH), 124.8 (CH), 121.54 (J_{PtC} = 891.3 Hz, CH), 121.46 (CH), 121.3 (CH), 121.2 (CH), 119.7 (CH), 119.63 (CH), 119.59 (CH). Elemental analysis calcd (%) for $C_{30}H_{20}N_2PtS_2$: C 53.97, H 3.02, N 4.20, S 9.60; found: C 53.88, H 3.28, N 4.15, S 9.73.

[Pt(thpy)$_2$(dFbph)] (2cc). White solid. Yield: 76%. ^{1}H NMR (300.1 MHz, CD_2Cl_2): δ 7.83-7.73 (m, 3H), 7.67-7.50 (m, 2H), 7.58 (d with satellites, J_{PtH} = 9.8 Hz, J_{HH} = 5.5 Hz, 1H), 7.48-7.43 (m, 1H), 7.40-7.34 (m, 2H), 7.31 (d with satellites, J_{PtH} = 15.0 Hz, J_{HH} = 4.8 Hz, 1H), 6.98 (t, J_{HH} = 6.9 Hz, 1H), 6.90 (t, J_{HH} = 6.9 Hz, 1H), 6.77-6.70 (m, 2H), 6.50 (d with satellites, J_{PtH} = 13.6 Hz, J_{HH} = 4.8 Hz, 1H), 6.38 (d with satellites, J_{PtH} = 20.4 Hz, J_{HH} = 4.8 Hz, 1H), 6.30 (dd with satellites, J_{PtH} = 55.1 Hz, J_{FH} = 9.5, J_{HH} = 2.8 Hz, 1H), 6.20 (dd with satellites, J_{PtH} = 24.3 Hz, J_{FH} = 8.4, J_{HH} = 2.8 Hz, 1H). ^{19}F NMR (282.4 MHz, CD_2Cl_2): δ –116.9 (m, 2F). ^{13}C NMR (151 MHz, CD_2Cl_2): δ 171.7 (J_{PtC} = 600.3 Hz, C), 162.6 (d, J_{CF} = 247.8 Hz, C), 161.9 (C), 161.8 (C), 161.1 (J_{PtC} = 600.0 Hz, C), 161.09 (d, J_{CF} = 247.8 Hz, C), 159.0 (C), 149.3 (CH), 148.7 (J_{PtC} = 42.4 Hz, C), 147.2 (J_{PtC} = 58.8 Hz, C), 146.8 (CH), 142.0 (C), 140.8 (C), 140.2 (CH), 139.4 (CH), 139.1 (C), 133.5 (J_{PtC} = 54.5 Hz, CH), 131.0 (J_{PtC} = 91.8 Hz, CH), 130.6 (J_{PtC} = 34.6 Hz, CH), 129.2 (J_{PtC} = 75.3 Hz, CH), 122.2 (CH), 121.7 (CH), 121.5 (CH), 120.5 (J_{PtC} = 45.2 Hz, CH), 120.4 (J_{PtC} = 45.2 Hz, CH), 119.9 (CH), 119.85 (CH), 117.8 (CH), 117.7 (CH), 111.2 (CH). Elemental analysis calcd (%) for $C_{30}H_{18}F_2N_2S_2Pt$: C 51.21, H 2.58, N 3.98; found: C 51.11, H 2.57, N 3.84.

[Pt(tpy)$_2$(dFbphI-κ^2*C,C*)] (2bc'). To a suspension of **1b** (100 mg, 0.19 mmol) in MeCN (10 mL) was added 3,7-difluorodibenzo-5-iodolium triflate (88 mg, 0.19 mmol) and the mixture was stirred and irradiated under N_2 with blue light until a pale yellow solution was obtained (2 h). γ-Picoline (55 μL, 0.57 mmol mmol) was then added and the solution was stirred at 50 C for 12 h, whereupon a white solid gradually precipitated, which was collected by filtration, washed with MeCN (3 × 2 mL) and vacuum-dried to give **2bc'**. Yield: 64%. ^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.76 (dd, J_{FH} = 6.0 Hz, J_{HH} = 8.9 Hz, 1H), 8.00 (d, J_{HH} = 8.4 Hz, 1H), 7.97 (d, J_{HH} = 8.2 Hz, 1H), 7.86-7.80 (m, 3H), 7.71 (d, J_{HH} = 8.0 Hz, 1H), 7.65 (d, J_{FH} = 8.0 Hz, 1H), 7.46-7.38 (m, 2H), 7.08-7.02 (m, 2H), 7.01-6.95 (m, 2H), 6.79 (dt, J = 8.7, 2.9 Hz, 1H), 6.58 (s with satellites, J_{PtH} = 26.3 Hz, 1H), 6.44 (s with satellites, J_{PtH} = 48.6 Hz, 1H), 6.40 (dd with satellites, J_{PtH} = 57.0 Hz, J_{FH} = 9.8, J_{HH} = 2.6 Hz, 1H), 6.11 (d with satellites, J_{PtH} = 23.8 Hz, J_{FH} = 7.1 Hz, J_{HH} = 2.6 Hz, 1H), 2.18 (s, 3H), 2.14 (s, 3H). ^{19}F NMR (282.4 MHz, CD_2Cl_2): δ –115.8 (m, 1F), –117.1 (m, 1F). ^{13}C NMR (151 MHz, CD_2Cl_2): δ 168.2 (J_{PtC} = 545.0 Hz, C), 166.93 (J_{PtC} = 605.5 Hz, C), 166.86 (C), 163.1 (J_{PtC} = 49.4 Hz, C), 161.7 (d, J_{CF} = 245.6 Hz, C), 160.4 (d, J_{CF} = 255.1 Hz, C), 148.9 (CH), 147.7 (J_{PtC} = 30.5 Hz, C), 146.7 (J_{PtC} = 71.6 Hz, C), 146.2 (C), 145.9 (CH), 143.6 (J_{PtC} = 863.7 Hz, C), 142.5 (J_{PtC} = 60.9 Hz, C), 142.1 (J_{PtC} = 38.0 Hz, C), 141.4 (C), 139.7 (CH), 138.9 (CH), 137.9 (C), 134.9 (J_{PtC} = 37.9 Hz, CH), 132.5 (J_{PtC} = 56.8 Hz, CH), 127.5 (J_{PtC} = 51.3 Hz, J_{CF} = 10.5 Hz, CH), 125.8 (CH), 125.5 (CH), 125.3 (CH), 125.27 (CH), 125.1 (CH), 123.7 (CH), 123.4 (CH), 120.82 (CH), 120.78 (CH), 119.7 (d, J_{PtC} = 49.3 Hz, J_{CF} = 19.3 Hz, CH), 117.3 (J_{CF} = 14.1 Hz, CH), 109.1 (J_{CF} = 20.3 Hz, CH), 89.9 (J_{PtC} = 45.7 Hz, J_{CF} = 5.3 Hz, C), 22.2 (CH_3), 22.1 (CH_3). Elemental analysis calcd (%) for $C_{36}H_{25}F_2IN_2Pt$: C 51.14, H 2.98, N 3.31; found: C 50.99, H 3.25, N 3.42.

[Pt(tpy)$_2$(dFbphI-κ^2*C,I*)]OTf (3bc). To a suspension of **1b** (50 mg, 0.09 mmol) in MeCN (10 mL) was added 3,7-difluorodibenzo-5-iodolium triflate (44 mg, 0.09 mmol) and the suspension was irradiated with blue light until a pale yellow solution was obtained (4 h). The solvent was evaporated under reduced pressure and the residue was treated with CH_2Cl_2 (1 mL) and Et_2O (5 mL) to give a pale brown precipitate, which was separated by filtration. The filtrate was evaporated under reduced pressure and

the residue was treated with CH_2Cl_2 (1 mL) and pentane (20 mL) to give a pale yellow precipitate, which was collected by filtration and vacuum-dried to give **3bc**. Yield: 50%. ^{1}H NMR (600 MHz, CD_2Cl_2): δ 9.25 (d, J_{HH} = 5.3 Hz, 1H), 8.30 (d, J_{HH} = 8.2 Hz, 1H), 8.25 (dt, J_{HH} = 7.8, 1.5 Hz, 1H), 7.91 (d, J_{HH} = 8.0 Hz, 1H), 7.86 (dt, J = 7.3, 1.5 Hz, 1H), 7.78 (d with satellites, J_{PtH} = 22.5, J_{HH} = 7.8 Hz, 1H), 7.62-7.56 (m, 2H), 7.50 (d, J_{HH} = 8.0 Hz, 1H), 7.40 (d, J_{PtH} = 10.7 Hz, J_{HH} = 5.2 Hz, 1H), 7.35-7.30 (m, 1H), 7.22 (dt, J = 8.3, 2.7 Hz, 1H), 7.13-7.10 (m, 1H), 7.09 (dd, J_{FH} = 7.3, J_{HH} = 2.7 Hz, 1H), 7.05 (d, J_{HH} = 7.7 Hz, 1H), 6.93 (d, J_{HH} = 7.9 Hz, 1H), 6.89 (m, 1H), 6.64 (s with satellites, J_{PtH} = 40.2 Hz, 1H), 6.27 (s with satellites, J_{PtH} = 64.8 Hz, 1H), 6.14 (dd with satellites, J_{PtH} = 60.0 Hz, J_{FH} = 10.9, J_{HH} = 2.7 Hz, 1H), 2.09 (s, 3H), 2.02 (s, 3H). ^{19}F NMR (282.4 MHz, CD_2Cl_2): δ –78.9 (s, 3F), –114.5 (m, 1F), –115.8 (m, 1F). ^{13}C NMR (151 MHz, CD_2Cl_2): δ 162.9 (C), 161.7 (J_{PtC} = 150.8 Hz, C), 161.2 (J_{PtC} = 251.0 Hz, C), 160.4 (J_{PtC} = 61.8 Hz, C), 160 (C), 159.3 (J_{PtC} = 47.7 Hz, C), 152.8 (CH), 149.1 (CH), 146.6 (C), 146.1 (J_{PtC} = 28.1 Hz, C), 143 (C), 142.7 (C), 141.8 (C), 141.5 (CH), 141.0 (CH), 140.9 (C), 139.0 (C), 136.4 (C), 135.9 (J_{PtC} = 42.2 Hz, CH), 135.3 (CH), 135.2 (CH), 133.7 (CH), 133.6 (CH), 132.2 (J_{PtC} = 59.3 Hz, CH), 128.5 (CH), 127.4 (CH), 126.9 (CH), 124.8 (CH), 122.8 (CH), 122.1 (CH), 121.9 (CH), 120.9 (CH), 117.9 (CH), 113.9 (CH), 101.3 (C), 22.2 (CH_3), 22.1 (CH_3). Elemental analysis calcd (%) for $C_{37}H_{27}F_5IN_2O_3PtS$: C 44.63, H 2.63, N 2.81, S 3.22; found: C 44.92, H 2.68, N 2.81, S 3.02.

1.4. X-ray structure determinations

Single crystals of **2ba**·0.5CH_2Cl_2, **2bc'**, and **3bc**·Et_2O suitable for X-ray diffraction were obtained by slow diffusion of Et_2O into solutions of the complexes in CH_2Cl_2. The data were collected on a Bruker D8 QUEST diffractometer with monochromated Mo-*K*α radiation performing *φ* and *ω* scans. The structures were solved by direct methods and refined anisotropically on F^2 using the program SHELXL-2018 (G. M. Sheldrick, University of Göttingen).[5,6] Numerical details are given in Table S1. Methyl hydrogens were included as part of rigid idealized methyl groups allowed to rotate but not tip; other hydrogens were included using a riding model. *Special features of refinement:* In the case of **2ba**·0.5CH_2Cl_2, there are two independent molecules of the complex and one resolved CH_2Cl_2 molecule in the asymmetric unit; additionally, there is a poorly-resolved region of residual electron density that could not be adequately modelled and was "removed" using the program SQUEEZE,[7] which is part of the PLATON system; the void volume per cell was 325 Å^3, with a void electron count per cell of 9; this additional solvent was not taken into account when calculating derived parameters such as the formula weight, because its nature was uncertain.

Table S1. Crystallographic data for **2ba**·0.5CH_2Cl_2, **2bc'** and **3bc**·Et_2O.

	2ba·0.5CH_2Cl_2	**2bc'**	**3bc**·Et_2O
formula	$C_{44.5}H_{45}ClN_2Pt$	$C_{36}H_{25}F_2IN_2Pt$	$C_{41}H_{36}F_5IN_2O_4PtS$
fw	838.36	845.57	1069.77
T (K)	100(2)	100(2)	100(2)
λ (Å)	0.71073	0.71073	0.71073
cryst syst	Monoclinic	Orthorhombic	Monoclinic
space group	$P2_1/n$	Pbca	$P2_1/c$
a (Å)	10.9752(8) Å	17.1359(10)	16.2963(10)
b (Å)	29.683(2) Å	18.0068(10)	21.4916(13)
c (Å)	23.6145(16) Å	18.8414(11)	11.4378(7)
α (°)	90	90	90
β (°)	91.371(2)	90	101.459(2)
γ (°)	90	90	90
V (Å^3)	7690.8(10)	5813.8(6)	3926.1(4)
Z	8	8	4
ρ_{calcd} (Mg m^{-3})	1.448	1.932	1.810
μ (mm^{-1})	3.751	5.931	4.481
R1[a]	0.0268	0.0179	0.0355
wR2[b]	0.0593	0.0395	0.0817

[a]$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$ for reflections with $I > 2\sigma(I)$. [b]$wR2 = [\Sigma[w(F_o^2-F_c^2)^2/\Sigma[w(F_o^2)^2]]^{0.5}$ for all reflections; $w^{-1} = \sigma^2(F^2) + (aP)^2 + bP$, where $P = (2F_c^2 + F_o^2)/3$ and a and b are constants set by the program.

1.5. Photophysical characterization

Electronic absorption spectra were registered with a Perkin-Elmer Lambda 750S spectrophotometer. Excitation and emission spectra were recorded on a Jobin Yvon Fluorolog 3-22 spectrofluorometer with a 450 W xenon lamp, double-grating monochromators, and a TBX-04 photomultiplier. Measurements in solution were performed using 10 mm quartz fluorescence cells (298 K) or 5 mm quartz NMR tubes (77 K). A liquid nitrogen Dewar with quartz windows was employed for measurements at 77 K. Emission data in PMMA matrices were registered using quartz slides as sample holders. Emission lifetimes were measured using an IBH FluoroHub controller in MCS mode and the Fluorolog's FL-1040 phosphorimeter pulsed xenon lamp as excitation source; the estimated uncertainty is ±10% or better. Emission quantum yields (Φ) were measured using a Hamamatsu C11347 Absolute PL Quantum Yield Spectrometer; the estimated uncertainty is ±5% or better. All emission data were registered under rigorous exclusion of oxygen.

1.6. Computational methods

DFT calculations were carried out with the Gaussian 09 package,[8] using the hybrid B3LYP functional[9,10] and the 6-31G**[11,12] basis set for the light atoms, and the LANL2DZ[13] basis set and effective core potential for the Pt atom. Geometry optimizations were performed using "tight" convergence criteria and "ultrafine" integration grid. No symmetry restrictions were applied. Vertical excitation energies at the ground-state geometries were obtained from TDDFT calculations. Triplet-state geometries were optimized through spin-unrestricted DFT (UB3LYP), following a previously described methodology.[14] The solvent effect (CH_2Cl_2) was accounted for in all cases by using the integral equation formalism variant of the polarizable continuum solvation model (IEFPCM).[15] Frequency calculations were performed in all cases to confirm the optimized geometries as minima on the potential energy surface (zero imaginary frequencies). Natural spin densities were calculated using the NBO 5.9 program.[16]

2. NMR spectra of new compounds

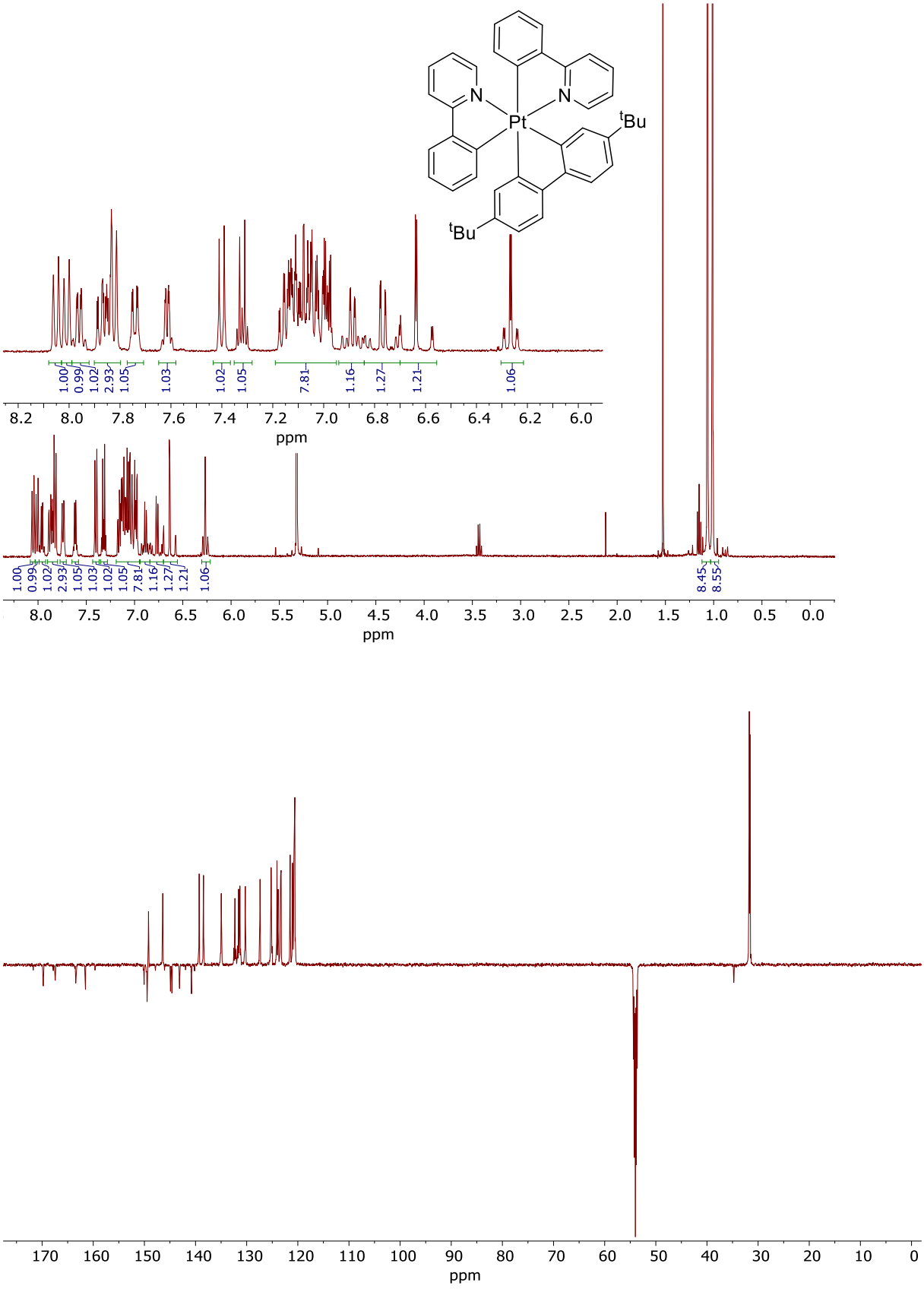


Figure S1. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2aa** (CD_2Cl_2, 400 and 151 MHz, respectively).

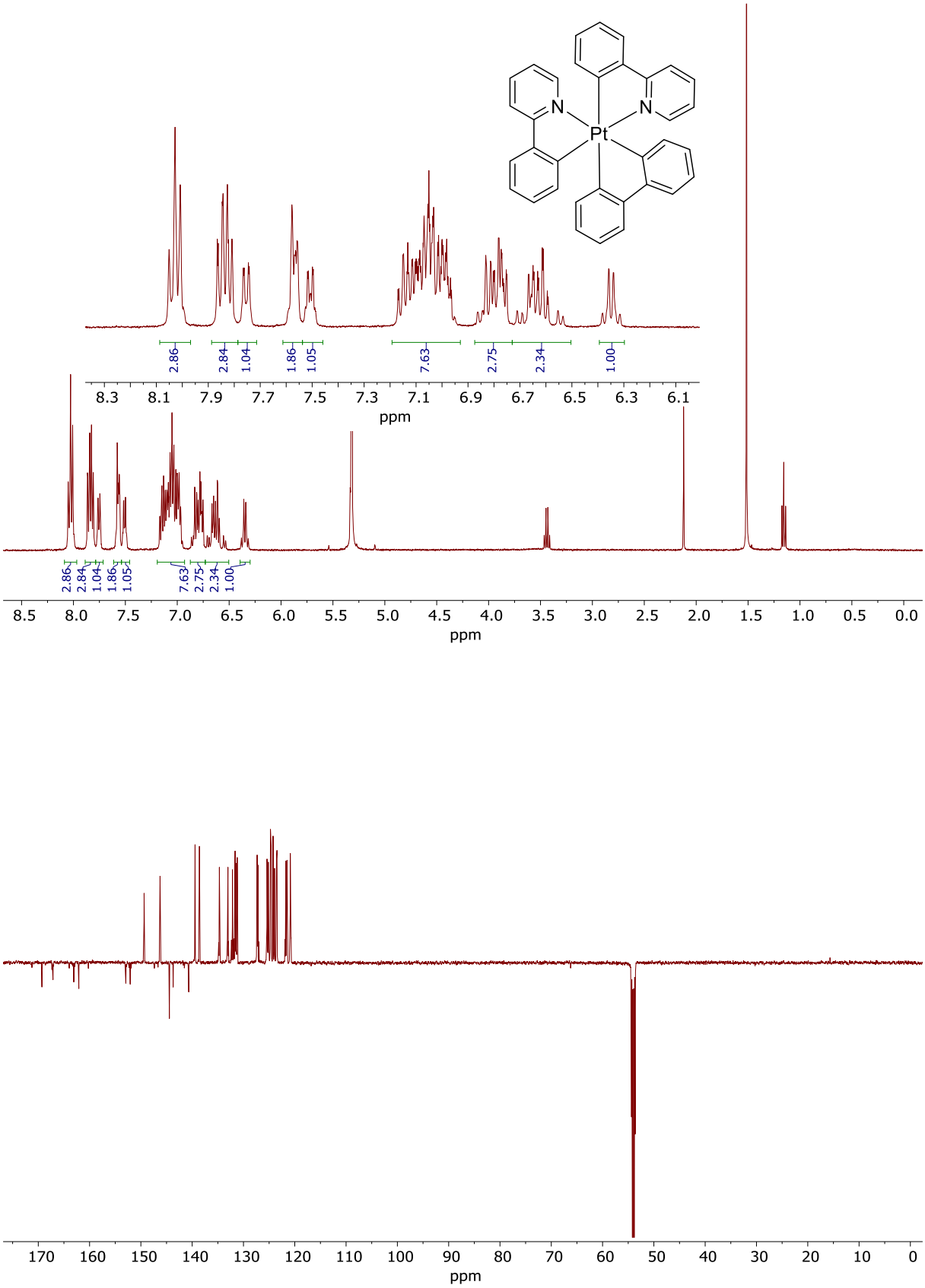


Figure S2. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2ab** (CD_2Cl_2, 400 and 151 MHz, respectively).

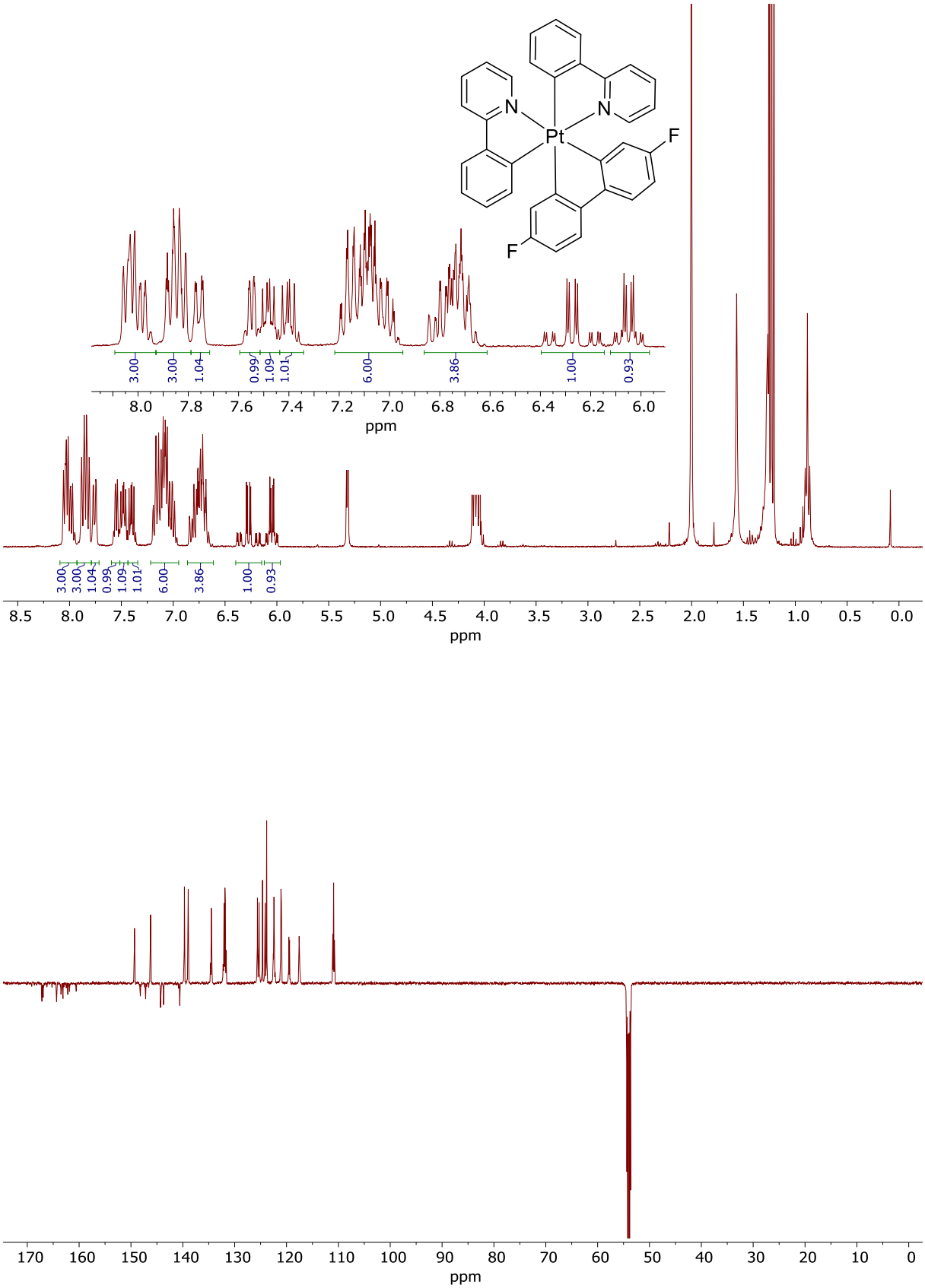


Figure S3. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2ac** (CD_2Cl_2, 400 and 151 MHz, respectively).

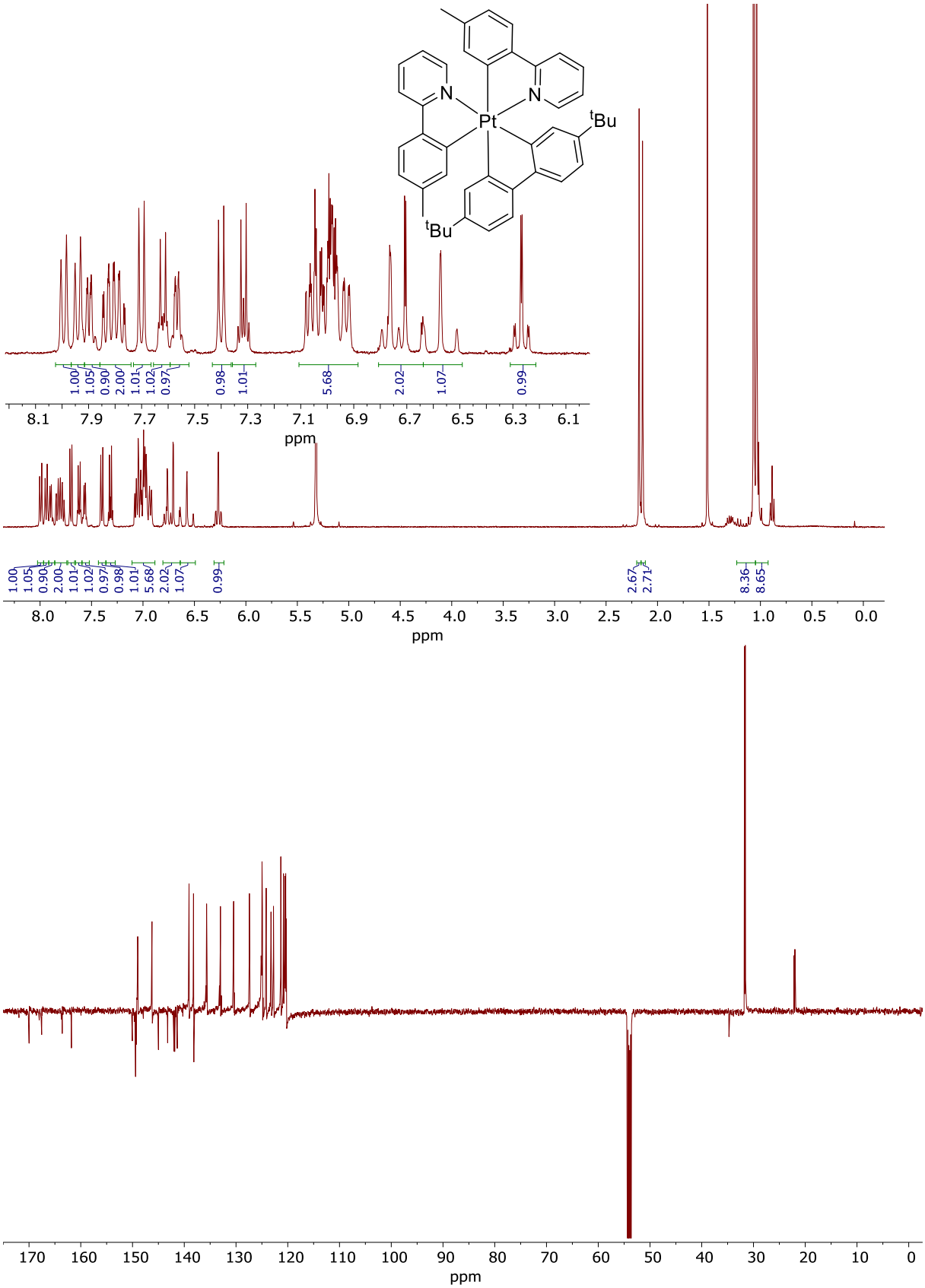


Figure S4. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2ba** (CD_2Cl_2, 400 and 151 MHz, respectively).

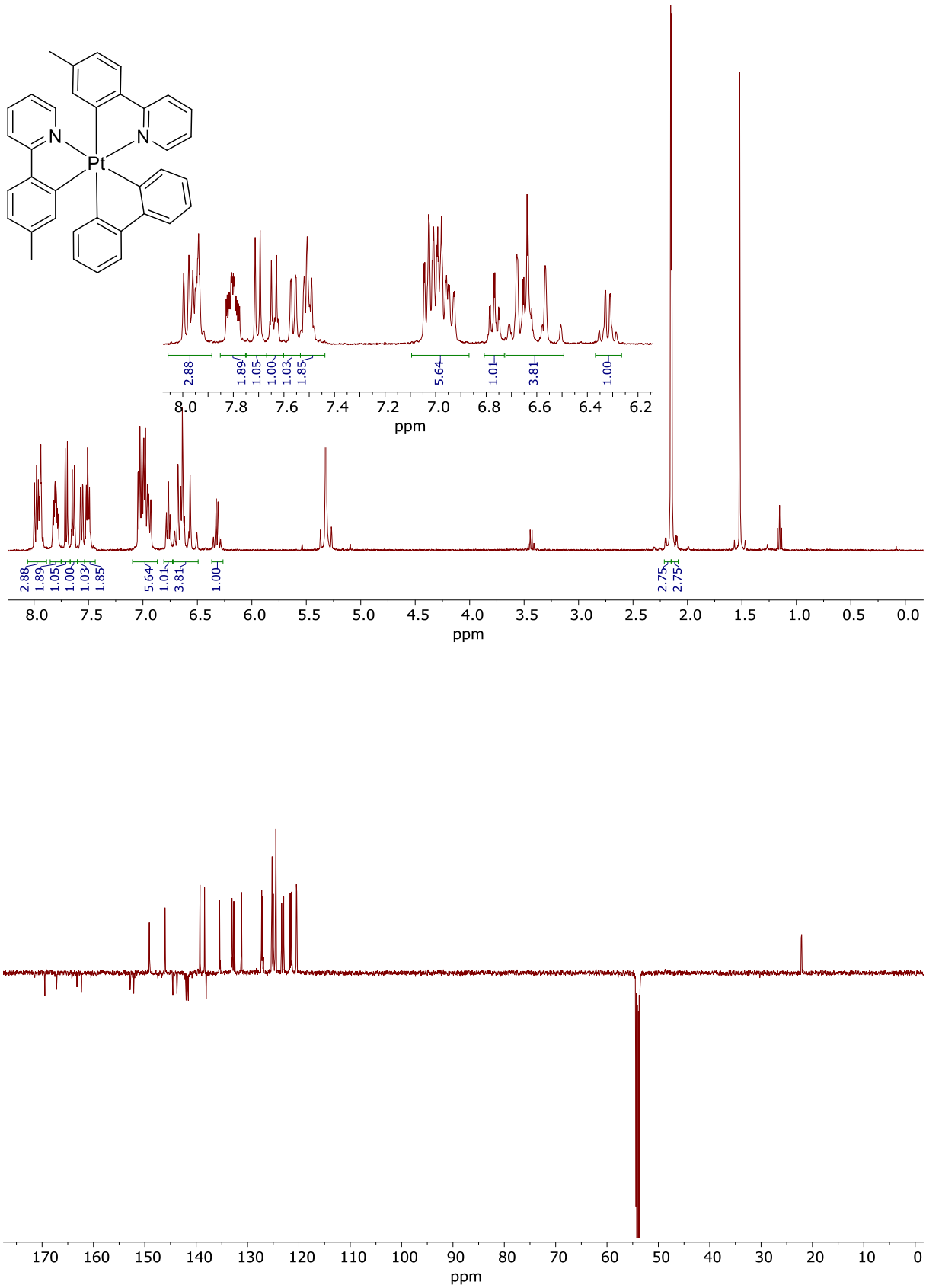


Figure S5. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2bb** (CD_2Cl_2, 400 and 151 MHz, respectively).

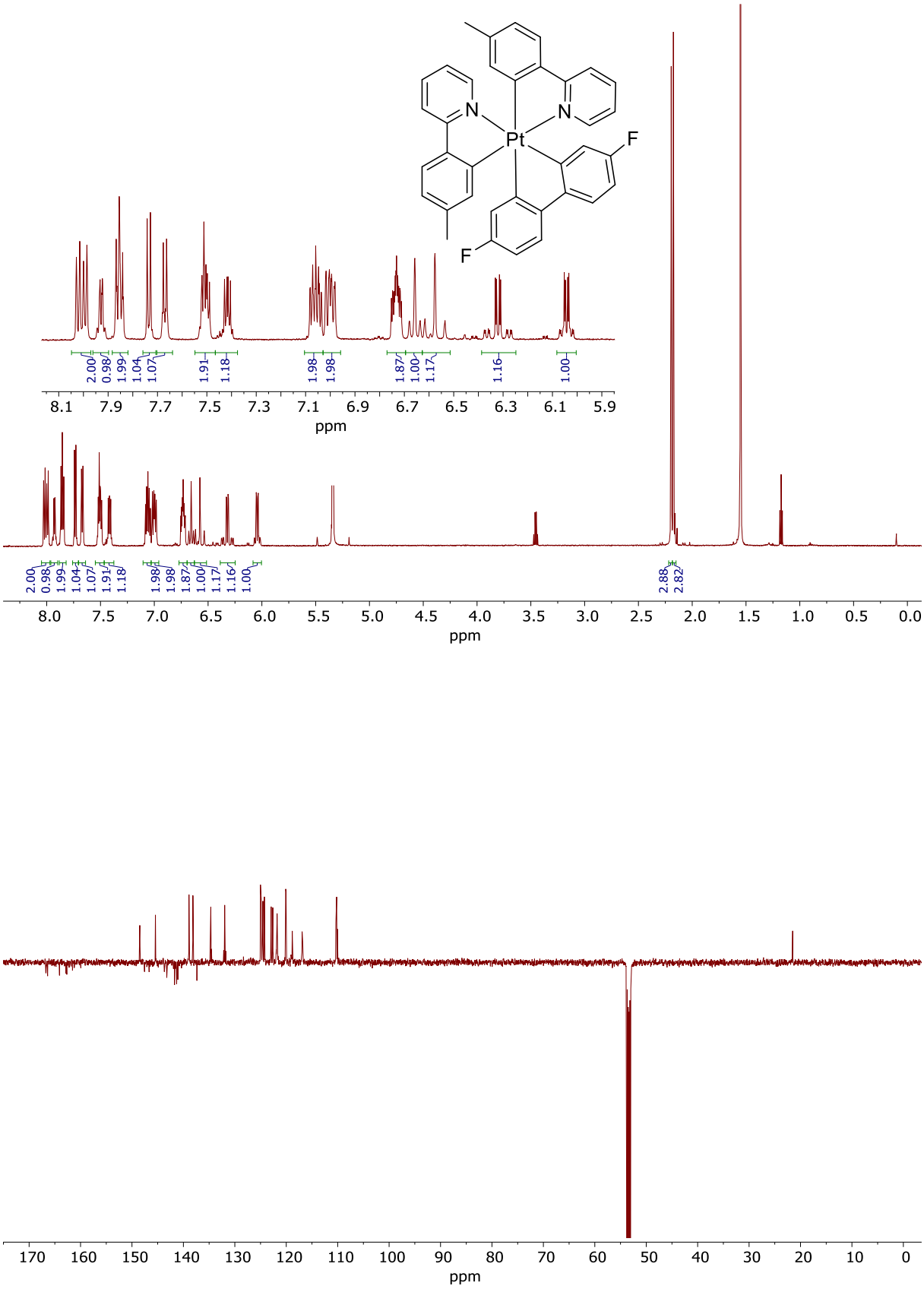


Figure S6. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2bc** (CD_2Cl_2, 600 and 151 MHz, respectively).

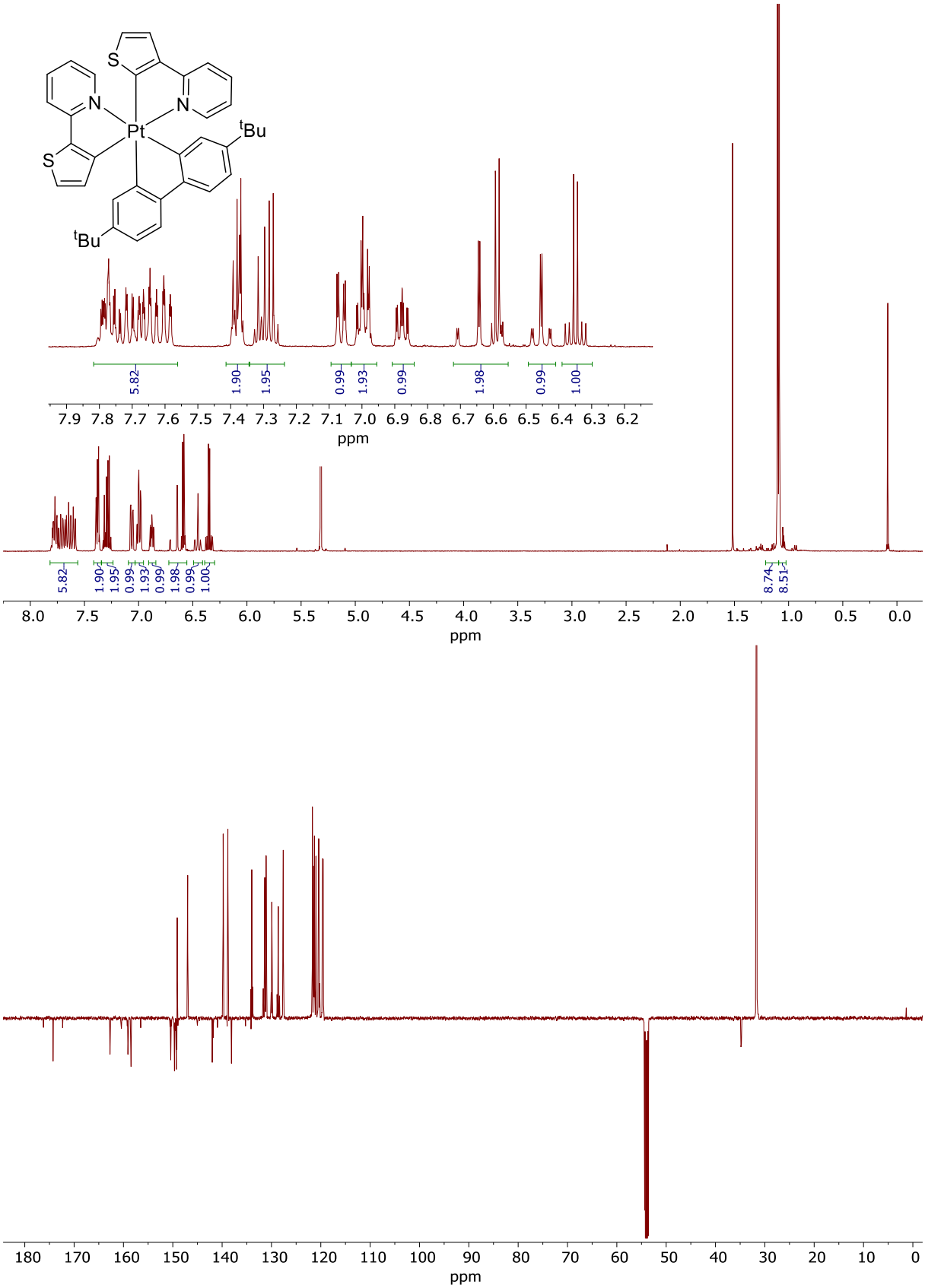


Figure S7. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2ca** (CD_2Cl_2, 400 and 151 MHz, respectively).

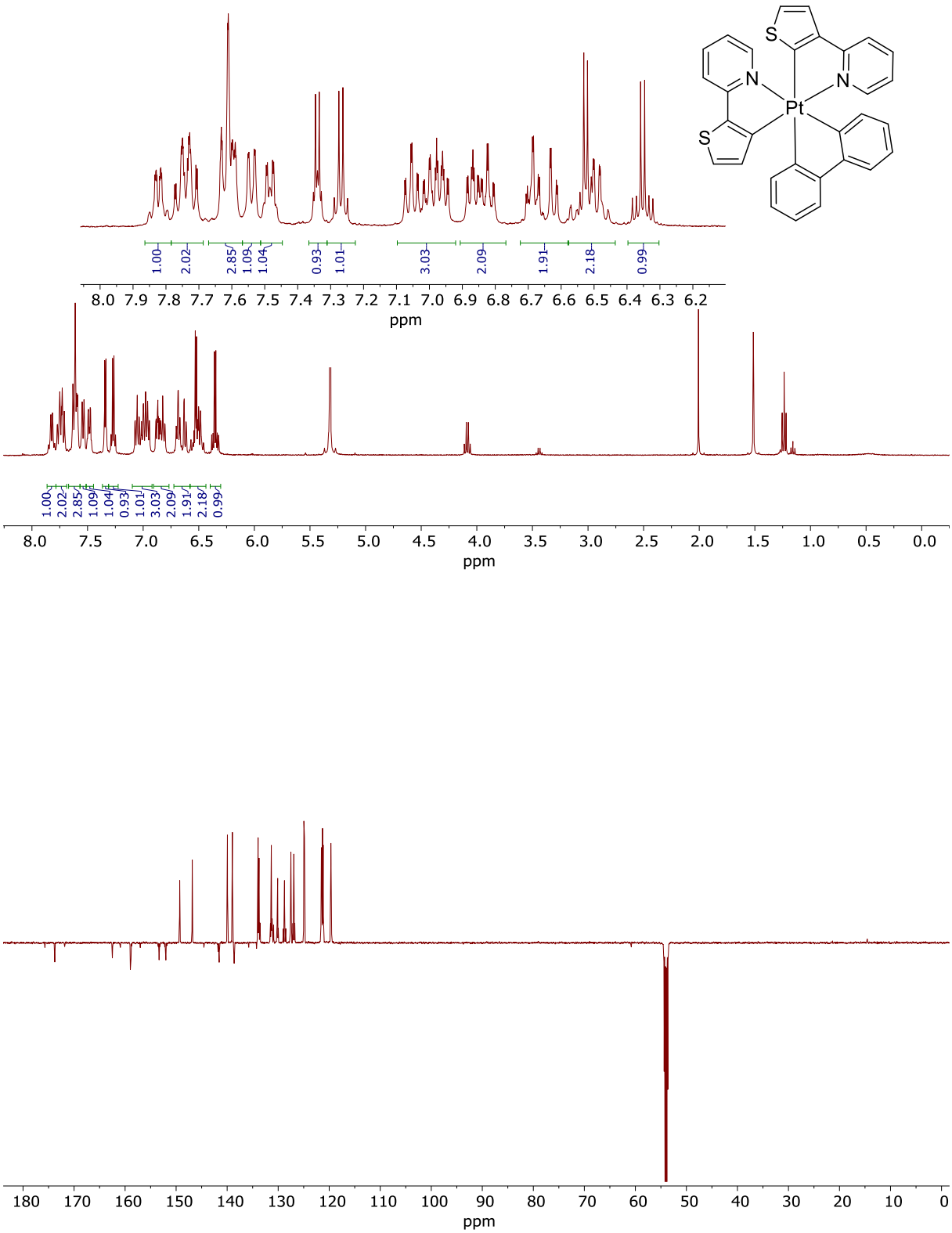


Figure S8. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2cb** (CD_2Cl_2, 400 and 151 MHz, respectively).

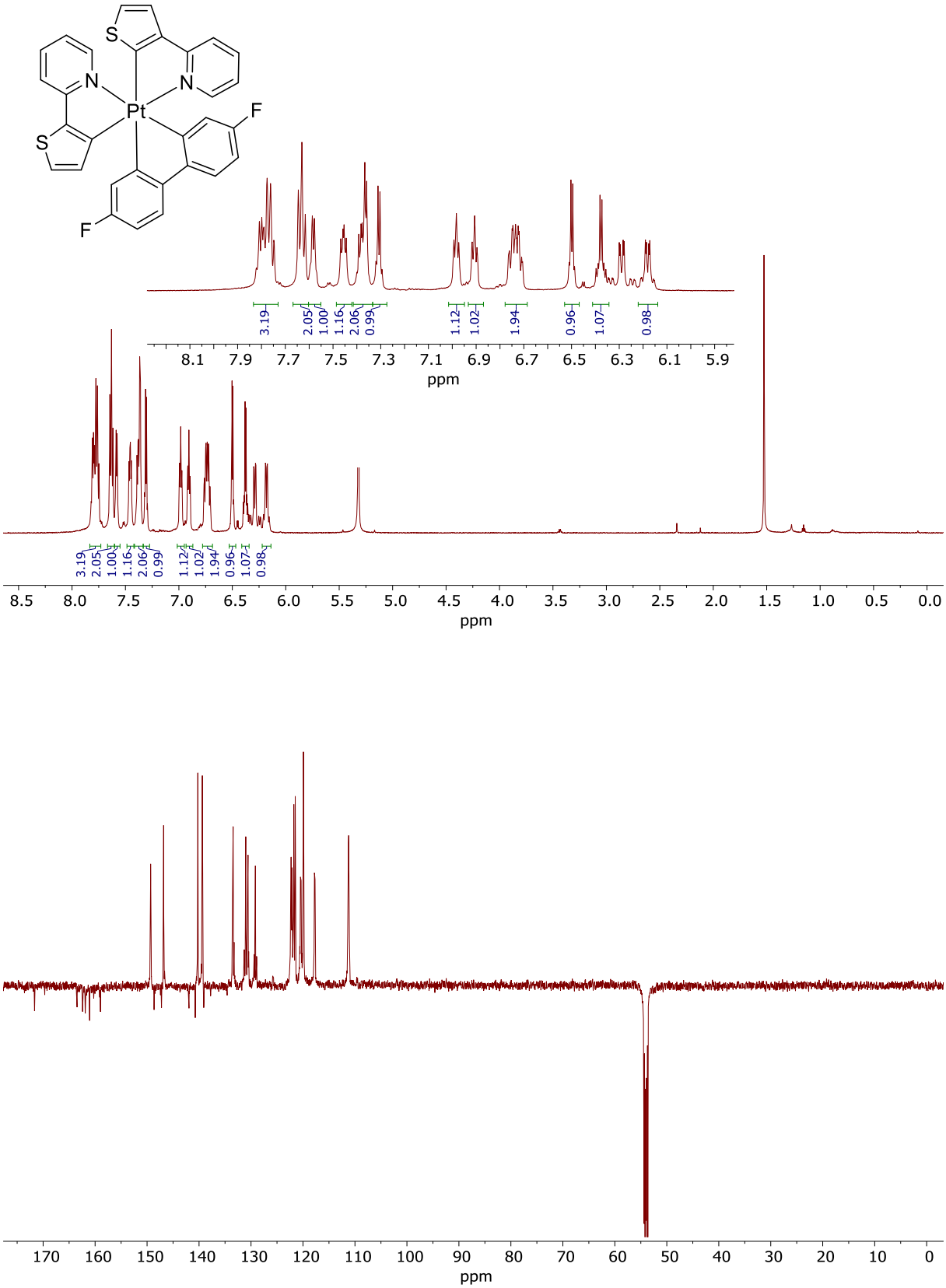


Figure S9. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2cc** (CD_2Cl_2, 400 and 151 MHz, respectively).

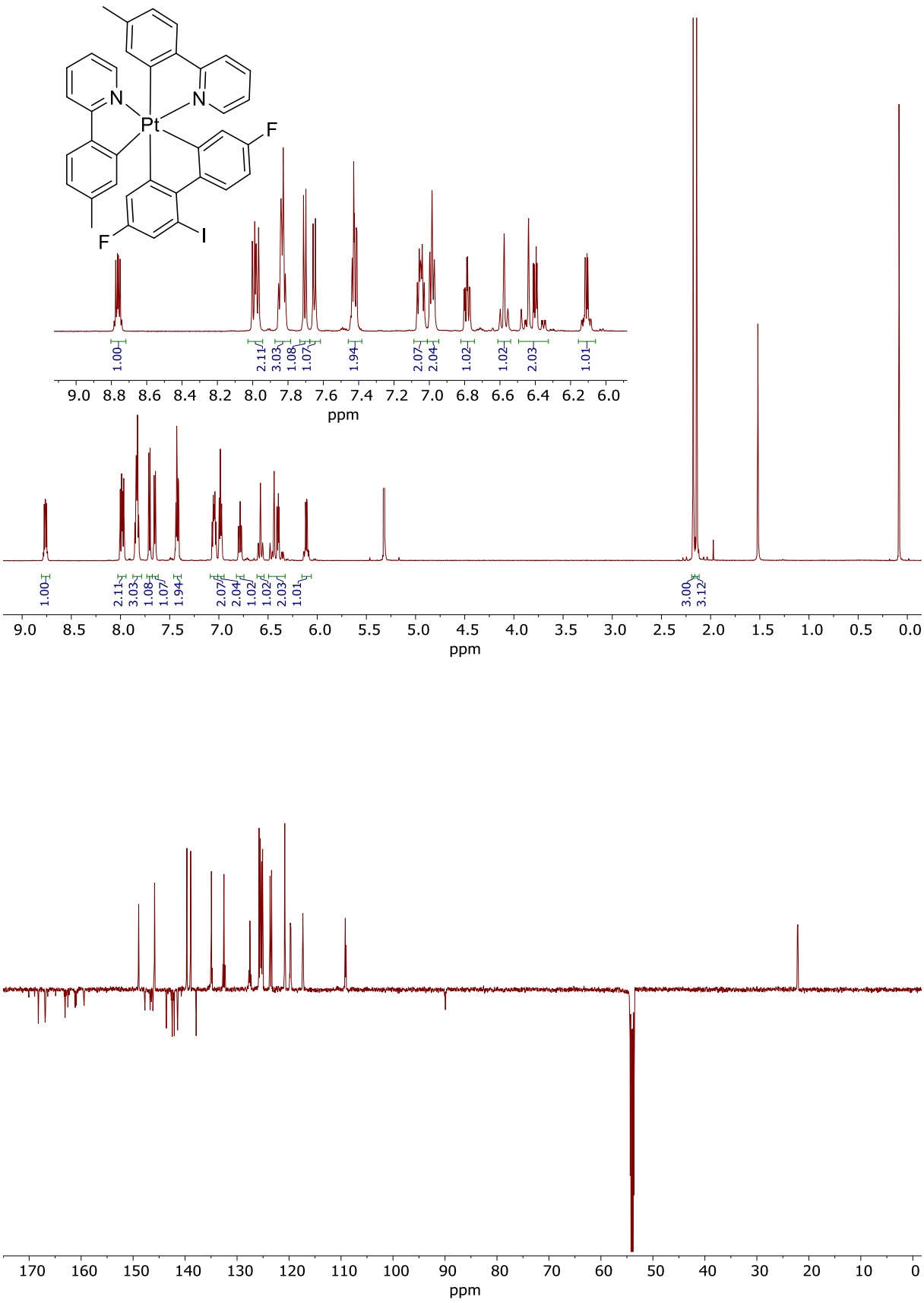


Figure S10. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2bc'** (CD_2Cl_2, 400 and 151 MHz, respectively).

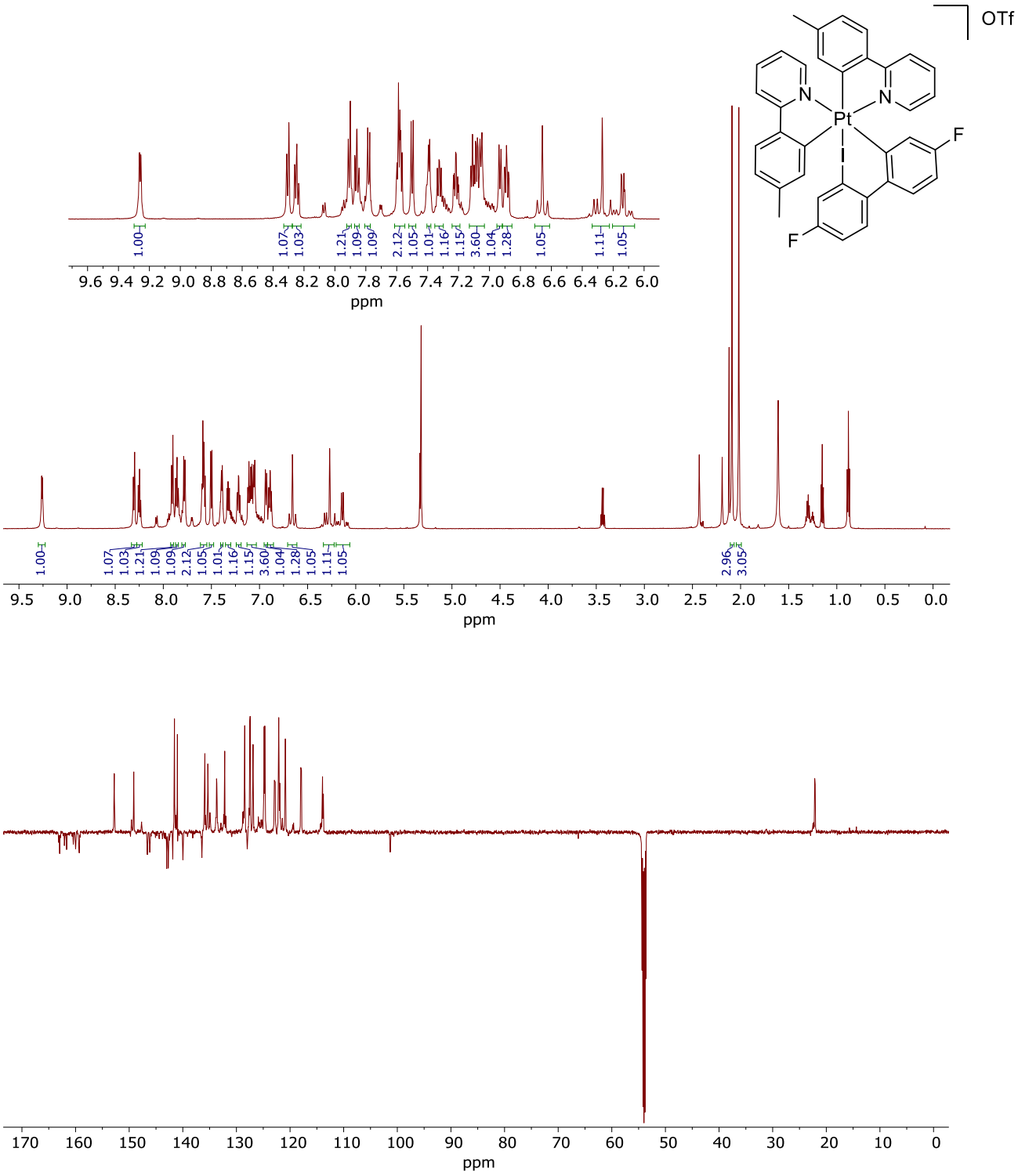


Figure S11. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **3bc** (CD_2Cl_2, 600 and 151 MHz, respectively). **Note:** Analytically pure samples this compound always showed additional signals corresponding to a secondary, minor product, possibly resulting from the decoordination of the iodine atom.

3. Additional discussion on NMR data

The ^{1}NMR spectra of complexes **2** and **3bc** show a series of resonances flanked by Pt satellites corresponding to inequivalent aromatic protons ortho to the metalated carbon atoms or the coordinated nitrogen atoms, whose chemical shifts are compiled in Table S2. They could be assigned as shown in Figure S12. The assignment to *c* or *d*, or *e* or *f* protons is based on the different values of Pt-H coupling constants, which are assumed to be larger for the protons ortho to shorter C–Pt bonds (*i.e.*, trans to N). The *a* and *b* protons could be distinguished because proton *a* in **3bc** is not shielded by any orthogonal aromatic ring and appears at 9.28 ppm, leaving proton *b* relatively unchanged with respect to the rest of complexes. The *f* resonance is absent for **3bc**. The main difference found for **2bc'** with respect to **2bc** is a resonance at 8.76 ppm arising from proton *g*, which is significantly downfield shifted relative to the analogous protons of **2bc** (*ca.* 7.50, 7.42 ppm) because it is directed toward the C–I bond and undergoes a strong through-space deshielding.

Table S2. Chemical shifts (ppm) of the assignable resonances of the protons ortho to the metalated carbon atoms or coordinated nitrogen atoms for the complexes described in this work (see Figure S12 for atom labeling).

Complex	H*a*	H*b*	H*c*	H*d*	H*e*	H*f*
2aa	7.96	7.62	6.89	6.77	6.64	6.27
2ab	–[a]	7.51	6.82	6.66	6.60	6.35
2ac	7.98	7.55	–[a]	–[a]	6.27	6.05
2ba	7.90	7.57	6.76	6.57	6.71	6.26
2bb	7.94	7.51	6.68	6.57	6.65	6.32
2bc	7.93	7.52	6.66	6.58	6.30	6.02
2ca	7.78	–[a]	6.59	6.35	6.64	6.45
2cb	7.82	7.48	6.52	6.35	6.62	6.49
2cc	7.80	7.58	6.50	6.38	6.29	6.18
2bc'	–[a]	7.43	6.58	6.44	6.40	6.11
3bc	9.25	7.40	6.64	6.27	6.14	–[b]

[a] This resonances could not be discerned. [b] Absent.

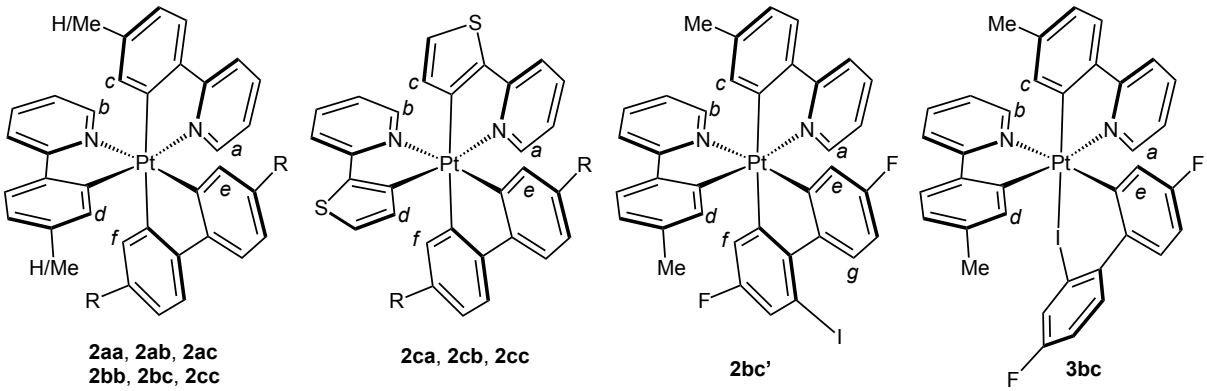


Figure S12. Labeling of aromatic H atoms for NMR assignments.

4. Additional photophysical data and discussion

Electronic absorption spectra

The electronic absorption spectra of complexes **2** in CH_2Cl_2 solution at 298 K (Figure S13, Table S3) show vibronically structured bands in the range 270-380 nm that are mainly attributable to singlet π-π* transitions within the C^N and C^C ligands (^{1}LC). By comparing the different spectra, the maxima of the lowest ^{1}LC(C^N) absorption band could be identified, which appear in the range 305-330 nm for ppy and tpy derivatives or 350-365 nm for thpy derivatives, being slightly blue-shifted with respect to those of other neutral Pt(IV) complexes bearing these ligands.[17,18] Additional maxima or shoulders in the 290-300 nm range (ppy and tpy derivatives) or 300-330 nm (thpy derivatives) are assignable to partially obscured ^{1}LC(C^C) absorptions. A more precise understanding was gained from DFT and TDDFT calculations on the ppy and thpy complexes (see the next section). The most intense absorptions are predicted to arise from ^{1}LC(C^C) and ^{1}LC(C^N) transitions, the former having higher energies in all cases. The ^{1}LC(C^C) energies are affected by the R substituent, increasing in the order *t*-Bu (dbbph) < H (bph) < F (dFbph). Additionaly, the calculations revealed the existence of relatively weak transitions of ligand-to-ligand charge-transfer character [^{1}LLCT, (C^C) → (C^N)], which emerge as the lowest-energy broad shoulder in the spectra of the ppy and tpy complexes at *ca.* 350 nm.

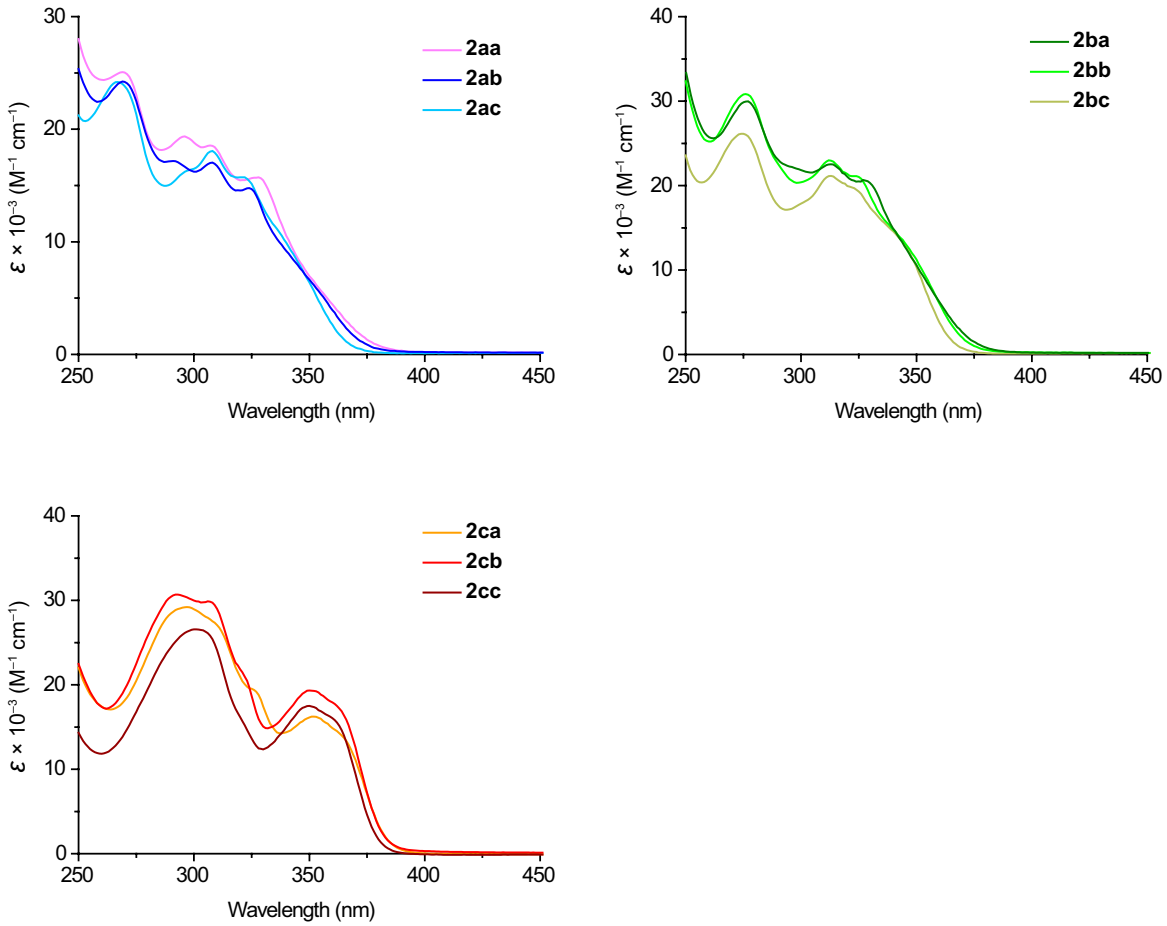


Figure S13. Electronic absorption spectra of complexes **2** in a CH_2Cl_2 solution at 298 K

Table S3. Electronic absorption data for complexes **2** in CH_2Cl_2 solution (*ca.* 5×10^{-5} M) at 298 K.

Complex	λ_{max} /nm ($\varepsilon \times 10^{-3}$/ M^{-1} cm^{-1})
2aa	269 (24.3), 297 (28.6), 307 (17.8), 329 (14.9), 352 (6.3)
2ab	270 (24.5), 292 (17.04), 307 (17.3), 325 (15.0), 346 (7.5)
2ac	268 (23.6), 297 (15.8), 308 (17.5), 322 (15.2), 342 (9.0)
2ba	277 (28.5), 299 (21.0), 313 (21.4), 330 (19.2), 349 (10.47)
2bb	276 (30.7), 313 (22.8), 326 (20.3), 347 (12.3)
2bc	275 (26.0), 314 (21.0), 324 (18.9), 345 (12.8)
2ca	296 (29.2), 327 (19.2), 352 (16.2), 366 (13.4)
2cb	292 (31.2), 308 (30.3), 323 (20.4), 350 (19.9), 365 (16.9)
2cc	302 (26.2), 348 (17.0), 362 (15.2)

Table S4. Complete listing of emission peaks for complexes **2** at 298 K.

Complex	Medium	λ_{em}/nm[a]
2aa	CH_2Cl_2	447, *461*, 477, 491
	PMMA	448, *462*, 479, 495
2ab	CH_2Cl_2	452, *477*, 513
	PMMA	452, *477*, 514
2ac	CH_2Cl_2	448, *476*, 507
	PMMA	*448*, 478, 503
2ba	CH_2Cl_2	456, *486*, 520
	PMMA	457, *484*, 520
2bb	CH_2Cl_2	*453*, 483, 513
	PMMA	*454*, 482, 516
2bc	CH_2Cl_2	*453*, 482, 513
	PMMA	*452*, 482, 511
2ca	CH_2Cl_2	514, 529, *556*
	PMMA	*513*, 528, 551
2cb	CH_2Cl_2	*514*, 531, 552
	PMMA	*513*, 527, 552
2cc	CH_2Cl_2	514, *554*
	PMMA	*513*, 528, 550

[a]The most intense peak is italicized.

Table S5. Emission data for complexes **2** in 2-MeTHF glasses at 77 K.

Complex	λ_{em}/nm[a]	τ/μs[b]
2aa	*456*, 474, 490, 510, 520, 531, 563	337 (25%), 525 (77%)
2ab	*452*, 467, 475, 484, 513, 526, 554	364
2ac	*444*, 466, 476, 502, 514, 546	308
2ba	*456*, 472, 489, 511, 519, 531, 561	488
2bb	*451*, 467, 475, 484, 511, 522, 557	317
2bc	*448*, 483, 503, 519, 548	262
2ca	*511*, 529, 550, 571, 597	293
2cb	*511*, 530, 551, 572, 597	316
2cc	*512*, 527, 549, 572, 596	355

[a] The most intense peak is italicized. [b] Emission lifetime.

Additional data and discussion on the dual emission of 2aa

The weak phosphorescence of **2aa** was assigned to a dual emission from ^{3}LC(ppy) and ^{3}LC(dbbph) excited states on the basis of its shape. The characteristic peaks of the ^{3}LC(ppy) emission at *ca.* 447 and 477 nm coincide with those of the corresponding emission of the other ppy derivatives and can be easily identified. The additional peaks correspond to the ^{3}LC(dbbph) emission. The shapes of the emission spectra measured in CH_2Cl_2, DMSO or MeOH solution, or in PMMA matrix, are very similar, but there are perceptible variations in the relative intensities of the observed peaks, suggesting that the two emissive states are affected differently by the medium (Figure S14). The emission spectra measured at different excitation wavelengths in CH_2Cl_2, DMSO or MeOH solutions are identical, but show some variations in the relative intensities of the different peaks when measured in PMMA (Figure S14), probably because the two emissive states are differently populated and their thermal equilibration is slower in the rigid medium.

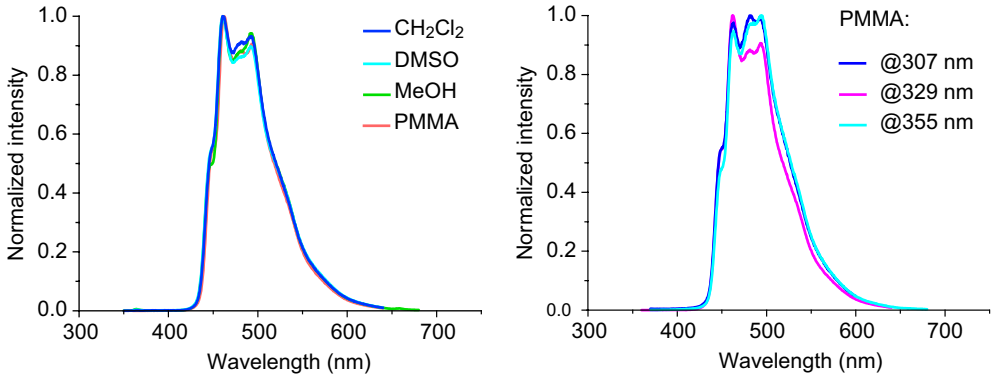


Figure S14. Emission spectra of complex **2aa** in PMMA and different solvents at 298 K upon excitation at 329 nm (left) and in PMMA at different excitation wavelengths (right).

The excitation spectra of **2aa** registered at different emission wavelengths can be correlated with the absorption spectrum, which demonstrates that the emissions arise from the complex and not from possible impurities or photodecomposition products. The maxima at *ca.* 297, 307, 329 and the shoulder

at *ca.* 355 nm observed in the absorption spectrum can be found in the excitation spectra. However, their relative intensities depend on the medium and the emission wavelength (Figure S15). The differences are mainly attributable to lowest-energy feature at *ca.* 355 nm, which arises from a ^{1}LLCT transition [(C^C) → (C^N)]. The relative contribution of this band to the excitation spectra is larger than expected, particularly in CH_2Cl_2. A possible explanation for this observation is that direct photoexcitation at the ^{1}LLCT band leads to a more effective population of the emissive excited states via intersystem crossing compared with photoexcitation at higher-lying ^{1}LC bands, probably because of slow internal conversion between singlet excited states. A similar behaviour has been previously observed for heteroleptic tris-cyclometalated Pt(IV) complexes.[19]

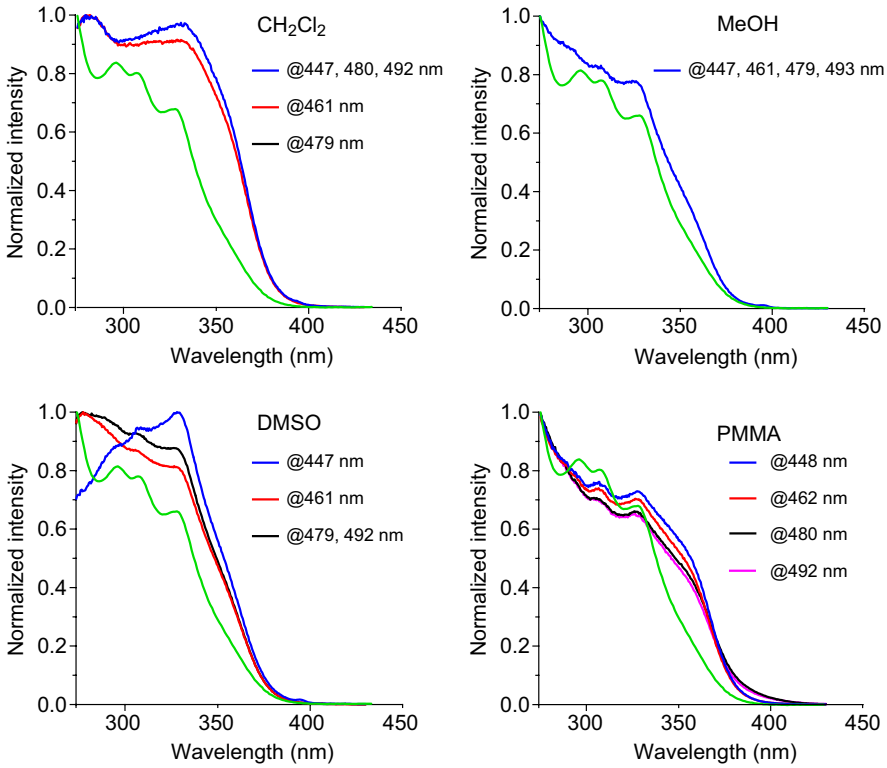


Figure S15. Excitation spectra of **2aa** in CH_2Cl_2, DMSO or MeOH solutions and in PMMA matrix at 298 K registered at the specified emission wavelengths compared with the absorption spectrum in CH_2Cl_2 (green line).

In addition, the biexponential decays observed for **2aa** can be clearly ascribed to the presence of two different emissive states. The proportions of the two lifetime components were found to vary depending on the excitation and emission wavelength employed for the measurement in PMMA (Table S6). This can be explained by the variations in the relative intensities of each of the emissions.

Table S6. Emission lifetimes of **2aa** determined at different excitation or emission wavelengths in PMMA at 298 K.

Excitation wavelength (nm)	Emission wavelength (nm)	τ / μs
328	448	94 (20%), 244 (80%)
328	462	88 (14%), 235 (86%)
307	462	87 (12%), 246 (88%)
352	462	84 (8%), 232 (92%)

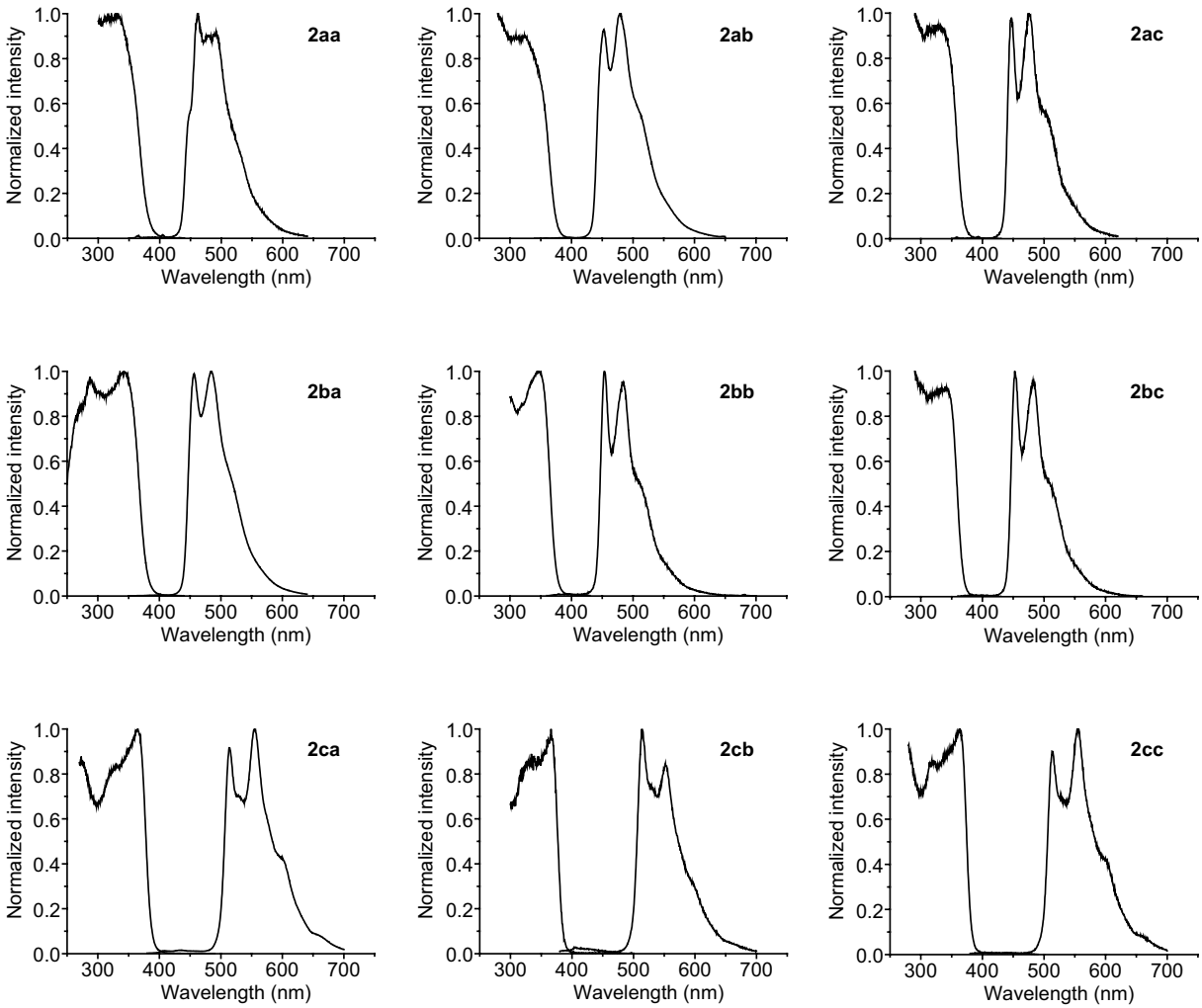


Figure S16. Excitation and emission spectra of complexes **2** in CH_2Cl_2 at 298 K.

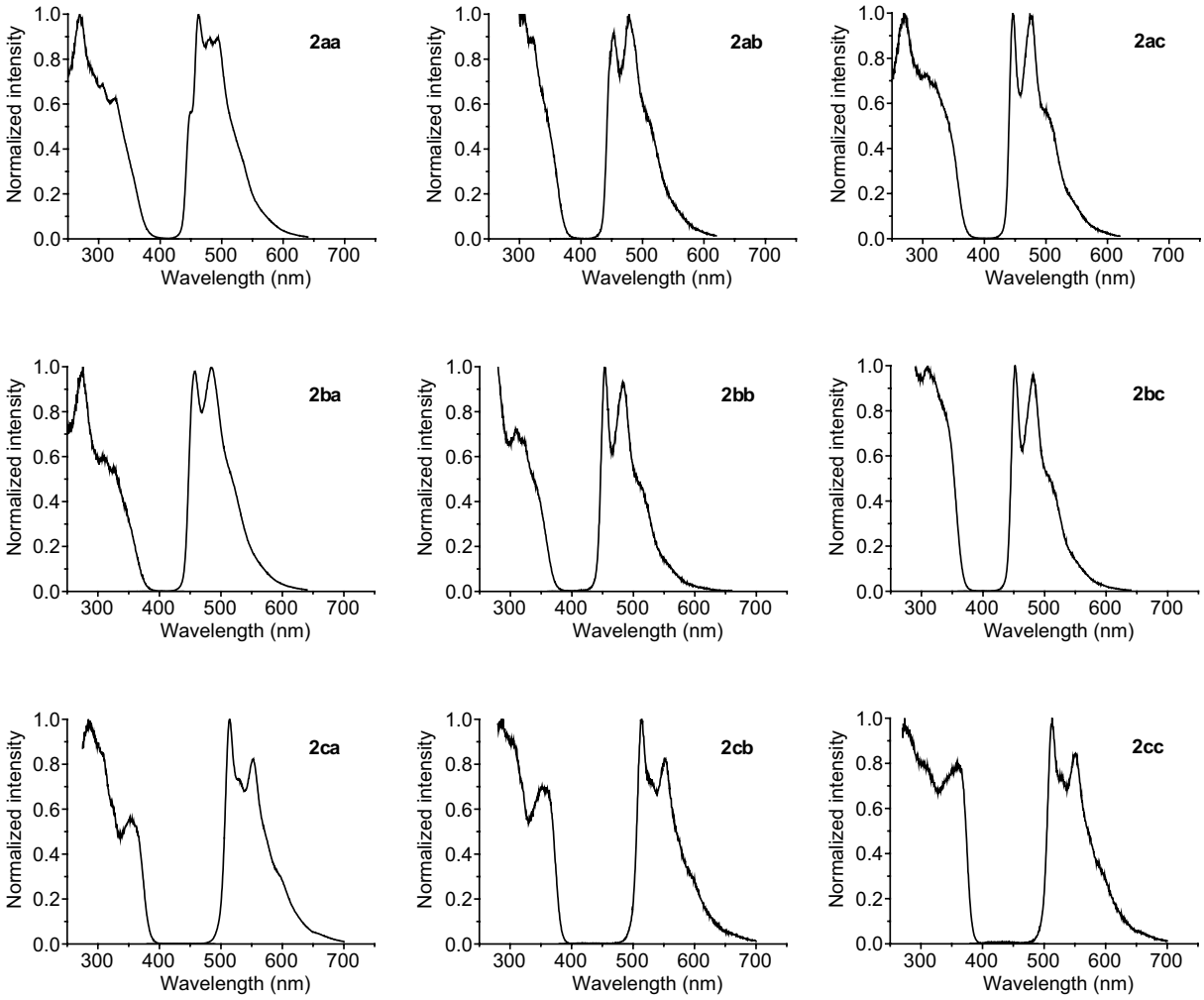


Figure S17. Excitation and emission spectra of complexes **2** in PMMA at 298 K.

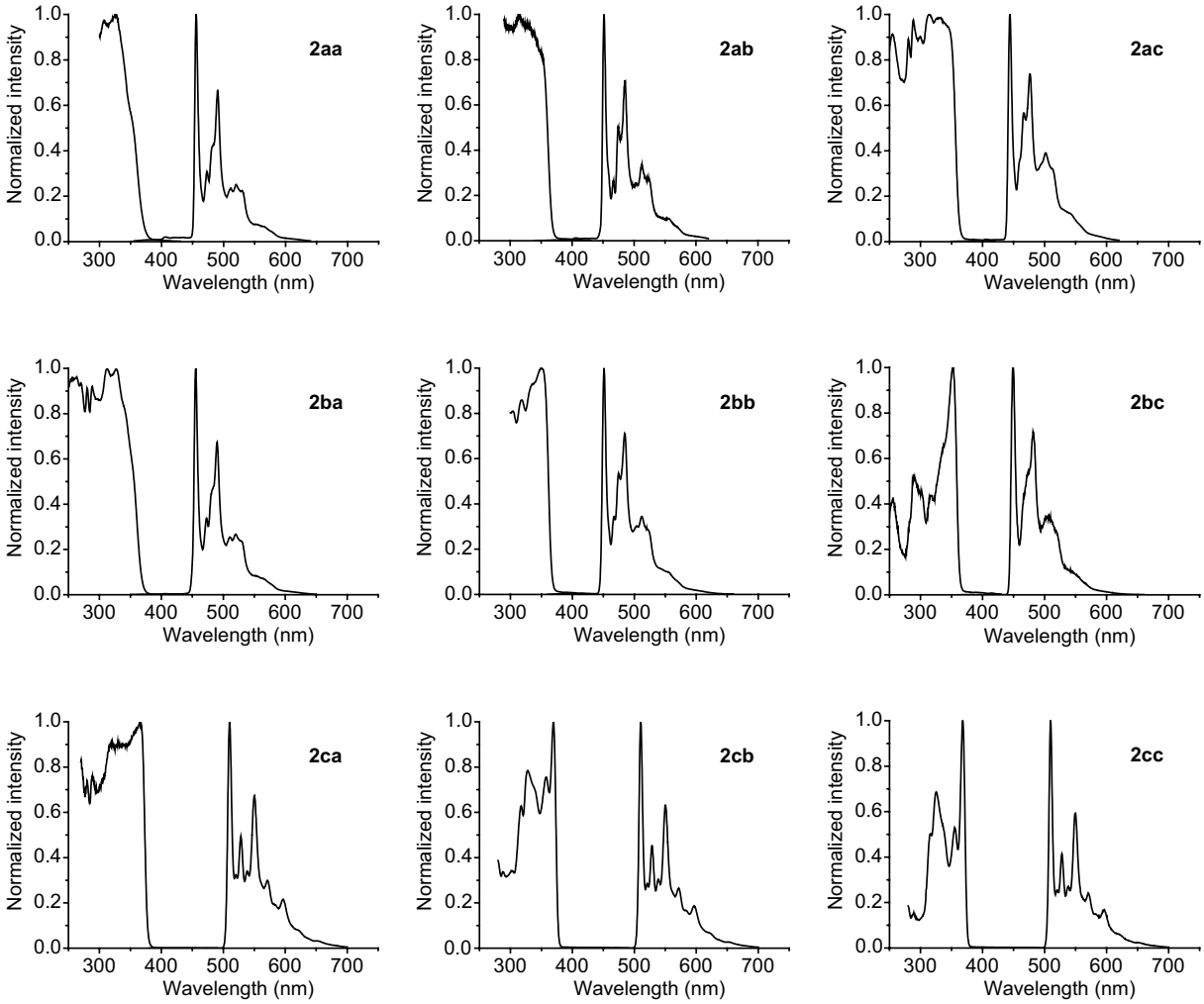


Figure S18. Excitation and emission spectra of complexes **2** in MeTHF at 298 K.

5. Computational data

5.1. Complex 2aa

Table S7. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **2aa** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	Pt
–0.003	168 (LUMO+5)	20	11	43	27
–0.018	167 (LUMO+4)	2	5	89	4
–0.034	166 (LUMO+3)	47	51	0	2
–0.040	165 (LUMO+2)	51	44	4	2
–0.055	164 (LUMO+1)	87	10	2	1
–0.056	163 (LUMO)	11	86	1	2
–0.191	162 (HOMO)	0	0	97	3
–0.210	161 (HOMO–1)	30	30	32	8
–0.222	160 (HOMO–2)	2	77	12	8
–0.225	159 (HOMO–3)	4	11	76	9
–0.226	158 (HOMO–4)	2	8	82	8
–0.231	157 (HOMO–5)	74	9	15	3

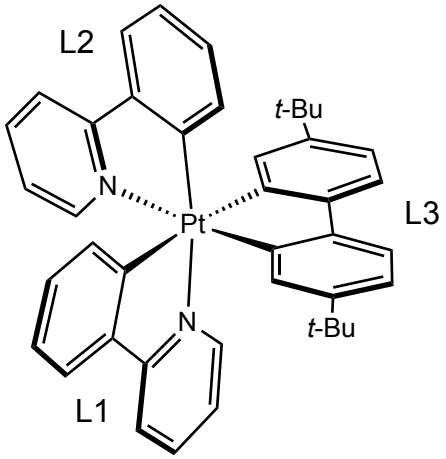
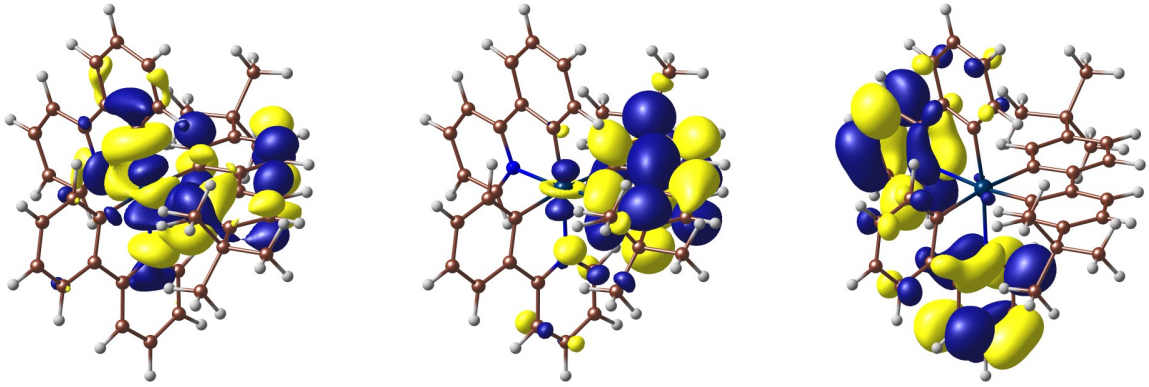
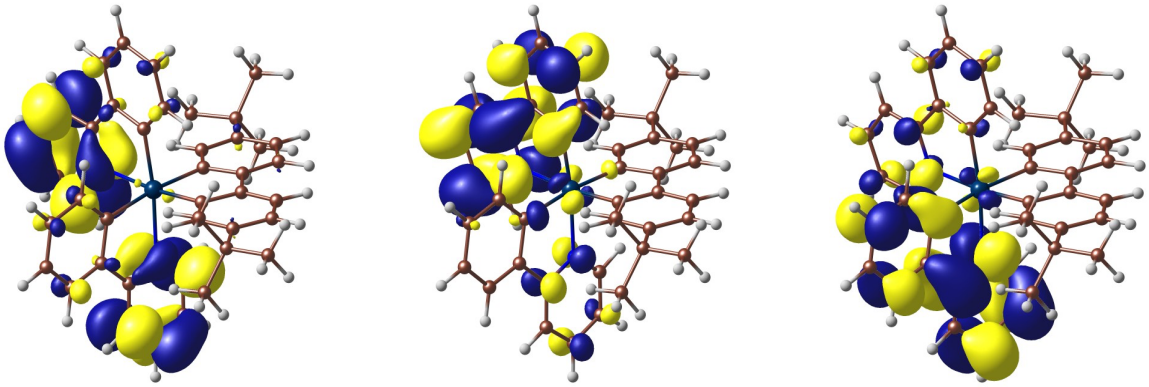


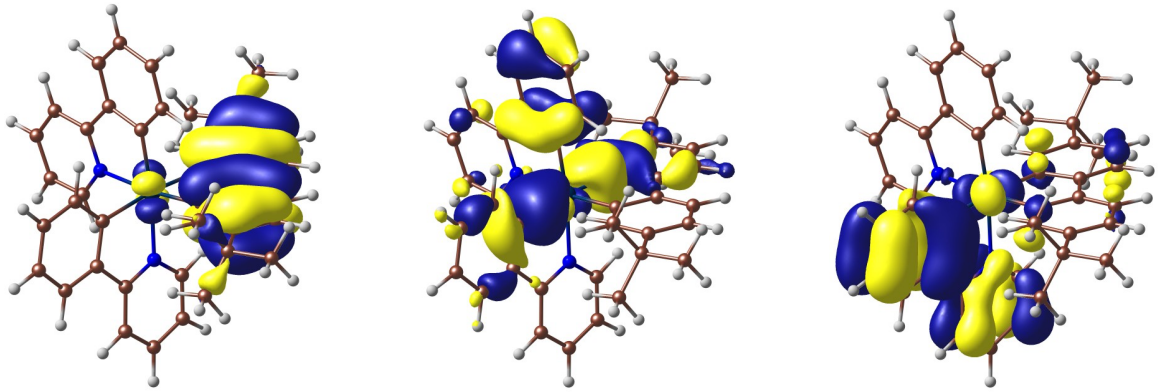
Figure S19. Ligand numbering in complex **2aa**.



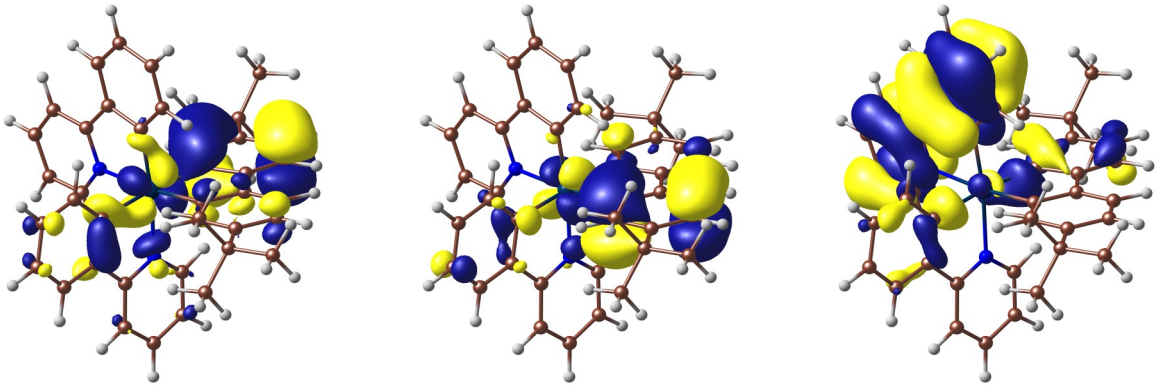
(LUMO+5) (LUMO+4) (LUMO+3)



(LUMO+2) (LUMO+1) (LUMO)



(HOMO) (HOMO–1) (HOMO–2)



(HOMO–3) (HOMO–4) (HOMO–5)

Figure S20. Molecular orbital isosurfaces of **2aa** (0.03 e bohr^{-3}).

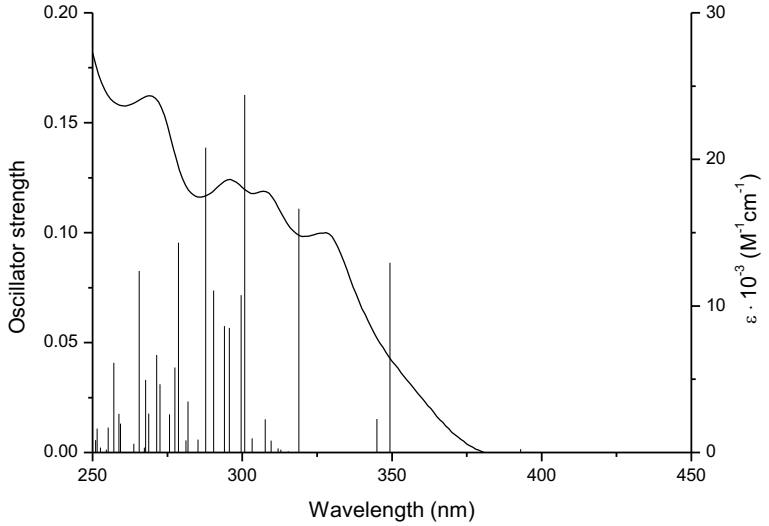


Figure S21. Calculated stick absorption spectrum of **2aa** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S8. Selected vertical singlet excitations of **2aa** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	monoexcitations[a]	ΔE/eV	λ/nm	oscillator strength	main character
S4:	H–1 -> L (8%) H–1 -> L+1 (90%)	3.552	349.0	0.0868	LC(C^N)
S5:	H -> L+2 (95%) H -> L+3 (4%)	3.597	344.7	0.0157	LLCT
S7:	H–6 -> L (2%) H–2 -> L (88%)	3.892	318.6	0.1114	LC(C^N)
S12:	H–4 -> L (39%) H–4 -> L+1 (5%) H–3 -> L (43%) H–3 -> L+1 (5%)	4.034	307.4	0.0156	LLCT
S14:	H–4 -> L+1 (5%) H–1 -> L+3 (19%) H -> L+4 (61%) H -> L+5 (7%)	4.126	300.5	0.1631	LC(C^C)
S15:	H–1 -> L+3 (75%) H -> L+4 (17%) H -> L+5 (2%)	4.143	299.3	0.0720	LLCT

[a] H = HOMO; L = LUMO.

Table S9. Lowest-energy vertical triplet excitations of **2aa** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**	**main character**
T1:	H–8 -> L+14 (2%) H -> L+2 (7%) H -> L+4 (75%)	2.888	429.3	LC(C^C)
T2:	H–6 -> L (10%) H–3 -> L (4%) H–2 -> L (54%) H–2 -> L+1 (5%) H–2 -> L+3 (3%)	2.957	419.3	LC(C^N)
T3:	H–5 -> L (7%) H–5 -> L+1 (40%) H–5 -> L+2 (2%) H–5 -> L+3 (2%) H–3 -> L+1 (2%) H–2 -> L+1 (3%) H–1 -> L (4%) H–1 -> L+1 (23%)	2.971	417.4	LC(C^N)

[a] H = HOMO; L = LUMO.

5.2. Complex 2ab

Table S10. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **2ab** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	Pt
–0.005	136 (LUMO+5)	19	10	44	27
–0.022	135 (LUMO+4)	2	6	88	4
–0.034	134 (LUMO+3)	48	49	1	2
–0.040	133 (LUMO+2)	49	44	5	2
–0.056	132 (LUMO+1)	87	11	0	1
–0.057	131 (LUMO)	12	86	0	2
–0.199	130 (HOMO)	0	0	95	4
–0.212	129 (HOMO–1)	33	29	30	8
–0.223	128 (HOMO–2)	2	86	4	8
–0.228	127 (HOMO–3)	9	10	72	10
–0.230	126 (HOMO–4)	2	4	87	7
–0.232	125 (HOMO–5)	69	8	21	2

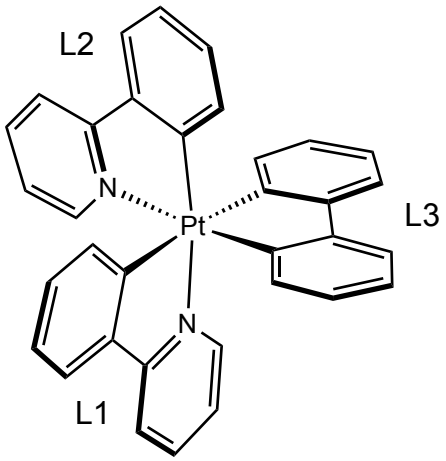


Figure S22. Ligand numbering in complex **2ab**.

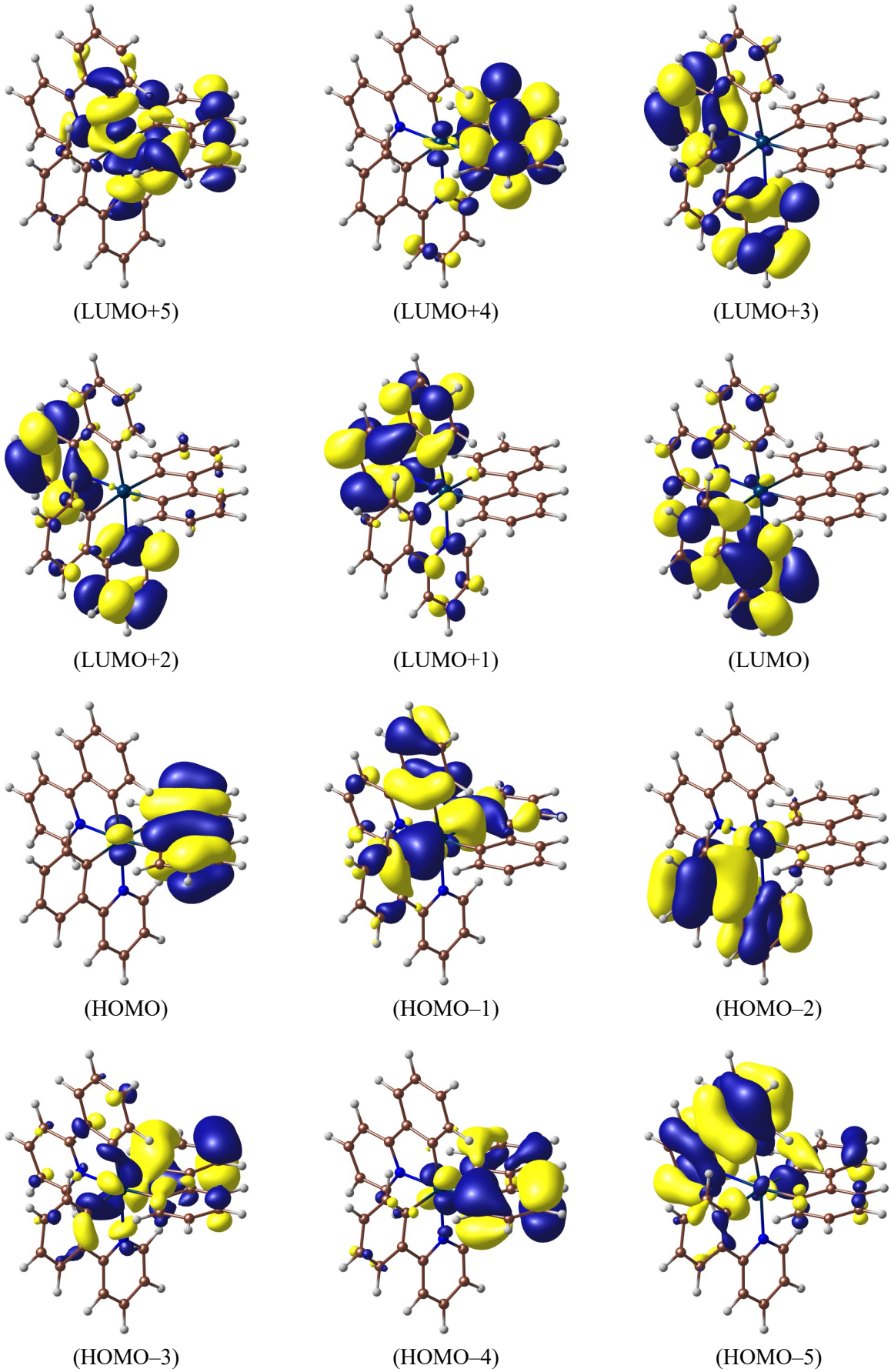


Figure S23. Molecular orbital isosurfaces of **2ab** (0.03 e bohr^{-3}).

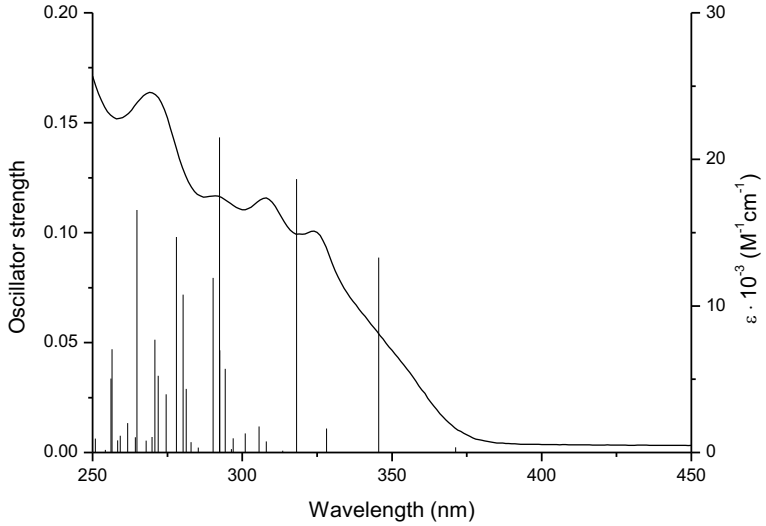


Figure S24. Calculated stick absorption spectrum of **2ab** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S11. Selected vertical singlet excitations of **2ab** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	monoexcitations	ΔE/eV	λ/nm	oscillator strength	main character
S4:	H–1 -> L (8%) H–1 -> L+1 (89%)	3.592	345.2	0.0891	LLCT/LC
S5:	H -> L+2 (95%) H -> L+3 (4%)	3.781	327.9	0.0113	LLCT
S6:	H–6 -> L (3%) H–2 -> L (88%)	3.902	317.8	0.1248	LC(C^N)
S11:	H–3 -> L (18%) H–3 -> L+1 (78%)	4.062	305.3	0.0123	LLCT
S15:	H–5 -> L (23%) H–5 -> L+1 (57%) H–4 -> L (4%) H–2 -> L+2 (4%) H -> L+4 (2%)	4.217	294.0	0.0385	LLCT
S16:	H–5 -> L (61%) H–5 -> L+1 (17%) H–4 -> L+1 (3%) H–1 -> L+3 (4%) H -> L+4 (8%)	4.243	292.2	0.0469	LLCT
S17:	H–5 -> L (4%) H–5 -> L+1 (8%) H -> L+4 (69%) H -> L+5 (9%)	4.245	292.1	0.1438	LC(C^C)

[a] H = HOMO; L = LUMO.

Table S12. Lowest-energy vertical triplet excitations of **2ab** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**	**main character**
T1:	H–8 -> L+13 (3%) H–4 -> L+5 (2%) H–3 -> L+9 (2%) H -> L+2 (8%) H -> L+4 (73%)	2.944	421.2	LC(C^C)
T2:	H–6 -> L (10%) H–2 -> L (58%) H–2 -> L+1 (6%) H–2 -> L+3 (3%)	2.956	419.4	LC(C^N)
T3:	H–7 -> L+7 (2%) H–5 -> L (6%) H–5 -> L+1 (37%) H–5 -> L+3 (2%) H–3 -> L+1 (6%) H–2 -> L+1 (2%) H–1 -> L (4%) H–1 -> L+1 (23%)	2.974	416.9	LC(C^N)

[a] H = HOMO; L = LUMO.

5.3. Complex 2ac

Table S13. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **2ac** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	Pt
–0.012	144 (LUMO+5)	14	8	56	21
–0.021	143 (LUMO+4)	2	5	87	5
–0.036	142 (LUMO+3)	47	51	0	2
–0.042	141 (LUMO+2)	51	44	3	2
–0.058	140 (LUMO+1)	83	14	0	2
–0.059	139 (LUMO)	15	82	0	2
–0.197	138 (HOMO)	0	0	97	3
–0.217	137 (HOMO–1)	39	27	27	8
–0.226	136 (HOMO–2)	2	90	2	7
–0.233	135 (HOMO–3)	61	17	17	6
–0.238	134 (HOMO–4)	2	25	67	6
–0.238	133 (HOMO–5)	20	12	60	9

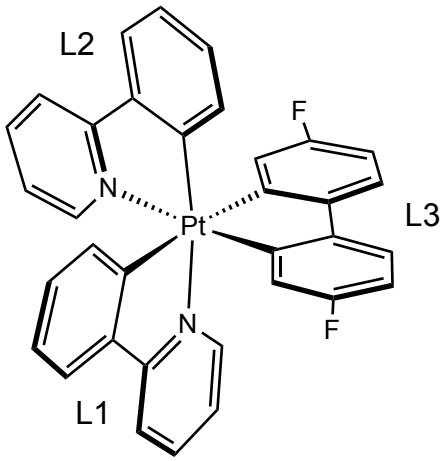


Figure S25. Ligand numbering in complex **2ac**.

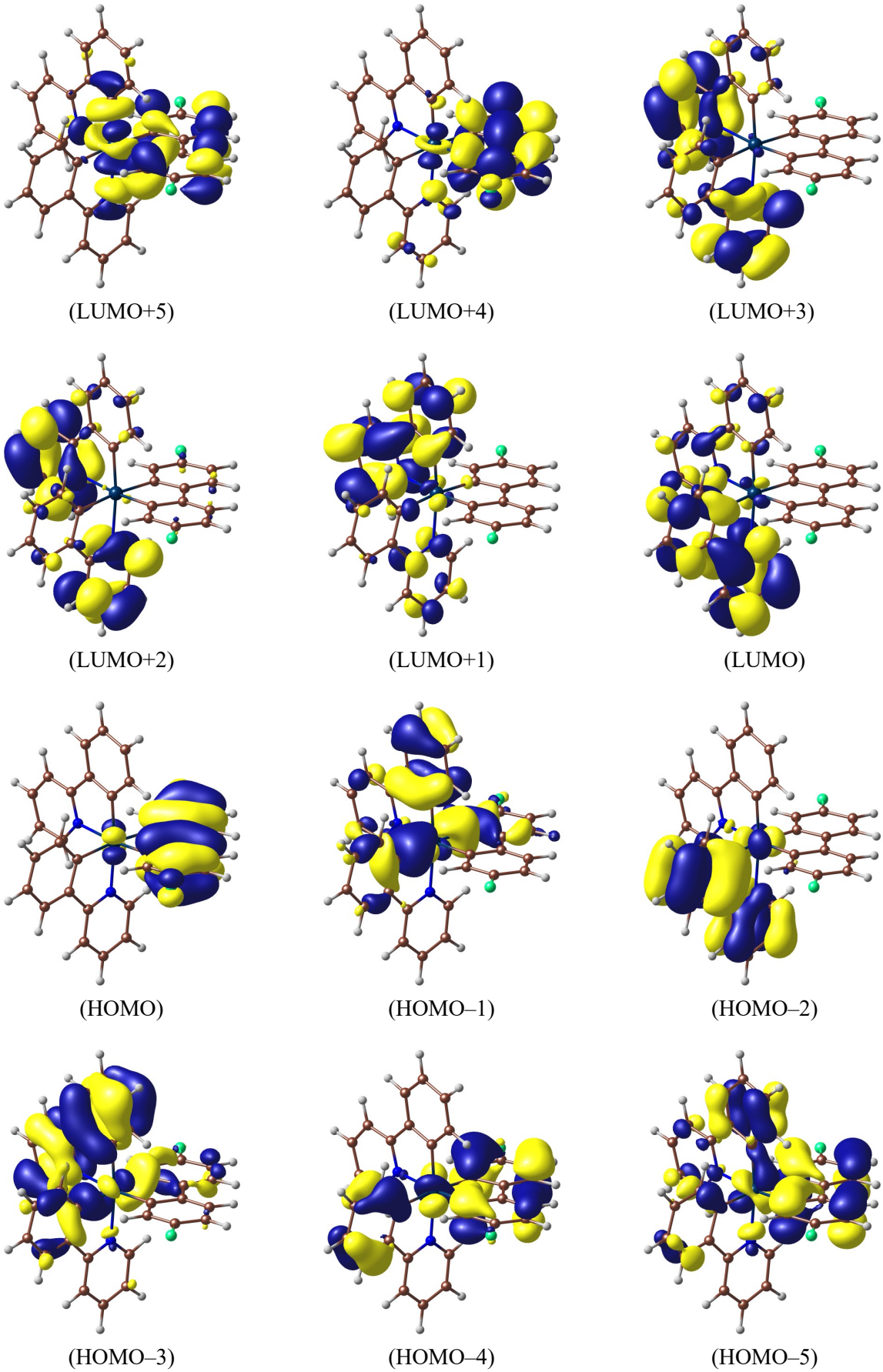


Figure S26. Molecular orbital isosurfaces of **2ac** (0.03 e bohr^{-3}).

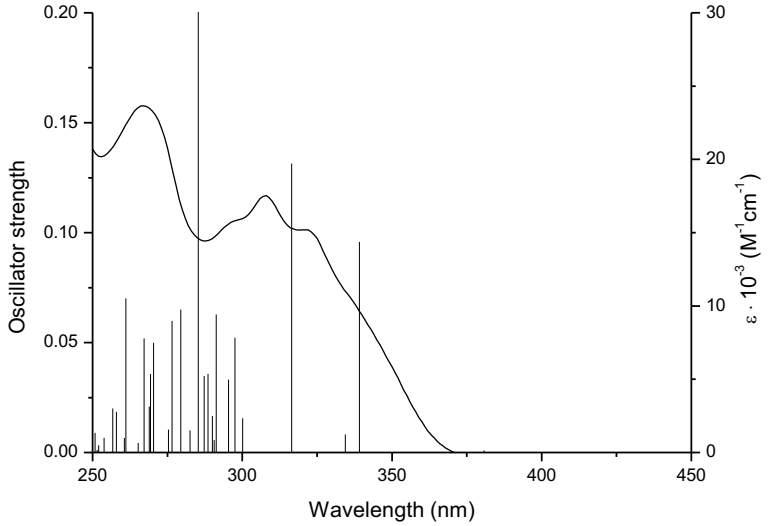


Figure S27. Calculated stick absorption spectrum of **2ac** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S14. Selected vertical singlet excitations of **2ac** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	monoexcitations	ΔE/eV	λ/nm	oscillator strength	main character
S4:	H–1 -> L (14%) H–1 -> L+1 (83%)	3.659	338.8	0.0962	LLCT/LC
S5:	H -> L+2 (96%) H -> L+3 (3%)	3.711	334.1	0.0087	LLCT
S7:	H–2 -> L (85%) H–2 -> L+1 (5%)	3.921	316.2	0.1319	LC(C^N)
S11:	H–5 -> L+1 (4%) H–4 -> L (3%) H–4 -> L+1 (3%) H–3 -> L (26%) H–3 -> L+1 (50%) H -> L+4 (4%)	4.172	297.2	0.0527	LLCT
S13:	H–5 -> L (24%) H–5 -> L+1 (7%) H–4 -> L (38%) H–4 -> L+1 (9%) H–2 -> L+2 (6%) H–1 -> L+3 (2%) H -> L+5 (3%)	4.261	291.0	0.0632	LLCT
S19:	H–4 -> L+4 (5%) H -> L+4 (43%) H -> L+5 (41%)	4.350	285.0	0.2033	LC(C^C)

[a] H = HOMO; L = LUMO.

Table S15. Lowest-energy vertical triplet excitations of **2ac** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**	**main character**
T1:	H–6 -> L (5%) H–2 -> L (55%) H–2 -> L+1 (11%) H–2 -> L+3 (4%) H -> L+4 (2%)	2.957	419.3	LC(C^N)
T2:	H–8 -> L+14 (3%) H–5 -> L+9 (2%) H–4 -> L+5 (3%) H -> L+2 (7%) H -> L+4 (71%)	2.961	418.8	LC(C^C)
T3:	H–7 -> L+7 (2%) H–5 -> L+1 (6%) H–3 -> L (9%) H–3 -> L+1 (33%) H–3 -> L+3 (2%) H–1 -> L (6%) H–1 -> L+1 (22%) H–1 -> L+7 (2%)	2.977	416.5	LC(C^N)

[a] H = HOMO; L = LUMO.

5.4. Complex 2ca

Table S16. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **2ca** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	Pt
–0.011	170 (LUMO+5)	25	9	43	24
–0.022	169 (LUMO+4)	4	8	79	9
–0.034	168 (LUMO+3)	47	50	1	2
–0.038	167 (LUMO+2)	50	44	4	2
–0.057	166 (LUMO+1)	96	1	0	2
–0.058	165 (LUMO)	2	95	0	3
–0.194	164 (HOMO)	0	0	97	3
–0.209	163 (HOMO–1)	70	11	12	6
–0.212	162 (HOMO–2)	1	94	1	4
–0.227	161 (HOMO–3)	2	7	86	5
–0.228	160 (HOMO–4)	47	17	31	5
–0.230	159 (HOMO–5)	2	3	86	9

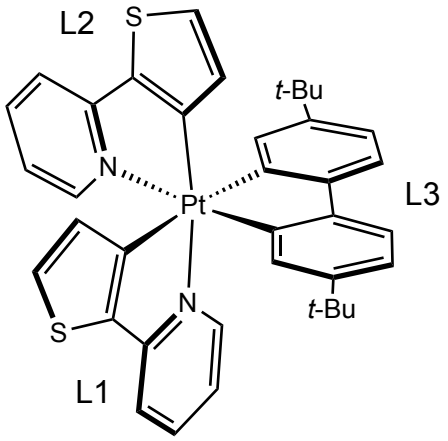
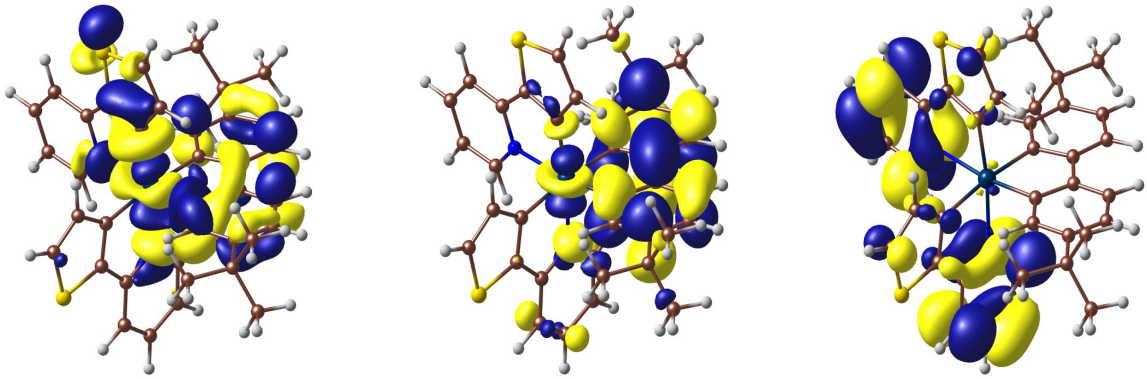
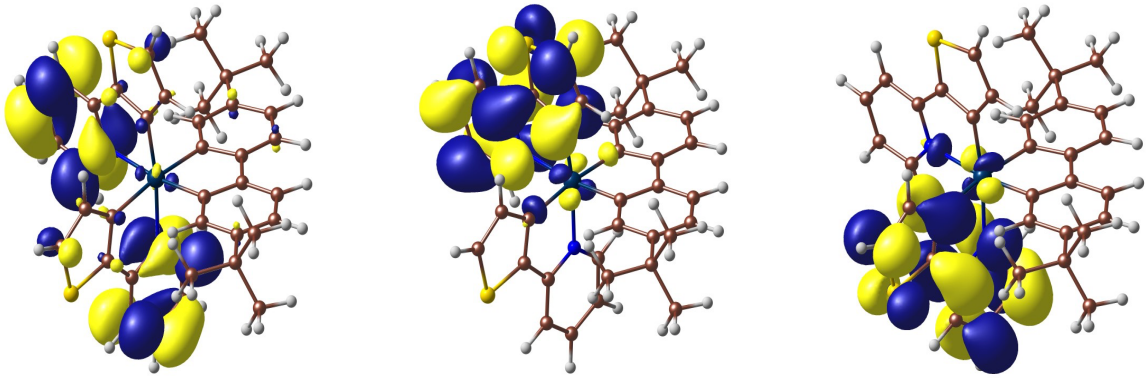


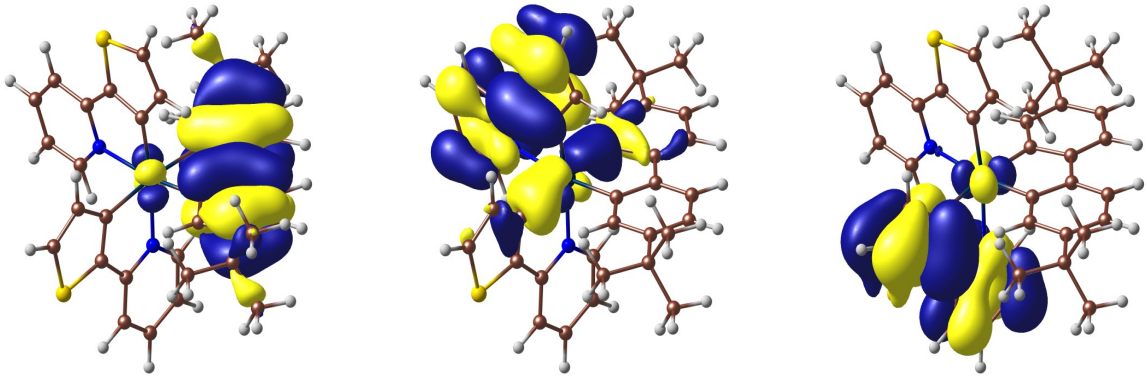
Figure S28. Ligand numbering in complex **2ca**.



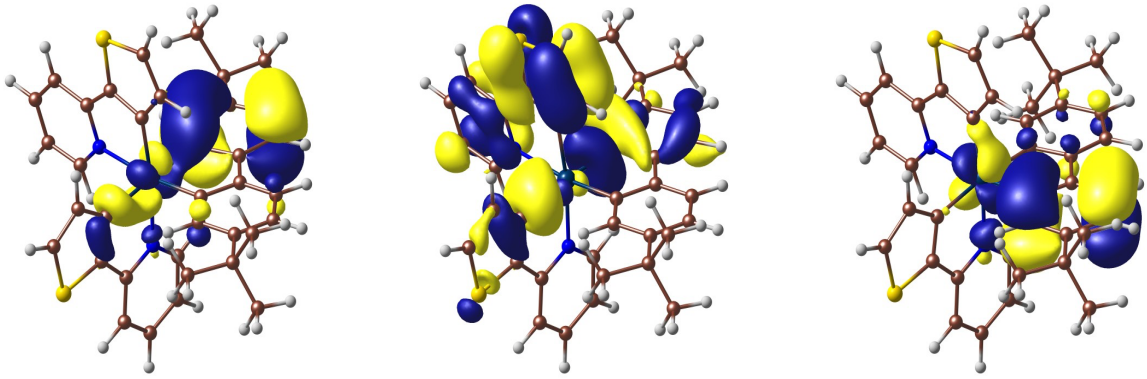
(LUMO+5) (LUMO+4) (LUMO+3)



(LUMO+2) (LUMO+1) (LUMO)



(HOMO) (HOMO–1) (HOMO–2)



(HOMO–3) (HOMO–4) (HOMO–5)

Figure S29. Molecular orbital isosurfaces of **2ca** (0.03 e bohr^{-3}).

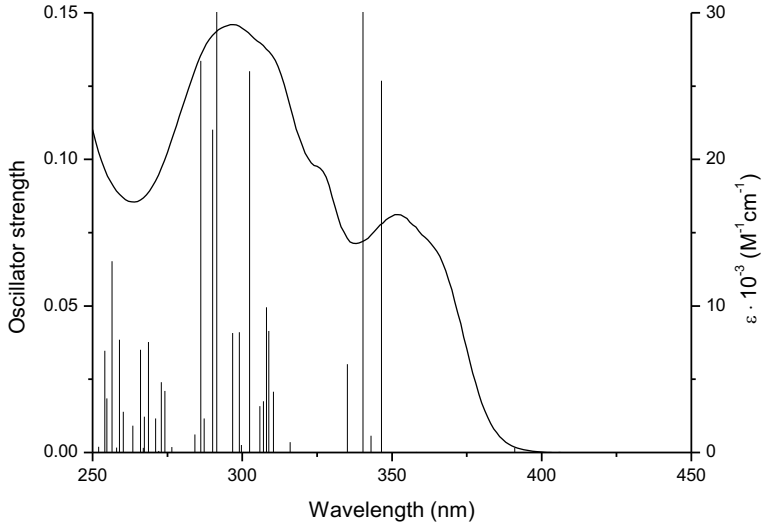


Figure S30. Calculated stick absorption spectrum of **2ca** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S17. Selected vertical singlet excitations of **2ca** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	monoexcitations[a]	ΔE/eV	λ/nm	Oscillator strength	main character
S4:	H–4 -> L+1 (3%) H–2 -> L (19%) H–2 -> L+1 (5%) H–1 -> L+1 (67%)	3.581	346.2	0.1272	LC(C^N)
S6:	H–2 -> L (70%) H–2 -> L+2 (4%) H–1 -> L+1 (18%)	3.647	340.0	0.1753	LC(C^N)
S7:	H -> L+2 (92%) H -> L+3 (6%)	3.703	334.8	0.0305	LLCT
S12:	H–5 -> L (30%) H–4 -> L (8%) H–4 -> L+1 (16%) H–1 -> L+2 (38%) H–1 -> L+3 (2%)	4.028	307.8	0.0499	LC(C^N)/LLCT
S15:	H–4 -> L+1 (68%) H–1 -> L+1 (3%) H–1 -> L+2 (18%)	4.104	302.1	0.1304	LC(C^N)
S17:	H–2 -> L (3%) H–2 -> L+2 (88%)	4.151	298.7	0.0414	LC(C^N)/LLCT
S18:	H–4 -> L+1 (3%) H–1 -> L+3 (81%) H–1 -> L+4 (4%) H–1 -> L+5 (3%)	4.182	296.5	0.0411	LC(C^N)/LLCT
S19:	H–3 -> L+4 (4%)	4.258	291.2	0.2343	LC(C^C)

	H–2 -> L+3 (12%) H–1 -> L+4 (2%) H -> L+4 (18%) H -> L+5 (53%)				
S20:	H–6 -> L (8%) H–2 -> L+3 (72%) H -> L+4 (4%) H -> L+5 (8%)	4.279	289.8	0.1105	LC(C^N)/LLCT

[a] H = HOMO; L = LUMO.

Table S18. Lowest-energy vertical triplet excitations of **2ca** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations[a]**	**ΔE/eV**	**λ/nm**	**main character**
T1:	H–2 -> L (84%) H–2 -> L+2 (3%) H–2 -> L+3 (5%)	2.494	497.2	LC(C^N)
T2:	H–4 -> L+1 (12%) H–1 -> L+1 (75%) H–1 -> L+2 (3%) H–1 -> L+3 (3%)	2.522	491.6	LC(C^N)
T3:	H -> L+2 (7%) H -> L+4 (71%) H -> L+5 (4%)	2.888	429.4	LC(C^C)

[a] H = HOMO; L = LUMO.

5.5. Complex 2cb

Table S19. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **2cb** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	Pt
–0.013	138 (LUMO+5)	25	9	42	24
–0.025	137 (LUMO+4)	3	10	79	7
–0.034	136 (LUMO+3)	51	46	1	2
–0.039	135 (LUMO+2)	46	46	6	2
–0.058	134 (LUMO+1)	96	1	0	2
–0.059	133 (LUMO)	2	95	0	3
–0.202	132 (HOMO)	0	0	95	4
–0.211	131 (HOMO–1)	72	11	11	6
–0.212	130 (HOMO–2)	2	93	1	4
–0.230	129 (HOMO–3)	44	24	28	5
–0.231	128 (HOMO–4)	5	2	87	6
–0.233	127 (HOMO–5)	1	3	87	8

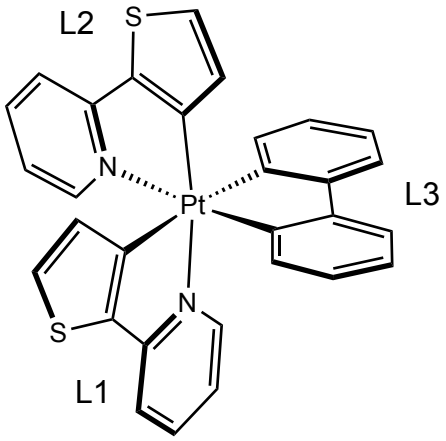
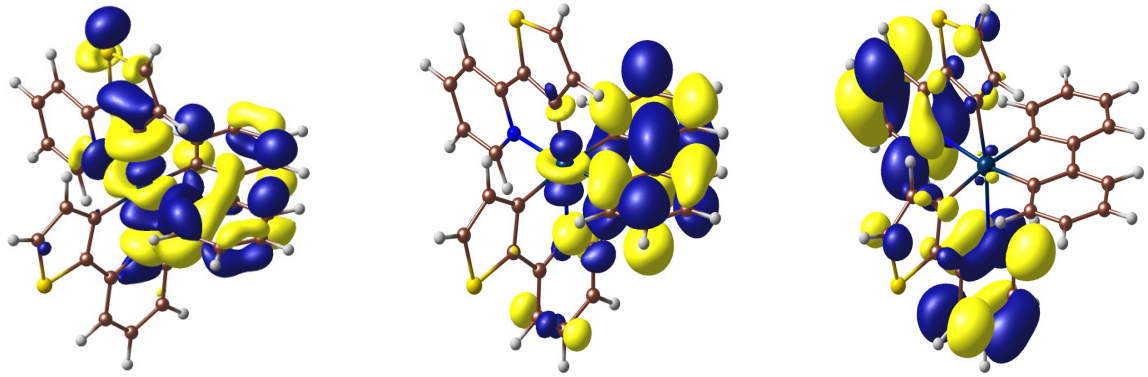
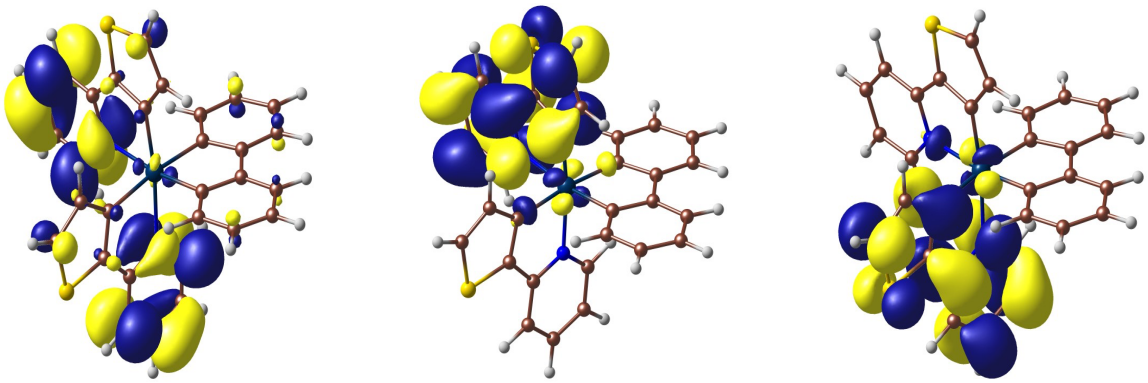


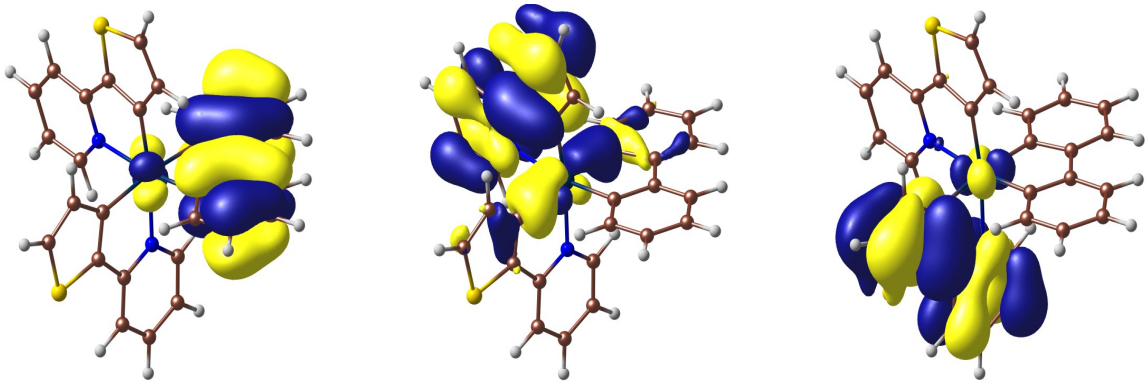
Figure S31. Ligand numbering in complex **2cb**.



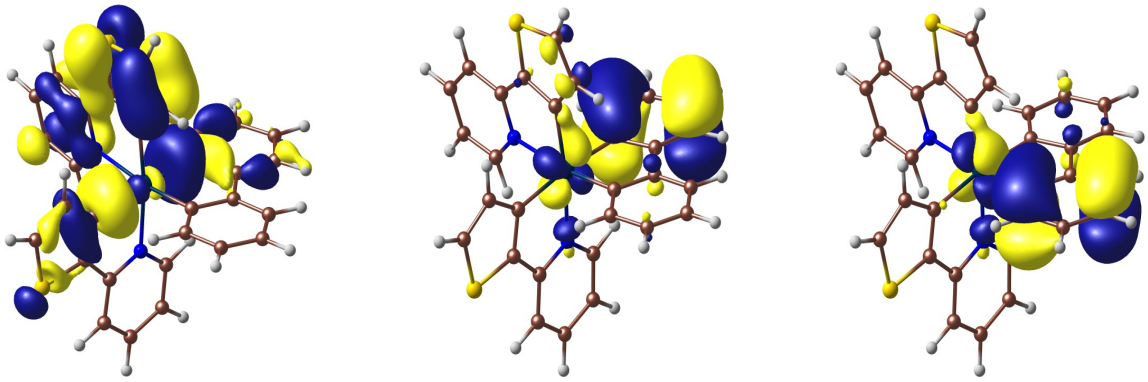
(LUMO+5) (LUMO+4) (LUMO+3)



(LUMO+2) (LUMO+1) (LUMO)



(HOMO) (HOMO–1) (HOMO–2)



(HOMO–3) (HOMO–4) (HOMO–5)

Figure S32. Molecular orbital isosurfaces of **2cb** (0.03 e bohr^{-3}).

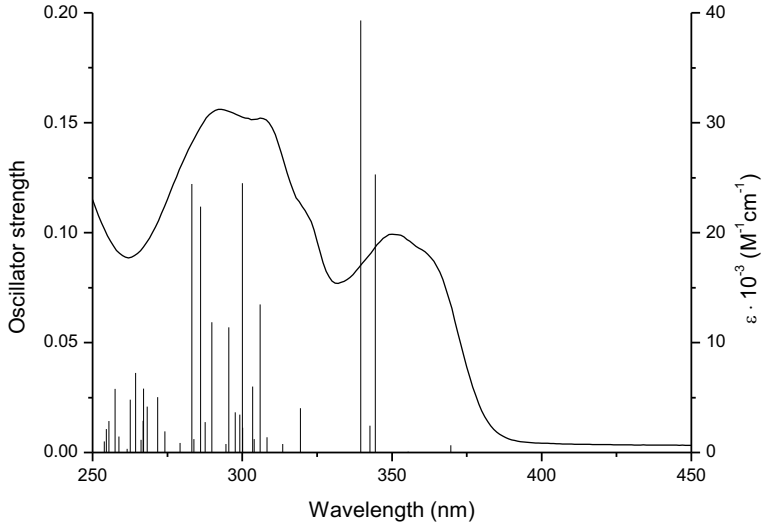


Figure S33. Calculated stick absorption spectrum of **2cb** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S20. Selected vertical singlet excitations of **2cb** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**	**oscillator strength**	**main character**
S4:	H–3 -> L+1 (3%) H–2 -> L (30%) H–2 -> L+1 (12%) H–1 -> L+1 (48%)	3.602	344.2	0.1269	LC(C^N)
S6:	H–2 -> L (57%) H–2 -> L+2 (4%) H–1 -> L+1 (31%)	3.655	339.2	0.1969	LC(C^N)
S10:	H–3 -> L+1 (27%) H–1 -> L+2 (57%) H -> L+3 (5%)	4.056	305.7	0.0678	LC(C^N)/LLCT
S14:	H–4 -> L (5%) H–4 -> L+1 (33%) H–3 -> L+1 (19%) H–2 -> L+2 (11%) H–1 -> L+2 (5%) H–1 -> L+3 (4%) H -> L+4 (9%) H -> L+5 (5%)	4.137	299.7	0.123	LLCT
S17:	H–5 -> L+1 (7%) H–4 -> L+1 (3%) H–3 -> L+1 (2%) H–1 -> L+3 (68%) H–1 -> L+4 (7%) H–1 -> L+5 (4%) H -> L+4 (2%)	4.201	295.1	0.0574	LC(C^N)/LLCT

S19:	H–6 -> L (9%) H–2 -> L+3 (82%)	4.283	289.5	0.0597	LC(C^N)/LLCT
S21:	H–6 -> L (79%) H–2 -> L+3 (10%) H–1 -> L+4 (3%)	4.339	285.8	0.1123	LC(C^N)
S23:	H–6 -> L+1 (8%) H–5 -> L+4 (3%) H–4 -> L+4 (4%) H–1 -> L+4 (4%) H -> L+4 (16%) H -> L+5 (55%)	4.383	282.9	0.1226	LC(C^C)

[a] H = HOMO; L = LUMO.

Table S21. Lowest-energy vertical triplet excitations of **2cb** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**	**main character**
T1:	H–2 -> L (83%) H–2 -> L+2 (3%) H–2 -> L+3 (5%) H–1 -> L (2%)	2.495	496.9	LC(C^N)
T2:	H–3 -> L+1 (9%) H–2 -> L+1 (2%) H–1 -> L+1 (75%) H–1 -> L+2 (3%) H–1 -> L+3 (3%)	2.525	491.0	LC(C^N)
T3:	H–8 -> L+13 (3%) H -> L+2 (8%) H -> L+4 (70%) H -> L+5 (3%)	2.945	421.0	LC(C^C)

[a] H = HOMO; L = LUMO.

5.6. Complex 2cc

Table S22. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **2cc** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	Pt
–0.018	146 (LUMO+5)	15	6	62	16
–0.025	145 (LUMO+4)	8	11	67	14
–0.036	144 (LUMO+3)	48	49	1	2
–0.041	143 (LUMO+2)	49	45	4	2
–0.060	142 (LUMO+1)	96	1	0	2
–0.061	141 (LUMO)	2	94	0	3
–0.200	140 (HOMO)	0	0	97	2
–0.213	139 (HOMO–1)	74	13	8	5
–0.214	138 (HOMO–2)	5	90	1	4
–0.233	137 (HOMO–3)	48	23	24	4
–0.240	136 (HOMO–4)	2	3	86	8
–0.241	135 (HOMO–5)	2	26	63	9

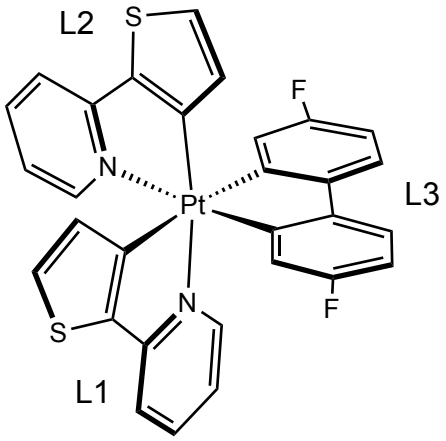


Figure S34. Ligand numbering in complex **2cc**.

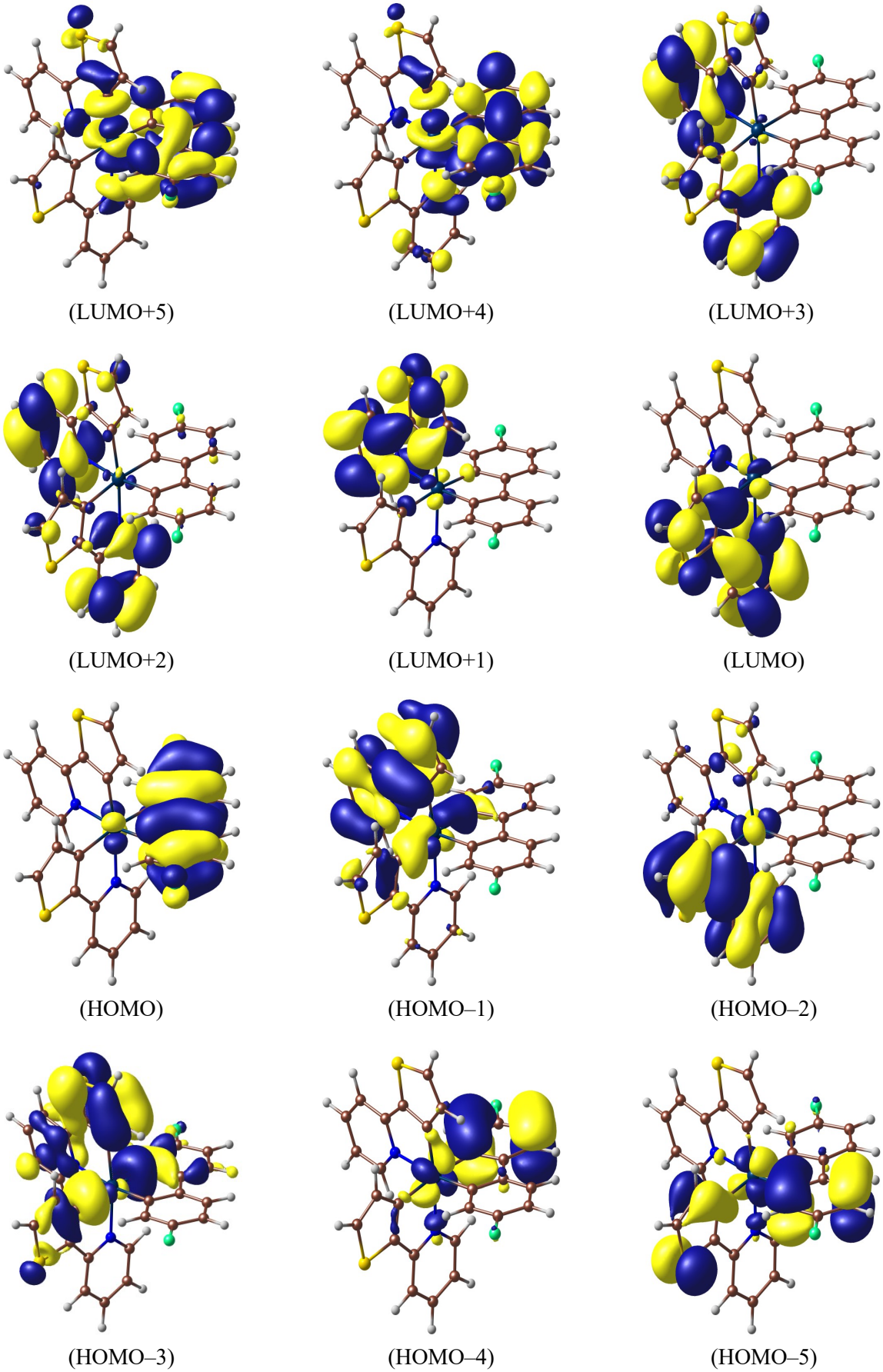


Figure S35. Molecular orbital isosurfaces of **2cc** (0.03 e bohr^{-3}).

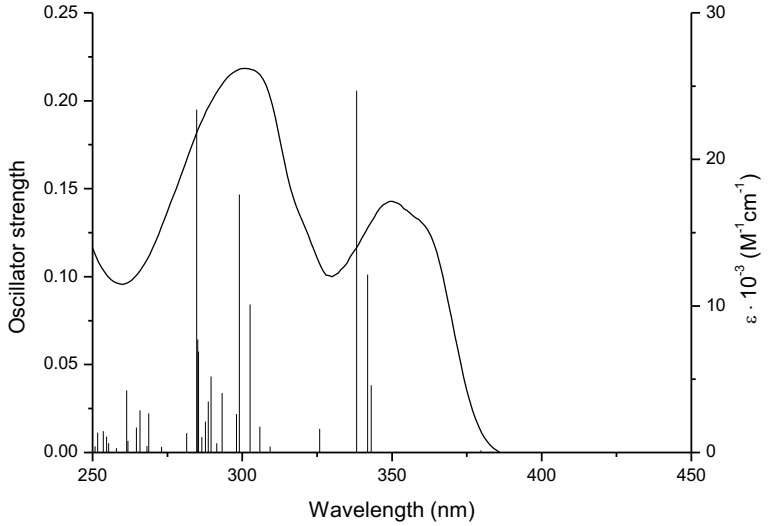


Figure S36. Calculated stick absorption spectrum of **2cc** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S23. Selected vertical singlet excitations of **2cc** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**	**Oscillator strength**	**main character**
S4:	H–2 -> L (18%) H–2 -> L+1 (75%) H–1 -> L (2%)	3.618	342.7	0.0388	LLCT
S5:	H–2 -> L (36%) H–2 -> L+1 (19%) H–1 -> L+1 (36%)	3.630	341.5	0.1018	LC(C^N)/LLCT
S6:	H–2 -> L (32%) H–2 -> L+1 (4%) H–2 -> L+2 (4%) H–1 -> L+1 (53%)	3.669	337.9	0.2062	LC(C^N)
S7:	H -> L+2 (93%) H -> L+3 (6%)	3.809	325.5	0.0141	LLCT
S11:	H–3 -> L+1 (24%) H–1 -> L+2 (63%) H–1 -> L+3 (3%) H -> L+4 (3%)	4.102	302.3	0.0848	LC(C^N)/LLCT
S12:	H–3 -> L+1 (57%) H–2 -> L+2 (9%) H–1 -> L+1 (4%) H–1 -> L+2 (20%)	4.151	298.7	0.1473	LC(C^N)
S14:	H–1 -> L+3 (64%) H–1 -> L+4 (16%) H–1 -> L+5 (7%)	4.233	292.9	0.0344	LC(C^N)/LLCT
S16:	H–6 -> L (4%)	4.286	289.3	0.0437	LLCT

	H–4 -> L (2%) H–4 -> L+1 (71%) H–2 -> L+3 (16%)				
S22:	H–6 -> L+1 (6%) H–5 -> L+1 (5%) H–4 -> L+4 (3%) H–1 -> L+4 (3%) H -> L+4 (20%) H -> L+5 (48%)	4.359	284.4	0.1956	LC(C^C)

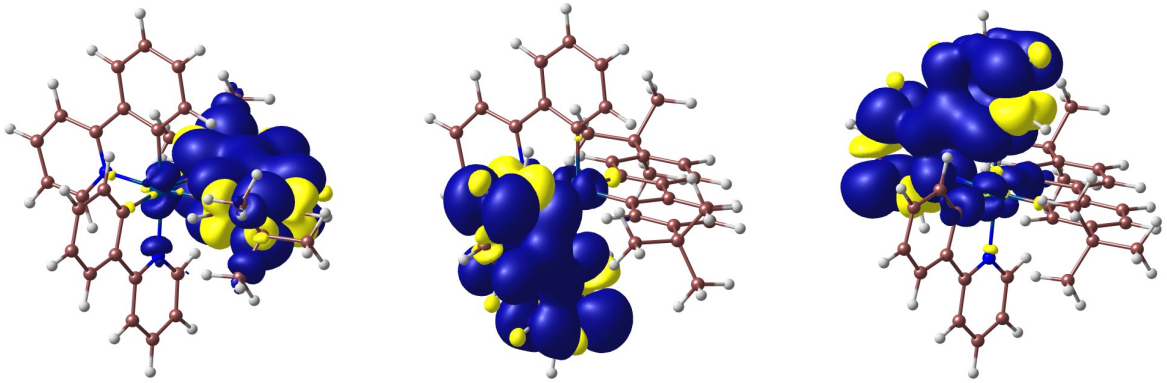
[a] H = HOMO; L = LUMO.

Table S24. Lowest-energy vertical triplet excitations of **2cc** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

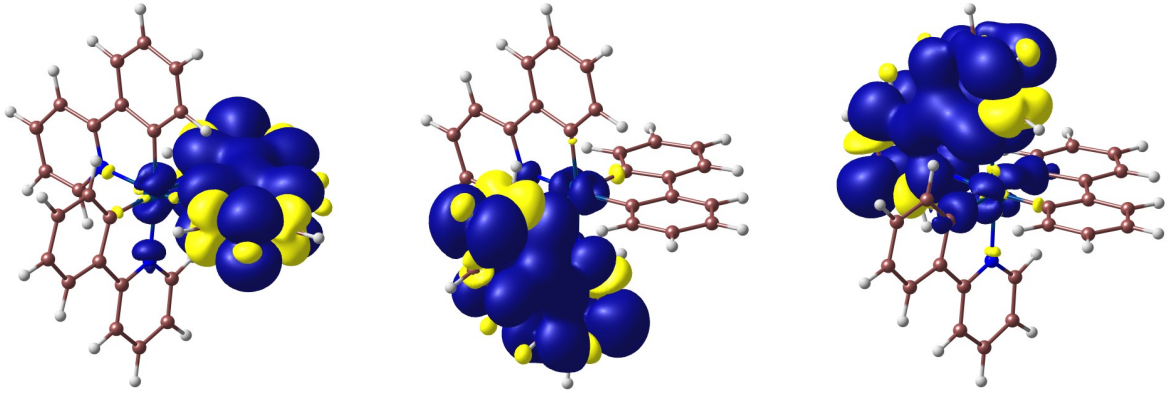
state	**monoexcitations[a]**	**ΔE/eV**	**λ/nm**	**main character**
T1:	H–2 -> L (79%) H–2 -> L+2 (3%) H–2 -> L+3 (5%) H–1 -> L (6%)	2.498	496.4	LC(C^N)
T2:	H–3 -> L+1 (7%) H–2 -> L+1 (6%) H–1 -> L+1 (75%) H–1 -> L+2 (3%) H–1 -> L+3 (3%)	2.529	490.2	LC(C^N)
T3:	H–4 -> L+8 (2%) H -> L+2 (6%) H -> L+4 (62%) H -> L+5 (12%)	2.960	418.8	LC(C^C)

[a] H = HOMO; L = LUMO.

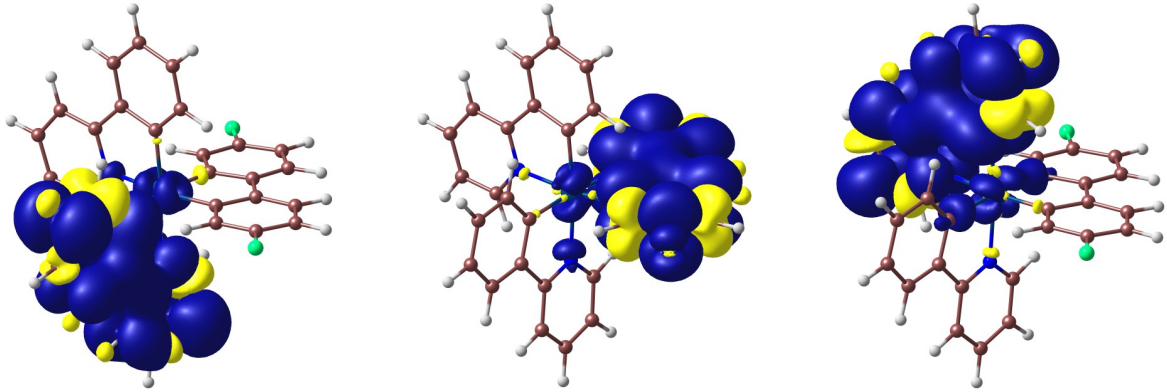
5.7. Spin densities



2aa (T_1) **2aa** (T_2) **2aa** (T_3)

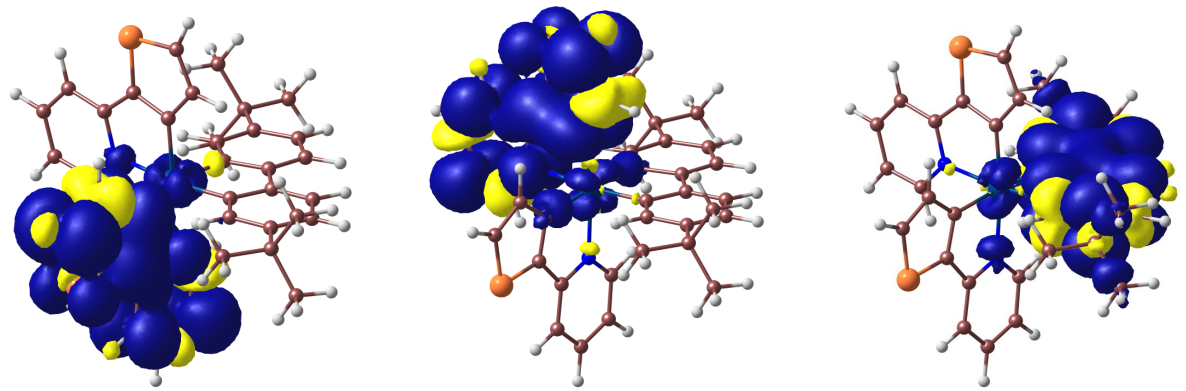


2ab (T_1) **2ab** (T_2) **2ab** (T_3)

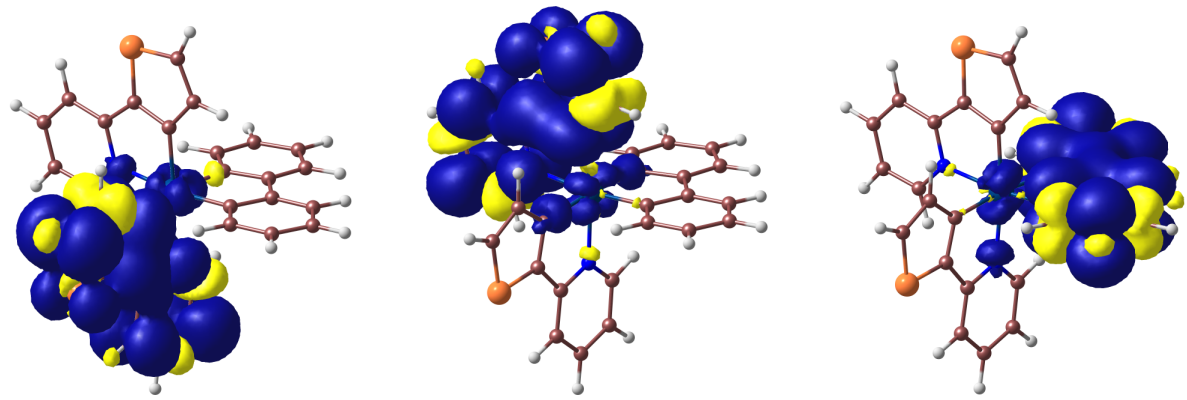


2ac (T_1) **2ac** (T_2) **2ac** (T_3)

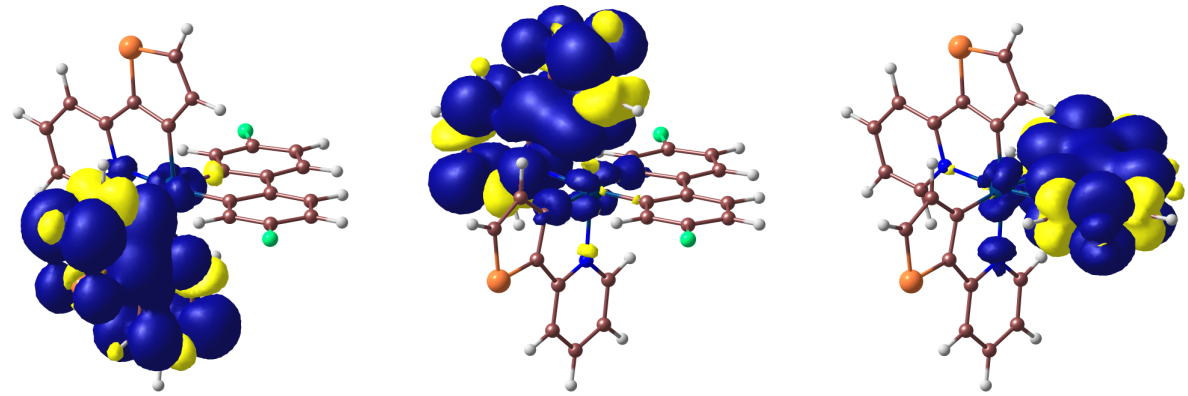
Figure S37. Spin density distributions (0.001 e $bohr^{-3}$) for the lowest triplet excited states of complexes **2aa**, **2ab** and **2ac**.



2ca (T_1) **2ca** (T_2) **2ca** (T_3)



2cb (T_1) **2cb** (T_2) **2cb** (T_3)



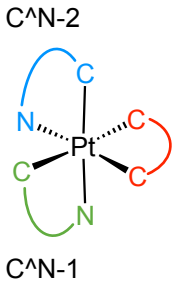
2cc (T_1) **2cc** (T_2) **2cc** (T_3)

Figure S38. Spin density distributions (0.001 e $bohr^{-3}$) for the lowest triplet excited states of complexes **2ca**, **2cb** and **2cc**.

Table S25. Natural spin densities on the Pt atom for the lowest triplet excited states of complexes **2** (ppy and thpy derivatives).

Complex	State	Involved ligand[a]	Spin density on Pt
2aa	T_1	C^C	0.0167
	T_2	C^N-1	0.0265
	T_3	C^N-2	0.0349
2ab	T_1	C^C	0.0188
	T_2	C^N-1	0.0255
	T_3	C^N-2	0.0322
2ac	T_1	C^N-1	0.0230
	T_2	C^C	0.0168
	T_3	C^N-2	0.0281
2ca	T_1	C^N-1	0.0228
	T_2	C^N-2	0.0246
	T_3	C^C	0.0200
2cb	T_1	C^N-1	0.0223
	T_2	C^N-2	0.0235
	T_3	C^C	0.0215
2cc	T_1	C^N-1	0.0208
	T_2	C^N-2	0.0213
	T_3	C^C	0.0215

[a] See figure for ligand numeration.



5.8. Supplementary computational data

Table S26. Energies, free energies, enthalpies and entropies of the optimized structures in CH_2Cl_2 solution.[a]

Structure	E_0 [b]	ZPE [c]	G [d]	H [e]	S [f]
2aa (S_0)	-1853.327077	-1852.621434	-1852.694237	-1852.580303	239.793
2aa (T_1)	-1853.224788	-1852.523787	-1852.598844	-1852.481913	246.103
2aa (T_2)	-1853.223010	-1852.522242	-1852.597497	-1852.480319	246.621
2aa (T_3)	-1853.222399	-1852.521494	-1852.596239	-1852.479630	245.425
2ab (S_0)	-1538.801482	-1538.320320	-1538.379900	-1538.290568	188.014
2ab (T_1)	-1538.697214	-1538.220954	-1538.282534	-1538.190458	193.789
2ab (T_2)	-1538.697391	-1538.221068	-1538.282831	-1538.190550	194.222
2ab (T_3)	-1538.696663	-1538.220212	-1538.281696	-1538.189743	193.533
2ac (S_0)	-1737.267245	-1736.802667	-1736.864667	-1736.771109	196.910
2ac (T_1)	-1737.163096	-1736.703309	-1736.767330	-1736.671010	202.721
2ac (T_2)	-1737.162589	-1736.702936	-1736.767182	-1736.670505	203.474
2ac (T_3)	-1737.162255	-1736.702388	-1736.766232	-1736.670126	202.272
2ca (S_0)	-2494.832350	-2494.194017	-2494.266868	-2494.153317	238.987
2ca (T_1)	-2494.746407	-2494.112052	-2494.186630	-2494.070683	244.031
2ca (T_2)	-2494.745436	-2494.111084	-2494.185702	-2494.069696	244.155
2ca (T_3)	-2494.730039	-2494.096397	-2494.171547	-2494.054915	245.472
2cb (S_0)	-2180.306685	-2179.892808	-2179.952322	-2179.863503	186.936
2cb (T_1)	-2180.220695	-2179.810796	-2179.872039	-2179.780821	191.984
2cb (T_2)	-2180.219677	-2179.809816	-2179.871164	-2179.779810	192.272
2cb (T_3)	-2180.202321	-2179.793356	-2179.854825	-2179.763295	192.641
2cc (S_0)	-2378.771947	-2378.374642	-2378.436526	-2378.343547	195.690
2cc (T_1)	-2378.685888	-2378.292550	-2378.356151	-2378.260788	200.708
2cc (T_2)	-2378.684821	-2378.291536	-2378.355250	-2378.259740	201.016
2cc (T_3)	-2378.667279	-2378.274941	-2378.339099	-2378.242940	202.384

[a] Thermal corrections from vibrational calculations at 298.15 K. [b] Electronic energy (Hartrees). [c] Sum of electronic and zero-point energies (Hartrees). [d] Free Energy (Hartrees). [e] Enthalpy (Hartrees). [f] Entropy (cal mol^{-1} K^{-1}).

Table S27. Cartesian coordinates (Å) of the optimized structures at the B3LYP(6-31G**+LANL2DZ) level in CH_2Cl_2 solution.

2aa (S_0)

Pt	-0.521953696	-0.011695575	0.177410158
C	-0.075123501	1.180723461	1.743365848
C	-0.097387839	0.826229501	3.097818941
C	0.216758994	1.756414290	4.091260139
C	0.563410117	3.067688038	3.751279219
C	0.591598696	3.441137127	2.412248420
C	0.276045579	2.513831507	1.402335469
C	0.286241819	2.871661761	-0.023379453
C	0.610918417	4.135507088	-0.542698252
C	0.580725722	4.349055545	-1.914916925
C	0.224691145	3.299538842	-2.766435346
C	-0.087214197	2.071806640	-2.197485056
H	-0.363546069	-0.185328356	3.382019588
H	0.191555109	1.455221051	5.135371529
H	0.808785480	3.790967290	4.523004114
H	0.859357071	4.461541880	2.155844940
H	0.885025088	4.943181047	0.124584040
H	0.831802102	5.324921264	-2.318508951
H	0.188161926	3.425350103	-3.842352020
H	-0.372154991	1.219925568	-2.804910623
N	-0.054583901	1.867277188	-0.871934862
C	-2.576146060	0.475952030	0.071119592
C	-3.313577930	1.311219291	0.920692926
C	-4.674856066	1.554795837	0.713467433
C	-5.338268173	0.961963285	-0.365314828
C	-4.633500557	0.128944062	-1.229289624
C	-3.263527166	-0.117987388	-1.019174394
C	-2.486679687	-1.000248296	-1.910708728
C	-3.010414412	-1.692276785	-3.015263019
C	-2.184829994	-2.499278297	-3.788274429
C	-0.833127427	-2.617287765	-3.456820237
C	-0.366465518	-1.914475639	-2.353631525
H	-2.820590441	1.780320835	1.768409431
H	-5.220122203	2.206295201	1.392399579
H	-6.395163941	1.148286076	-0.532393572
H	-5.159846400	-0.323098480	-2.064785585
H	-4.060366533	-1.600681945	-3.263869411
H	-2.592344006	-3.033884671	-4.640720344
H	-0.155845504	-3.237978086	-4.031979010
H	0.668966553	-1.964251782	-2.036048349
N	-1.165575778	-1.131371380	-1.610519911
C	-0.777969906	-1.711152442	1.281271832
C	-1.977792120	-2.150325446	1.835365625

C	-2.074388924	-3.352011259	2.569130445
C	-0.904978881	-4.105716742	2.728164348
C	0.307779580	-3.679909136	2.180471642
C	0.396459729	-2.486367256	1.454739336
C	1.624175885	-1.946920475	0.844499123
C	2.886921534	-2.556619912	0.885775583
C	3.983186073	-1.955304156	0.271458284
C	3.862708109	-0.728035254	-0.403927442
C	2.587795924	-0.132135157	-0.435947337
H	-2.866228481	-1.544363488	1.698963352
H	-0.922253517	-5.037415629	3.282566043
H	1.192778209	-4.293870476	2.328547655
H	3.026837824	-3.506044712	1.397602507
H	4.947291680	-2.453818881	0.323947314
H	2.464629760	0.816245815	-0.948031847
C	5.101814908	-0.094902411	-1.066157000
C	1.469574471	-0.715235319	0.170387812
C	6.184559862	0.167320942	0.008381844
H	6.489874603	-0.755309346	0.510876104
H	7.077426611	0.610455382	-0.448048389
H	5.815644261	0.858978561	0.773347035
C	5.669450367	-1.061857450	-2.133109501
H	6.557651466	-0.629168058	-2.608223615
H	5.959137392	-2.022769281	-1.697547057
H	4.928545322	-1.258558465	-2.915703802
C	4.782790550	1.244448568	-1.757774688
H	4.041437788	1.125567528	-2.554925438
H	4.404516512	1.988796970	-1.049502183
H	5.693472421	1.650731423	-2.210694019
C	-3.434592099	-3.778637693	3.152405902
C	-3.350383309	-5.110987137	3.921556334
H	-4.338139772	-5.372035714	4.315816695
H	-3.023583622	-5.933580407	3.276785892
H	-2.661231978	-5.048464109	4.770271904
C	-3.943961371	-2.691033028	4.128662313
H	-3.244005807	-2.553881097	4.959975894
H	-4.067454021	-1.724687923	3.630999003
H	-4.915551660	-2.978263687	4.547303515
C	-4.458193093	-3.950209181	2.004058151
H	-4.592742192	-3.023483222	1.438464982
H	-4.131972179	-4.726662254	1.303572790
H	-5.435789613	-4.243472804	2.404187129

2aa (T_1)

$\langle S^2 \rangle$ = 2.033636

Pt	-0.527272792	0.015975358	0.184935710
C	-0.075969603	1.203110913	1.752901516
C	-0.090049618	0.841107123	3.105151644
C	0.230365158	1.767052525	4.101045653
C	0.576099412	3.079312575	3.764365497
C	0.599552277	3.458462417	2.426682116
C	0.277873721	2.535838851	1.414207243
C	0.284352814	2.897431666	-0.010419322
C	0.609518410	4.162471987	-0.527007062
C	0.573670747	4.380466972	-1.898314958
C	0.210445373	3.334884194	-2.751812491
C	-0.101938496	2.105874616	-2.185534112
H	-0.355286929	-0.171649823	3.385743657
H	0.210791073	1.461461406	5.143969887
H	0.826200131	3.799091643	4.537885403
H	0.870017992	4.478872461	2.173218797
H	0.888429476	4.967269481	0.141770425
H	0.825559038	5.356999513	-2.299838689
H	0.169203919	3.464530075	-3.827094496
H	-0.392581347	1.256639071	-2.793879077
N	-0.062419617	1.896617108	-0.861005865
C	-2.584749006	0.495881205	0.075524341
C	-3.321687905	1.334188303	0.922344504
C	-4.684564648	1.572689182	0.719004521
C	-5.350269860	0.970199384	-0.352777146
C	-4.646074660	0.133476718	-1.213861959
C	-3.274298796	-0.107397787	-1.008589156
C	-2.499434272	-0.991407199	-1.901456461
C	-3.028193825	-1.697450858	-2.994698424
C	-2.202318016	-2.505810889	-3.767205036
C	-0.845981999	-2.606991871	-3.450113312
C	-0.374154189	-1.885565030	-2.360498399
H	-2.826745260	1.809945871	1.765267272
H	-5.228992187	2.227291182	1.395642064
H	-6.408480475	1.151789377	-0.516922553
H	-5.174493074	-0.326359692	-2.043794213
H	-4.080934197	-1.616768981	-3.235320622
H	-2.613795005	-3.053811772	-4.609244199
H	-0.169391221	-3.227432272	-4.026527542
H	0.667420630	-1.911764595	-2.058378179
N	-1.174582227	-1.106528863	-1.616077722
C	-0.792353251	-1.674900059	1.281679944
C	-1.968234349	-2.129802836	1.817897738
C	-2.059216698	-3.351948821	2.568854384
C	-0.855413398	-4.090780746	2.767192583
C	0.347816743	-3.673096524	2.258223465
C	0.446268299	-2.445940178	1.478865061
C	1.600940575	-1.940004721	0.903495719
C	2.922495401	-2.546658240	0.964346255
C	3.982053015	-1.956212484	0.334115370
C	3.855835102	-0.728043377	-0.400169457
C	2.559519988	-0.127019118	-0.449199232
H	-2.869623121	-1.545593005	1.672432066
H	-0.882485180	-5.012733506	3.338275024
H	1.241004396	-4.263062602	2.440064098
H	3.069757190	-3.474396547	1.509723884
H	4.955831764	-2.435221878	0.394985523
H	2.445179210	0.808384189	-0.987106618
C	5.089894370	-0.128804497	-1.082150398
C	1.454409521	-0.678195240	0.160684141
C	6.182145544	0.163185872	-0.021348933
H	6.480218124	-0.741523273	0.516884829
H	7.077938485	0.576353724	-0.499926460
H	5.824643872	0.889892847	0.715830913
C	5.652320053	-1.135789264	-2.118316779
H	6.546961186	-0.726387968	-2.602254755
H	5.931288540	-2.085975265	-1.653046991
H	4.912112013	-1.347978128	-2.897317480
C	4.777996527	1.188352070	-1.818591325
H	4.033604986	1.046645123	-2.609035939
H	4.406382947	1.958546373	-1.134912253
H	5.689866343	1.573171856	-2.287466678
C	-3.418956785	-3.800195385	3.113436628

C	-3.336014511	-5.130850869	3.886307758
H	-4.330695074	-5.408065170	4.250896695
H	-2.976467061	-5.948211999	3.252360484
H	-2.674358135	-5.056687614	4.755733103
C	-3.976716336	-2.719717441	4.075095255
H	-3.307601297	-2.576516606	4.930303762
H	-4.095488101	-1.753737473	3.575676786
H	-4.958692613	-3.020890994	4.458625754
C	-4.412736910	-3.988605515	1.938484056
H	-4.542510942	-3.066517477	1.364409827
H	-4.060621257	-4.765747555	1.251600758
H	-5.397060083	-4.289463758	2.316253169

2aa (T_2)

$\langle S^2 \rangle = 2.030253$

Pt	-0.5182075951	-0.0130363119	0.1848706926
C	-0.0682889884	1.1901737137	1.747325974
C	-0.0905403263	0.8438853089	3.1038374976
C	0.226044274	1.778290284	4.0927006436
C	0.5748592221	3.0869261734	3.7453050212
C	0.6028295119	3.4530984659	2.404108384
C	0.285119701	2.5210527296	1.3992012091
C	0.2971858371	2.8737271495	-0.0287986203
C	0.6247437438	4.1351522267	-0.5524312468
C	0.5965266663	4.3433397567	-1.9257616363
C	0.2410884349	3.2912771082	-2.7743434073
C	-0.0721322135	2.0656109311	-2.2010805122
H	-0.3587543102	-0.165821521	3.393505224
H	0.2009253287	1.482811964	5.1384719398
H	0.8220766473	3.814040458	4.5128660732
H	0.8722076472	4.4717918413	2.1425934279
H	0.8997891427	4.9451789515	0.1116220797
H	0.8493603566	5.3174797853	-2.3324952238
H	0.2066346257	3.4135863542	-3.8507627074
H	-0.3551713922	1.2093473585	-2.8035636377
N	-0.0429046813	1.8676540939	-0.8749939369
C	-2.5578685108	0.4797487723	0.1002087555
C	-3.2988694771	1.2970944319	0.9326419447
C	-4.6764013843	1.5318709435	0.7326300416
C	-5.3548642254	0.9056169972	-0.3608280319
C	-4.6879395249	0.0859925351	-1.2250406219
C	-3.2622752132	-0.1612153319	-1.0464679496
C	-2.5194358939	-0.9733619451	-1.9025645683
C	-3.0388931643	-1.6770819904	-3.0541385403
C	-2.2250636035	-2.4664849479	-3.8220268779
C	-0.8519867881	-2.5914924346	-3.4730126631
C	-0.375876221	-1.8906603792	-2.3509923914
H	-2.8111652141	1.7748836618	1.7785866897
H	-5.2284936199	2.1815184625	1.4049441278
H	-6.4168863494	1.0877692409	-0.5009746842
H	-5.223923004	-0.3798258654	-2.0444776793
H	-4.0878797188	-1.5738889518	-3.3046230763
H	-2.6210966125	-2.9927079761	-4.6842494582
H	-0.1714606751	-3.2086654452	-4.047067403
H	0.6656807887	-1.962681377	-2.0526370177
N	-1.137621075	-1.112603761	-1.5992761026
C	-0.7732856549	-1.7105149504	1.2890228741
C	-1.974963841	-2.1499097154	1.8386749391
C	-2.074224184	-3.3525080737	2.5703369383
C	-0.9050458944	-4.1060236243	2.7322679107
C	0.3093347244	-3.6799650028	2.18838044
C	0.4004106435	-2.4860513491	1.4636261742
C	1.6279261259	-1.9472371629	0.8533396987
C	2.8912217958	-2.5554769074	0.8971908732
C	3.9871084796	-1.9545878757	0.2819459889
C	3.8654487326	-0.7291643548	-0.3965871003
C	2.5900067981	-0.1346242865	-0.4309912306
H	-2.8621327731	-1.5412945388	1.7027006693
H	-0.9240168824	-5.0382433758	3.2856833383
H	1.193630595	-4.2946399631	2.3375362818
H	3.0316588243	-3.5033463353	1.4117331324
H	4.9517830703	-2.4517768419	0.3362719228
H	2.4661200475	0.8120985916	-0.9457315566
C	5.1042142113	-0.0961872389	-1.0596191687
C	1.4721299136	-0.7174486316	0.176153552
C	6.1858667379	0.1700401633	0.0150428633
H	6.49197411	-0.7509408608	0.5200782317
H	7.0785114101	0.6131376405	-0.4418543078
H	5.8155339615	0.8631759308	0.777995801
C	5.6737179151	-1.0651278453	-2.1237610738
H	6.5617073941	-0.6325400556	-2.5993632666
H	5.9642847483	-2.0245899524	-1.6855995877
H	4.9335583571	-1.2646914755	-2.9063209547
C	4.7840669962	1.2410634479	-1.7547702512
H	4.0433834432	1.1193397625	-2.5521001102
H	4.404464126	1.9867289546	-1.0485879218
H	5.694581026	1.6472834617	-2.2080828055
C	-3.4360580111	-3.779894109	3.1492805136
C	-3.3544486206	-5.1150038446	3.9139192578
H	-4.3433655078	-5.37689991	4.3046640649
H	-3.0263870776	-5.9353942245	3.2670143185
H	-2.6675332771	-5.0558610086	4.7646681766
C	-3.9462383563	-2.6952539985	4.1284066013
H	-3.2477225677	-2.5615927529	4.9614770212
H	-4.0679100401	-1.7269944349	3.6339374621
H	-4.9188748121	-2.983018902	4.5442278498
C	-4.4576766358	-3.9467255517	1.99852092
H	-4.5914126538	-3.0177739645	1.4363830437
H	-4.1304035281	-4.7202428436	1.295353051
H	-5.4359349253	-4.2414626163	2.3959023465

2aa (T_3)

$\langle S^2 \rangle = 2.028266$

Pt	-0.537457296	-0.010407936	0.197088597
C	-0.108774566	1.157206570	1.758231675
C	-0.167287377	0.835674092	3.104613460
C	0.167656731	1.767783144	4.100539151
C	0.594007775	3.086456960	3.731923619
C	0.671164385	3.465799618	2.423492791
C	0.313629220	2.536620155	1.365691071
C	0.332304112	2.868555168	0.011095844
C	0.700935516	4.149978646	-0.541009139
C	0.655808005	4.364953057	-1.895404504
C	0.242119525	3.313527076	-2.753472668
C	-0.099568201	2.075737680	-2.176522906
H	-0.477117164	-0.160821323	3.398147138
H	0.112257934	1.493797708	5.148961563
H	0.859695665	3.793607043	4.512992789

H	0.996091593	4.468945176	2.171557562
H	1.013663680	4.944305072	0.126043085
H	0.932475957	5.330064444	-2.307272460
H	0.187393097	3.439763500	-3.827856707
H	-0.415893197	1.246480852	-2.802645506
N	-0.056779986	1.844392108	-0.877472501
C	-2.594502240	0.462921673	0.063900778
C	-3.343204453	1.284347776	0.916810966
C	-4.702009537	1.527194507	0.693477133
C	-5.348944430	0.946333506	-0.401560134
C	-4.631277568	0.124274918	-1.265347767
C	-3.263493039	-0.121714494	-1.040860628
C	-2.472465753	-0.995339531	-1.927560954
C	-2.979039874	-1.678435736	-3.045294606
C	-2.141343647	-2.479999502	-3.810918490
C	-0.795326264	-2.600418013	-3.458432603
C	-0.345982681	-1.905422152	-2.343124642
H	-2.862927468	1.739065182	1.779372655
H	-5.257778847	2.168948517	1.373075258
H	-6.403854883	1.132426808	-0.580633201
H	-5.145690803	-0.321103549	-2.111669996
H	-4.024813018	-1.584096191	-3.309934016
H	-2.535060744	-3.008142479	-4.673783831
H	-0.108706325	-3.216763677	-4.027127624
H	0.684673285	-1.956908654	-2.011205208
N	-1.156660084	-1.128099731	-1.606531565
C	-0.789798293	-1.713688243	1.301101549
C	-1.986879814	-2.157451839	1.856863445
C	-2.077875631	-3.361043537	2.588357666
C	-0.905616804	-4.111392243	2.742466528
C	0.304379340	-3.681264999	2.192111166
C	0.387316085	-2.485866363	1.468896071
C	1.612167049	-1.944933113	0.853541000
C	2.876422488	-2.552689972	0.886202264
C	3.967594130	-1.950204840	0.263910261
C	3.842805361	-0.723948540	-0.412794294
C	2.567071893	-0.129127528	-0.438127004
H	-2.877513657	-1.553611464	1.724231862
H	-0.918546620	-5.044176864	3.295093854
H	1.191339540	-4.293253625	2.336246639
H	3.020700310	-3.502152942	1.396579814
H	4.932303544	-2.448064364	0.310378762
H	2.435328216	0.818194547	-0.949824224
C	5.076953700	-0.090082838	-1.083041125
C	1.458213406	-0.714943123	0.178257065
C	6.164656818	0.176902831	-0.014739009
H	6.474207781	-0.743860585	0.488642651
H	7.054273202	0.620325416	-0.477094121
H	5.798538236	0.870096786	0.750165701
C	5.640643492	-1.058768235	-2.150537869
H	6.524992816	-0.625036194	-2.631736246
H	5.935358972	-2.017777214	-1.714139759
H	4.895815476	-1.259283570	-2.928390663
C	4.750613102	1.246669096	-1.776166508
H	4.005100171	1.123846840	-2.568821495
H	4.374314440	1.991891445	-1.067820410
H	5.657662203	1.654066711	-2.235242250
C	-3.434825810	-3.793183193	3.174985186
C	-3.343787596	-5.126368684	3.941896209
H	-4.329466668	-5.391177060	4.338779717
H	-3.016345652	-5.946960759	3.294922543
H	-2.652276907	-5.062808533	4.788610071
C	-3.944825411	-2.708719783	4.154421333
H	-3.242706878	-2.570278664	4.983695127
H	-4.073517169	-1.742113015	3.658576789
H	-4.913997408	-3.000065901	4.575734690
C	-4.461143362	-3.966418568	2.029336890
H	-4.600640872	-3.039238093	1.465690321
H	-4.134363996	-4.740605206	1.326635647
H	-5.436480189	-4.263674506	2.431951657

2ab (S_0)

Pt	-0.523682299	-0.013684574	0.177278959
C	-0.078810172	1.179497082	1.744143908
C	-0.098791449	0.824654542	3.098324675
C	0.213555522	1.755842090	4.091513048
C	0.556135231	3.067948663	3.751086011
C	0.582193168	3.441475023	2.412002130
C	0.268328436	2.513308288	1.402447326
C	0.276409381	2.870686694	-0.023341359
C	0.595535002	4.135543294	-0.543197641
C	0.564686482	4.348220345	-1.915535629
C	0.213392530	3.296732980	-2.766513215
C	-0.093716465	2.068036643	-2.197180679
H	-0.361422132	-0.187563363	3.383432957
H	0.190105416	1.454558850	5.135602642
H	0.800164457	3.791950777	4.522526367
H	0.847030125	4.462536924	2.155309121
H	0.866091825	4.944665262	0.123748402
H	0.811631257	5.324921052	-2.319606227
H	0.176863626	3.421671861	-3.842510715
H	-0.375023353	1.214826040	-2.804327343
N	-0.060511565	1.864493975	-0.871417094
C	-2.576444728	0.476215584	0.070905565
C	-3.312699978	1.311029602	0.921682959
C	-4.671258343	1.564397557	0.708627297
C	-5.332511253	0.982624815	-0.377421968
C	-4.628821354	0.149393696	-1.241930674
C	-3.262005580	-0.108490327	-1.025447119
C	-2.486942122	-0.992859468	-1.916192079
C	-3.011065564	-1.681108816	-3.022878282
C	-2.187434604	-2.491396149	-3.794499712
C	-0.837253771	-2.616499424	-3.459509960
C	-0.370082494	-1.917264303	-2.354361239
H	-2.821099520	1.772674996	1.774237022
H	-5.215907618	2.215376004	1.388506014
H	-6.387067423	1.177412092	-0.549448564
H	-5.153521325	-0.294372412	-2.082852844
H	-4.059956706	-1.584334712	-3.273891478
H	-2.595304843	-3.023122624	-4.648552892
H	-0.161432721	-3.239833990	-4.033490827
H	0.664413310	-1.972696953	-2.034911550
N	-1.167278560	-1.130946536	-1.612447809
C	-0.774585950	-1.711425021	1.281660936
C	-1.975795746	-2.151724046	1.842172046
C	-2.031187581	-3.348343113	2.569373718
C	-0.878362964	-4.116067439	2.739894768
C	0.327928841	-3.686058456	2.185834515

C	0.399003894	-2.488253180	1.457358187
C	1.628869719	-1.948411766	0.844518126
C	2.887200463	-2.568159251	0.893187748
C	3.990901282	-1.973439892	0.278620126
C	3.842051082	-0.755189021	-0.387681446
C	2.585708309	-0.134805143	-0.437873566
H	-2.877889637	-1.561973550	1.720384923
H	-0.915821823	-5.045095346	3.302367400
H	1.220485242	-4.289842363	2.326584344
H	3.016374752	-3.516544420	1.408785700
H	4.962153723	-2.459273301	0.322044955
H	2.492095181	0.814713942	-0.960555917
C	1.467024456	-0.713893902	0.168697579
H	4.699849684	-0.287936910	-0.865935924
H	-2.974512894	-3.674462293	3.000197242

2ab (T_1)

$\langle S^2 \rangle = 2.037652$

Pt	-0.529931686	-0.003957239	0.168548630
C	-0.079699924	1.180340416	1.739982484
C	-0.093579117	0.815228297	3.091173549
C	0.225408190	1.739612229	4.088936807
C	0.569124189	3.052943742	3.754869459
C	0.591879763	3.434916612	2.417959830
C	0.271709408	2.514008633	1.403682193
C	0.278182470	2.878059218	-0.020380453
C	0.599681127	4.144742914	-0.534369938
C	0.566008478	4.364452037	-1.905522050
C	0.208704336	3.318654640	-2.761013978
C	-0.101002133	2.087878192	-2.197290800
H	-0.357633511	-0.198256691	3.370377948
H	0.206242262	1.431770022	5.131156760
H	0.818143630	3.771511083	4.529802967
H	0.860578756	4.456263379	2.166582211
H	0.874368633	4.949534624	0.136115577
H	0.815172384	5.342399407	-2.305218527
H	0.169751440	3.449358568	-3.836233218
H	-0.387351935	1.238705963	-2.807613211
N	-0.064019841	1.877265964	-0.872794855
C	-2.584785662	0.483103094	0.057981406
C	-3.319591321	1.319932321	0.907818192
C	-4.678967323	1.571826221	0.697768734
C	-5.342591022	0.985215804	-0.384019720
C	-4.640313931	0.149477215	-1.247451818
C	-3.272469605	-0.106102328	-1.034916005
C	-2.500282590	-0.990921515	-1.929056034
C	-3.029630467	-1.687720966	-3.027870731
C	-2.206275246	-2.496733827	-3.802157426
C	-0.851628770	-2.608294033	-3.481054084
C	-0.379318940	-1.896978547	-2.385251707
H	-2.825981630	1.784492181	1.757675277
H	-5.222135923	2.224946201	1.376784246
H	-6.397870841	1.178130302	-0.553850450
H	-5.167136701	-0.298147080	-2.085001267
H	-4.081080319	-1.599347703	-3.271313967
H	-2.618249783	-3.037165089	-4.648799113
H	-0.176778452	-3.229086586	-4.059063333
H	0.661045293	-1.932328286	-2.080088486
N	-1.177363038	-1.117279692	-1.638931268
C	-0.795100511	-1.691481691	1.263101468
C	-1.972747204	-2.147884638	1.807800306
C	-2.021364750	-3.358092241	2.552884153
C	-0.834581521	-4.116890474	2.760265436
C	0.363080901	-3.700935142	2.244545138
C	0.447951107	-2.469098461	1.464160051
C	1.602602027	-1.963120708	0.889744900
C	2.924421680	-2.580400021	0.959824409
C	3.989015617	-1.996021970	0.326028098
C	3.832113917	-0.781460264	-0.400597833
C	2.556113558	-0.154790444	-0.469055271
H	-2.887220879	-1.579454385	1.675892235
H	-0.885288756	-5.036531718	3.337959486
H	1.261148444	-4.285727481	2.416259409
H	3.062395752	-3.504783164	1.512169747
H	4.970678298	-2.460862008	0.377628952
H	2.471386428	0.779999782	-1.019367766
C	1.449593876	-0.698993567	0.143518717
H	4.688529736	-0.333694791	-0.896364637
H	-2.965078558	-3.701889677	2.965192152

2ab (T_2)

$\langle S^2 \rangle = 2.030294$

Pt	-0.520140605	-0.018683543	0.186449748
C	-0.074076119	1.186669593	1.749160915
C	-0.095538027	0.841189304	3.105659606
C	0.217609316	1.777627386	4.093840354
C	0.562084798	3.086965589	3.745261267
C	0.589081008	3.452132483	2.403725068
C	0.274678965	2.518222631	1.399635808
C	0.285207338	2.869459791	-0.028656675
C	0.606861141	4.131692768	-0.553545808
C	0.578520016	4.338071339	-1.927148529
C	0.228764344	3.283293688	-2.774638462
C	-0.079237407	2.056861071	-2.200312297
H	-0.360118480	-0.169069327	3.396749142
H	0.193195096	1.482942859	5.139817015
H	0.806729187	3.815583785	4.512189181
H	0.855040821	4.471475738	2.141361628
H	0.877718458	4.943730460	0.109745127
H	0.826965401	5.312892642	-2.334910763
H	0.194829649	3.403983693	-3.851236578
H	-0.357707835	1.198670238	-2.802073259
N	-0.050070991	1.860827147	-0.873858178
C	-2.559071600	0.474681395	0.101860254
C	-3.303918043	1.273666576	0.947956657
C	-4.676657459	1.526787284	0.736013379
C	-5.344781815	0.941189183	-0.385787976
C	-4.674243987	0.136973427	-1.261437227
C	-3.256410229	-0.138913820	-1.063482919
C	-2.516074002	-0.957446535	-1.915548387
C	-3.034056633	-1.651639449	-3.073565668
C	-2.223847751	-2.450340768	-3.835573159
C	-0.855669684	-2.593771652	-3.474562974
C	-0.380504292	-1.901464663	-2.346973538
H	-2.822348929	1.727396786	1.810469238
H	-5.230830041	2.165885660	1.416639622
H	-6.401654829	1.142106259	-0.538442063
H	-5.202045466	-0.297687277	-2.102989139

H	-4.079950467	-1.536444441	-3.331538936
H	-2.619163207	-2.970530275	-4.701747668
H	-0.177738858	-3.217639720	-4.044408854
H	0.657875304	-1.986622290	-2.041312070
N	-1.138794012	-1.115376294	-1.600025468
C	-0.768986180	-1.714237148	1.292250704
C	-1.971973705	-2.156025940	1.847406381
C	-2.029057362	-3.352817090	2.573962685
C	-0.875706436	-4.118631705	2.749477994
C	0.332138387	-3.687298403	2.199827433
C	0.404635407	-2.489848152	1.470992264
C	1.634009046	-1.950016681	0.858268574
C	2.893662326	-2.566640412	0.910898003
C	3.996415023	-1.971821932	0.294910639
C	3.844997700	-0.756679285	-0.376503246
C	2.587385785	-0.139278171	-0.430356604
H	-2.873698585	-1.565533103	1.723817326
H	-0.914182765	-5.047609266	3.311923828
H	1.224746288	-4.290373969	2.343153413
H	3.024357618	-3.512537961	1.430653664
H	4.968839978	-2.455027082	0.341143971
H	2.492063071	0.807735142	-0.957024273
C	1.469626235	-0.718675336	0.177575954
H	4.701998694	-0.289365729	-0.856112981
H	-2.973800733	-3.680329906	3.000519850

2ab (T_3)

$\langle S^2 \rangle = 2.028907$

Pt	-0.543124128	-0.016072892	0.194913908
C	-0.109625075	1.154310997	1.755297630
C	-0.156370965	0.833000377	3.100958793
C	0.179069674	1.768628521	4.095134563
C	0.593040984	3.090243673	3.724160414
C	0.658775043	3.469331765	2.415337519
C	0.301338732	2.536003134	1.359733578
C	0.310619386	2.866756637	0.005704129
C	0.667305513	4.150948321	-0.549348835
C	0.615258406	4.364135520	-1.903583838
C	0.206290190	3.308635203	-2.758741792
C	-0.124412588	2.068448322	-2.179469016
H	-0.456872723	-0.165229632	3.398278178
H	0.132648155	1.493841143	5.143771509
H	0.858629140	3.799321290	4.503423201
H	0.974847344	4.474472940	2.160334723
H	0.976562322	4.948128669	0.115818108
H	0.882856499	5.330813600	-2.317657886
H	0.146865569	3.433074779	-3.833062340
H	-0.437177127	1.236772159	-2.804056886
N	-0.075258547	1.838631506	-0.880720083
C	-2.599720002	0.457998452	0.073755868
C	-3.343932252	1.279051574	0.930704960
C	-4.701692184	1.529337082	0.709439479
C	-5.352025458	0.956859646	-0.387981284
C	-4.639129574	0.134644099	-1.255466446
C	-3.272752906	-0.119625873	-1.032419976
C	-2.487207727	-0.994884148	-1.922226059
C	-2.999331392	-1.675899262	-3.038697004
C	-2.166694465	-2.479995242	-3.807132771
C	-0.820017362	-2.605213205	-3.458809033
C	-0.364919597	-1.912249544	-2.344679465
H	-2.860761704	1.728459967	1.794491953
H	-5.253930146	2.170699744	1.392250853
H	-6.405974185	1.149396708	-0.565850418
H	-5.156192342	-0.304370756	-2.103489180
H	-4.045659041	-1.578234441	-3.299845024
H	-2.564851772	-3.006523371	-4.668928942
H	-0.137205082	-3.223623571	-4.029807007
H	0.666695620	-1.967632102	-2.016533668
N	-1.170738193	-1.132360852	-1.605320305
C	-0.783129046	-1.717372545	1.301149794
C	-1.978983436	-2.164131649	1.867410070
C	-2.024674404	-3.362668259	2.592154090
C	-0.867214025	-4.125274880	2.754100913
C	0.333873248	-3.688824312	2.193776847
C	0.394989667	-2.489167598	1.467544828
C	1.619200143	-1.945418686	0.846038357
C	2.880230934	-2.560928166	0.883144366
C	3.976464601	-1.962430470	0.258846252
C	3.819489161	-0.745009699	-0.407276980
C	2.560795110	-0.128434796	-0.448223875
H	-2.884427241	-1.577929477	1.752374392
H	-0.897054949	-5.055617305	3.314799949
H	1.229769196	-4.289100298	2.327881903
H	3.016856510	-3.509260771	1.396779129
H	4.949358482	-2.445562504	0.294138416
H	2.455740842	0.820096881	-0.970113012
C	1.453050525	-0.712741878	0.169724336
H	4.672240972	-0.275587669	-0.892168251
H	-2.963822524	-3.694330253	3.027779358

2ac (S_0)

Pt	-0.523765036	-0.012903068	0.172435571
C	-0.080592592	1.180053750	1.742217390
C	-0.103519372	0.825002148	3.095645049
C	0.209266827	1.756632226	4.088585238
C	0.554751914	3.067591373	3.747383627
C	0.583589942	3.440493960	2.408093161
C	0.269370520	2.512138807	1.399073493
C	0.279607384	2.866444518	-0.027188587
C	0.601717422	4.129032059	-0.549864418
C	0.572663861	4.338228283	-1.922785283
C	0.220256789	3.285355966	-2.771482390
C	-0.089908797	2.058568736	-2.200053344
H	-0.368628888	-0.186208394	3.381994352
H	0.183598576	1.456283893	5.132797389
H	0.799000209	3.791625073	4.518640195
H	0.850745589	4.460786003	2.151008498
H	0.873393471	4.939034398	0.115485804
H	0.822066585	5.313319000	-2.329079695
H	0.185286265	3.407614765	-3.847780664
H	-0.372173148	1.204664260	-2.805489665
N	-0.058503085	1.858621309	-0.873366864
C	-2.573848394	0.473735968	0.073621718
C	-3.307142897	1.302528586	0.932086774
C	-4.667488077	1.552682763	0.726147081
C	-5.331892486	0.973573826	-0.359153472
C	-4.630338797	0.145435374	-1.230258399
C	-3.261981746	-0.109731943	-1.021490931

C	-2.488819098	-0.989895927	-1.917682469
C	-3.015364187	-1.675146460	-3.024858998
C	-2.192933793	-2.481942826	-3.801378191
C	-0.841576001	-2.606490523	-3.470854648
C	-0.371785294	-1.910239316	-2.365108199
H	-2.812834280	1.761597475	1.784219834
H	-5.210711658	2.198970795	1.411430391
H	-6.387773028	1.165905816	-0.525286780
H	-5.157897298	-0.297080166	-2.069912037
H	-4.065046095	-1.578722226	-3.272527291
H	-2.602592767	-3.011404550	-4.655917875
H	-0.166726005	-3.227035796	-4.048905400
H	0.664015798	-1.965781855	-2.050198978
N	-1.168020821	-1.127199077	-1.618372700
C	-0.776263130	-1.708802011	1.274772880
C	-1.982338393	-2.144663954	1.825679787
C	-2.010139175	-3.337060853	2.545612125
C	-0.880090902	-4.118864411	2.740099221
C	0.324384978	-3.680096544	2.188207827
C	0.398330029	-2.484460487	1.458037708
C	1.629561301	-1.944105723	0.849581923
C	2.889020796	-2.559157999	0.905755443
C	3.998659100	-1.969984190	0.295987894
C	3.818750546	-0.761757439	-0.364561784
C	2.580894733	-0.125762589	-0.438745940
H	-2.898260686	-1.576957849	1.712663772
H	-0.946581902	-5.041024576	3.307373809
H	1.214287317	-4.284952538	2.336823718
H	3.023099589	-3.504681859	1.424298309
H	4.980643139	-2.429828111	0.329749969
H	2.515215221	0.819259517	-0.970579227
C	1.467442389	-0.711467857	0.168339005
F	4.892140610	-0.178264191	-0.962603293
F	-3.191193213	-3.746672508	3.077611069

2ac (T_1)

$\langle S^2 \rangle = 2.030418$

Pt	-0.519783125	-0.018273011	0.183153490
C	-0.076120975	1.187073096	1.748565533
C	-0.100271040	0.841584436	3.104416839
C	0.212715185	1.778826851	4.092187681
C	0.559263918	3.087194834	3.742675278
C	0.588803206	3.451551897	2.400887709
C	0.274630679	2.517113248	1.397477712
C	0.287047612	2.865034271	-0.031297844
C	0.610656829	4.125129441	-0.559276216
C	0.584052152	4.327662365	-1.933492735
C	0.234120802	3.270998990	-2.778461032
C	-0.076053852	2.046396733	-2.201769032
H	-0.366683434	-0.167775384	3.396901132
H	0.186307067	1.485211426	5.138324968
H	0.803675892	3.816099579	4.509320807
H	0.856444045	4.470246751	2.137966290
H	0.881876224	4.938430305	0.102250094
H	0.834177764	5.300968162	-2.343693518
H	0.201767792	3.388699186	-3.855380311
H	-0.354785889	1.187128194	-2.801573848
N	-0.048620926	1.854302561	-0.874367538
C	-2.556858417	0.472097757	0.103872458
C	-3.300057970	1.261734942	0.958512642
C	-4.674788754	1.513446742	0.751484236
C	-5.343794265	0.937166717	-0.374169497
C	-4.673447195	0.141276407	-1.257381014
C	-3.255028235	-0.136104660	-1.062931442
C	-2.516969348	-0.953107504	-1.917789675
C	-3.037242095	-1.645135876	-3.076122986
C	-2.228390759	-2.442003078	-3.841440973
C	-0.859503097	-2.585714468	-3.483674421
C	-0.382016408	-1.896313593	-2.355407830
H	-2.817770265	1.709797632	1.823383655
H	-5.228334547	2.145323674	1.439172698
H	-6.400970232	1.138331442	-0.523700925
H	-5.201334823	-0.286601134	-2.102234739
H	-4.083792209	-1.530030289	-3.331243047
H	-2.625330662	-2.960675253	-4.707703283
H	-0.182458051	-3.207729860	-4.056519827
H	0.657253071	-1.982674569	-2.053343222
N	-1.139062543	-1.112203453	-1.604881342
C	-0.769558158	-1.711723530	1.287652519
C	-1.976156793	-2.147539556	1.837094944
C	-2.004936389	-3.340257894	2.556435081
C	-0.874897213	-4.121708998	2.752147259
C	0.330108180	-3.682695783	2.201545856
C	0.404808110	-2.487188597	1.471337250
C	1.634959189	-1.947022104	0.861616277
C	2.895473192	-2.559670931	0.919128747
C	4.003662783	-1.970191812	0.307174981
C	3.820965417	-0.764192962	-0.356704111
C	2.582023812	-0.130533395	-0.432110488
H	-2.891239298	-1.577718113	1.725943893
H	-0.941861551	-5.044015115	3.319109648
H	1.219888541	-4.287645679	2.350446190
H	3.031280860	-3.503430370	1.440417376
H	4.986554377	-2.428018442	0.341707379
H	2.514354430	0.812663730	-0.966714773
C	1.470063425	-0.716633670	0.177223340
F	4.892885956	-0.180330751	-0.956985436
F	-3.186672145	-3.749798702	3.086809641

2ac (T_2)

$\langle S^2 \rangle = 2.035925$

Pt	-0.531231018	-0.001049893	0.162561913
C	-0.081616817	1.181973965	1.737120366
C	-0.096819518	0.816162766	3.087539434
C	0.223632166	1.740546529	4.085212913
C	0.570197799	3.052837324	3.750610497
C	0.594991410	3.434636116	2.413603489
C	0.273271435	2.513967082	1.399718417
C	0.281367848	2.875436562	-0.024643460
C	0.606162648	4.140011392	-0.541250052
C	0.573338022	4.356894031	-1.912834195
C	0.213346806	3.310376471	-2.766328151
C	-0.099801911	2.081470268	-2.200738036
H	-0.362402449	-0.196592325	3.367777031
H	0.203143297	1.433229609	5.127485423
H	0.820250660	3.771075676	4.525457655
H	0.866648900	4.455087955	2.161978284
H	0.882872448	4.945260158	0.127796848

H	0.825286946	5.333268136	-2.314508186
H	0.175064916	3.438976936	-3.841771015
H	-0.388557440	1.232107175	-2.809404110
N	-0.063262723	1.873621134	-0.875483769
C	-2.583385962	0.482572095	0.059553460
C	-3.315019309	1.314081795	0.916721414
C	-4.676007841	1.563435756	0.713686586
C	-5.343060349	0.979461049	-0.367203740
C	-4.643283197	0.148140848	-1.236906993
C	-3.274034673	-0.105316144	-1.031921211
C	-2.504174710	-0.986803749	-1.931047730
C	-3.036802179	-1.682654739	-3.028626602
C	-2.215387064	-2.490324300	-3.806498743
C	-0.859563201	-2.601029276	-3.490264726
C	-0.383675823	-1.890014056	-2.395892123
H	-2.818428112	1.776233936	1.765934109
H	-5.217435448	2.212467943	1.397828572
H	-6.399534204	1.170479098	-0.531287671
H	-5.173101761	-0.298180320	-2.073143410
H	-4.089159887	-1.594901509	-3.268210496
H	-2.629833240	-3.030411750	-4.652097052
H	-0.186266078	-3.220790335	-4.071138962
H	0.658007382	-1.925221806	-2.095640312
N	-1.179973183	-1.111566509	-1.646026138
C	-0.797722616	-1.689661951	1.252761445
C	-1.977946217	-2.145546277	1.784495721
C	-1.991547686	-3.354213404	2.523053982
C	-0.832880338	-4.122837378	2.759698629
C	0.365589192	-3.694848233	2.249033836
C	0.445641461	-2.462839511	1.464196437
C	1.602303815	-1.955586388	0.893951049
C	2.925598110	-2.573915684	0.977243389
C	3.998532356	-1.992637336	0.348782060
C	3.808775592	-0.792579130	-0.367073383
C	2.551032414	-0.145601583	-0.466017366
H	-2.908666422	-1.603918953	1.662011032
H	-0.913268919	-5.035093504	3.342496710
H	1.263841416	-4.273906396	2.432968900
H	3.064994531	-3.494721557	1.533433036
H	4.991115541	-2.430467575	0.390353305
H	2.499134318	0.785220486	-1.024296343
C	1.449600231	-0.694742798	0.143910788
F	4.878341080	-0.234514442	-0.988228733
F	-3.173202542	-3.789710653	3.025478463

2ac (T_3)

$\langle S^2 \rangle = 2.029713$

Pt	-0.541320697	-0.017907501	0.186409221
C	-0.108993317	1.153719864	1.751328568
C	-0.155959708	0.832229281	3.094723873
C	0.178946012	1.769988157	4.090041793
C	0.591027031	3.091811631	3.720087749
C	0.656506095	3.470239146	2.411377352
C	0.300727573	2.534395965	1.355556777
C	0.311104800	2.862520880	0.002337387
C	0.666030847	4.146887135	-0.555272678
C	0.615788383	4.357130520	-1.909607129
C	0.210539062	3.298585164	-2.763017311
C	-0.119035663	2.058369723	-2.182763578
H	-0.455726659	-0.165555233	3.394311434
H	0.132124638	1.494371204	5.138400471
H	0.855216444	3.801048572	4.499499780
H	0.971241212	4.475396651	2.155138435
H	0.972231234	4.945743418	0.109160655
H	0.881963988	5.323263140	-2.325590867
H	0.153307877	3.420390305	-3.837707320
H	-0.429042066	1.225615488	-2.806997465
N	-0.071763076	1.830831253	-0.883537735
C	-2.594385101	0.456637517	0.075954240
C	-3.334513167	1.273688865	0.939559397
C	-4.693968678	1.522185151	0.726326969
C	-5.349137050	0.951697252	-0.369065939
C	-4.639916926	0.132888331	-1.242790327
C	-3.272079300	-0.119820198	-1.028070600
C	-2.489995808	-0.992076603	-1.923620928
C	-3.006017002	-1.670237293	-3.039875662
C	-2.175934969	-2.471794159	-3.813669079
C	-0.827767126	-2.597472850	-3.471104604
C	-0.368424131	-1.907443175	-2.357093847
H	-2.847310167	1.721450940	1.801835118
H	-5.243546287	2.160396864	1.414062148
H	-6.404386759	1.142705563	-0.540414577
H	-5.161050681	-0.305108259	-2.088738724
H	-4.053336418	-1.572232402	-3.296760714
H	-2.577169510	-2.996077878	-4.675349201
H	-0.147004064	-3.213918011	-4.046578386
H	0.664727457	-1.963692346	-2.034142814
N	-1.172017416	-1.129836290	-1.612565297
C	-0.783903597	-1.716898772	1.291090467
C	-1.985380718	-2.158805443	1.846739438
C	-2.004558758	-3.352581114	2.564774586
C	-0.869923290	-4.129423439	2.752566643
C	0.330025776	-3.684588518	2.195719440
C	0.395064185	-2.487444772	1.467177637
C	1.621590351	-1.943008432	0.851988711
C	2.883799748	-2.553607814	0.899420916
C	3.987157183	-1.960326387	0.282293288
C	3.800059042	-0.752906045	-0.378111536
C	2.559525010	-0.121228406	-0.445558884
H	-2.904266636	-1.594628787	1.738993653
H	-0.929586734	-5.052764315	3.318668033
H	1.223148252	-4.285885853	2.339247418
H	3.024566744	-3.499074157	1.416231129
H	4.970764411	-2.417100610	0.309828547
H	2.483029761	0.823183255	-0.976844469
C	1.455041554	-0.712140838	0.170091487
F	4.868173680	-0.166480392	-0.981857011
F	-3.180976986	-3.768472124	3.101736440

2ca (S_0)

C	-4.579170860	-6.484376240	-72.785424888
C	-4.200058378	-6.857748466	-74.061935882
C	-2.241190652	-6.563550470	-72.575934198
C	-3.436150823	-6.322237918	-71.943769002
C	-5.173360021	-7.086040665	-75.108316686
C	-7.472468964	-7.099878650	-75.583634275
C	-7.250866095	-7.456098019	-76.908572395
C	-5.930691469	-7.630510448	-77.336036485

C	-4.888954201	-7.445581680	-76.436684405
C	-6.690917242	-5.950638488	-70.609898370
C	-6.691294228	-7.079454630	-69.806353301
C	-6.676777997	-4.979373299	-68.489083487
C	-6.684246063	-4.748736068	-69.840688966
C	-6.695348784	-8.406221164	-70.376937082
C	-6.696953832	-9.570360047	-72.410716065
C	-6.697814115	-10.801907379	-71.766464461
C	-6.695780169	-10.818381513	-70.367185403
C	-6.693334365	-9.619153152	-69.667471790
C	-9.207555860	-4.859057729	-73.034381087
C	-10.578161607	-4.606684637	-73.156419415
C	-11.514633461	-5.607713057	-72.882322005
C	-11.112148760	-6.887838649	-72.478461866
C	-9.724773174	-7.124389399	-72.361834904
C	-8.129054102	-3.890623262	-73.291879795
C	-5.725203688	-3.515482001	-73.329821804
C	-5.899782385	-2.173132594	-73.713360478
C	-7.217104322	-1.714963645	-73.883452862
C	-8.308962514	-2.553984493	-73.677811408
H	-1.240458984	-6.508990232	-72.166824092
H	-3.489654982	-6.032800982	-70.899455693
H	-8.471093850	-6.947096976	-75.189524227
H	-8.089720781	-7.589826455	-77.581529220
H	-5.717546229	-7.906955818	-78.364001921
H	-3.858198000	-7.573478793	-76.749052443
H	-6.684683481	-3.754943411	-70.270715333
H	-6.695769798	-9.495276357	-73.492945453
H	-6.698841566	-11.717762593	-72.345850576
H	-6.695227338	-11.761046381	-69.828964515
H	-6.689822269	-9.609098255	-68.582913493
H	-6.671174909	-4.253515975	-67.686715838
H	-12.567655493	-5.371393875	-72.987616635
H	-9.390136669	-8.109588529	-72.047801016
H	-4.726166647	-3.905607419	-73.188267419
H	-7.400158480	-0.685967324	-74.179966221
H	-9.311900988	-2.158350409	-73.817009896
H	-10.934888775	-3.627218169	-73.466587664
N	-6.469799206	-6.923185784	-74.709161462
N	-6.698511677	-8.409107562	-71.740994631
S	-2.453767154	-7.005362566	-74.241138582
S	-6.679978355	-6.672165952	-68.100921921
Pt	-6.681220387	-6.331641239	-72.578470016
C	-4.716435644	-1.214452372	-73.946655147
C	-6.810634387	-4.369851809	-73.122769563
C	-4.752031614	-0.697850788	-75.405245449
H	-3.920823635	-0.006403400	-75.585741458
H	-4.663657558	-1.527064996	-76.115390204
H	-5.682252065	-0.165681062	-75.625604910
C	-4.827835345	-0.012078130	-72.978433822
H	-3.996816647	0.684715418	-73.137939487
H	-5.760012968	0.542053412	-73.123531049
H	-4.794970273	-0.345836928	-71.935706987
C	-3.352976976	-1.892303589	-73.712718056
H	-3.249353053	-2.256710330	-72.685442667
H	-3.196140206	-2.737366921	-74.390949190
H	-2.548663139	-1.170760578	-73.890852877
C	-12.110658391	-8.017307425	-72.161675727
C	-13.575176695	-7.577413597	-72.350563958
H	-14.244160192	-8.412047512	-72.115760604
H	-13.839072838	-6.745850180	-71.688881255
H	-13.778456325	-7.270303517	-73.381862153
C	-11.930565614	-8.469017200	-70.692218241
H	-10.917295960	-8.834693284	-70.501366762
H	-12.122714583	-7.639869001	-70.002853218
H	-12.629666229	-9.278774228	-70.452635358
C	-11.846940580	-9.220627649	-73.098855514
H	-11.978585010	-8.934731915	-74.148134622
H	-10.831669524	-9.611336940	-72.982137534
H	-12.545845664	-10.036286326	-72.879892552
C	-8.771705157	-6.144530144	-72.632682108

2ca (T_1)

$\langle S^2 \rangle = 2.033814$

C	-4.587649613	-6.465852178	-72.740395608
C	-4.192001855	-6.856075578	-74.116380812
C	-2.234848499	-6.554463756	-72.585519715
C	-3.468742791	-6.318680736	-71.946566762
C	-5.143271378	-7.083600681	-75.106258716
C	-7.460672915	-7.104965154	-75.559580523
C	-7.242812706	-7.463555185	-76.894512156
C	-5.913353824	-7.639974466	-77.344451462
C	-4.874477372	-7.452095587	-76.462983455
C	-6.695175108	-5.951937830	-70.596576862
C	-6.697779719	-7.084477845	-69.798515127
C	-6.687589670	-4.990350901	-68.470790359
C	-6.690727585	-4.753920417	-69.821471365
C	-6.702843416	-8.411235595	-70.371324628
C	-6.708952344	-9.574653103	-72.405312107
C	-6.713016795	-10.806886831	-71.761813522
C	-6.710637826	-10.823505378	-70.362623366
C	-6.705055324	-9.624424446	-69.662209122
C	-9.206442365	-4.853006492	-73.026135976
C	-10.577316246	-4.600852776	-73.145187099
C	-11.512618036	-5.603772221	-72.874373233
C	-11.108406154	-6.885340879	-72.476847875
C	-9.720782543	-7.121208832	-72.362245546
C	-8.128933926	-3.883896922	-73.283264789
C	-5.724778653	-3.509391970	-73.327007110
C	-5.899445511	-2.168354796	-73.714832120
C	-7.216993989	-1.710051790	-73.882431550
C	-8.308712689	-2.548078493	-73.672132278
H	-1.238246208	-6.501139993	-72.168250225
H	-3.504836982	-6.036723191	-70.898796339
H	-8.464620689	-6.958610867	-75.174283922
H	-8.088723705	-7.598928727	-77.557790857
H	-5.715835187	-7.917908676	-78.374633622
H	-3.844349072	-7.576254646	-76.780359627
H	-6.689817189	-3.758071579	-70.246958449
H	-6.709660912	-9.497563620	-73.487665323
H	-6.717198777	-11.722694472	-72.341326111
H	-6.712954882	-11.766316405	-69.824620499
H	-6.702975604	-9.615311484	-68.577604787
H	-6.684591087	-4.268238511	-67.665030154
H	-12.565964983	-5.367933532	-72.977379701
H	-9.385171029	-8.107430333	-72.052866301
H	-4.725954701	-3.899260297	-73.181608252
H	-7.400320885	-0.681873239	-74.181528352

H	-9.311766630	-2.152801382	-73.811314891
H	-10.935006305	-3.620258758	-73.450609157
N	-6.474538888	-6.924461683	-74.684822484
N	-6.705131737	-8.414416744	-71.734804315
S	-2.430416911	-6.993362307	-74.304798076
S	-6.692082649	-6.684870016	-68.090851678
Pt	-6.677746232	-6.322988768	-72.570165108
C	-4.716065950	-1.211289062	-73.954119721
C	-6.810331962	-4.362036258	-73.114331303
C	-4.754795602	-0.699642175	-75.414347827
H	-3.923778169	-0.009082001	-75.598982002
H	-4.668341169	-1.531246629	-76.121908610
H	-5.685347963	-0.167901135	-75.634299821
C	-4.824469307	-0.005660402	-72.989596816
H	-3.993191333	0.689856862	-73.153182438
H	-5.756448800	0.548808894	-73.134582916
H	-4.789704960	-0.335997857	-71.945846552
C	-3.352572150	-1.889307472	-73.720849394
H	-3.246720788	-2.249140254	-72.692146285
H	-3.197996925	-2.737326888	-74.395944094
H	-2.548112895	-1.169227609	-73.904050558
C	-12.105462664	-8.017569580	-72.165347158
C	-13.570635402	-7.577917850	-72.349663298
H	-14.238524507	-8.414494851	-72.118692775
H	-13.834343052	-6.750378985	-71.682870860
H	-13.775667296	-7.265138376	-73.378903523
C	-11.923090404	-8.478067877	-70.698910216
H	-10.909286068	-8.844030087	-70.511495214
H	-12.115161107	-7.653343071	-70.004235429
H	-12.621176638	-9.289907006	-70.463467087
C	-11.841779197	-9.214882319	-73.110224358
H	-11.975009942	-8.922674029	-74.157558740
H	-10.825962507	-9.605249602	-72.997182572
H	-12.539619153	-10.032549700	-72.895390037
C	-8.768704405	-6.139454540	-72.629839368

2ca (T_2)

$\langle S^2 \rangle = 2.035877$

C	-4.567933141	-6.473399622	-72.791068034
C	-4.196383279	-6.860375778	-74.065266523
C	-2.229650989	-6.547329652	-72.593216069
C	-3.421226611	-6.299164520	-71.957310648
C	-5.175397883	-7.097314998	-75.104223500
C	-7.476764719	-7.112104337	-75.567721915
C	-7.262122383	-7.479884642	-76.890599419
C	-5.944451136	-7.660036316	-77.323209758
C	-4.898025839	-7.468902891	-76.430641200
C	-6.674038393	-5.906357677	-70.626395470
C	-6.706151938	-7.134636440	-69.786070995
C	-6.668748896	-4.997900271	-68.467833846
C	-6.656682914	-4.764290074	-69.851895353
C	-6.723165304	-8.403819440	-70.356432522
C	-6.699615699	-9.553683026	-72.411617783
C	-6.721474053	-10.800167867	-71.769360119
C	-6.751413262	-10.832438419	-70.357865005
C	-6.752100504	-9.649247304	-69.652992971
C	-9.200342222	-4.852307374	-73.031079021
C	-10.571595311	-4.604146624	-73.155149390
C	-11.505563733	-5.608136240	-72.882886637
C	-11.100940045	-6.888018569	-72.480436226
C	-9.712960879	-7.121525068	-72.363151497
C	-8.123636703	-3.881812794	-73.289377316
C	-5.720491524	-3.500853452	-73.330638324
C	-5.898681167	-2.159567580	-73.716180463
C	-7.217383304	-1.705050658	-73.885464794
C	-8.307102773	-2.546200777	-73.677208146
H	-1.226788579	-6.488361579	-72.189996235
H	-3.469725108	-5.995372857	-70.916788894
H	-8.473280093	-6.955139411	-75.170183327
H	-8.104575792	-7.618114101	-77.558107835
H	-5.736868713	-7.945744510	-78.349763349
H	-3.868995396	-7.601148678	-76.746796031
H	-6.636484271	-3.760113267	-70.258346344
H	-6.678629588	-9.487271969	-73.495171173
H	-6.716214243	-11.709184894	-72.358651374
H	-6.772461392	-11.781951740	-69.832812692
H	-6.773422696	-9.645149831	-68.568315080
H	-6.657362007	-4.276016020	-67.663286515
H	-12.559023448	-5.374329009	-72.989250205
H	-9.374145568	-8.106172531	-72.051920132
H	-4.720463842	-3.888503717	-73.188925715
H	-7.403281367	-0.676948064	-74.183244474
H	-9.311044250	-2.152982271	-73.815774796
H	-10.930735686	-3.625955933	-73.466423619
N	-6.469493130	-6.929246980	-74.699638918
N	-6.705392833	-8.401267272	-71.755440640
S	-2.451096893	-7.008526093	-74.251890405
S	-6.708419674	-6.742893085	-68.063639267
Pt	-6.670972446	-6.318566486	-72.572465971
C	-4.717975719	-1.198255903	-73.951760649
C	-6.803759898	-4.357032448	-73.121646649
C	-4.756760046	-0.682755478	-75.410648878
H	-3.927371203	0.010455976	-75.592641401
H	-4.667408917	-1.512227089	-76.120361295
H	-5.688453069	-0.152815160	-75.630136255
C	-4.831058315	0.004442059	-72.984128828
H	-4.001936670	0.703113228	-73.145188686
H	-5.764763974	0.556219704	-73.128356087
H	-4.795993501	-0.328567047	-71.941233714
C	-3.352638043	-1.872783584	-73.719159731
H	-3.246650084	-2.235968752	-72.691688546
H	-3.194813818	-2.718081564	-74.396875976
H	-2.550265520	-1.149548968	-73.899092696
C	-12.096907455	-8.020169216	-72.165848818
C	-13.562270697	-7.583233329	-72.354973592
H	-14.229471925	-8.419654488	-72.121558799
H	-13.828351337	-6.753118694	-71.692346308
H	-13.765722098	-7.275324086	-73.385998731
C	-11.916337679	-8.473459219	-70.696940619
H	-10.902219065	-8.836789143	-70.506106073
H	-12.111137931	-7.645856747	-70.006461677
H	-12.613402972	-9.285410587	-70.458988131
C	-11.829626695	-9.221438402	-73.104629896
H	-11.961088558	-8.934323972	-74.153592556
H	-10.813622516	-9.610163701	-72.987574301
H	-12.526869421	-10.038931260	-72.887356597
C	-8.764451672	-6.137569240	-72.630363253

2ca (T_3)

$\langle S^2 \rangle$ = 2.034087

C	-4.567039874	-6.499055087	-72.764836718
C	-4.185034750	-6.870757707	-74.041047139
C	-2.228883238	-6.576554101	-72.549825122
C	-3.425657587	-6.336803363	-71.920725979
C	-5.152389325	-7.099194265	-75.094430017
C	-7.449092453	-7.130416357	-75.577179900
C	-7.220527252	-7.470395965	-76.905792627
C	-5.897318377	-7.628943978	-77.329661487
C	-4.859520129	-7.445325399	-76.424429718
C	-6.680154465	-5.955644717	-70.585059848
C	-6.692334326	-7.083226817	-69.780073300
C	-6.675412825	-4.979683915	-68.467005683
C	-6.673822595	-4.751867072	-69.819278984
C	-6.699719577	-8.410987570	-70.348495921
C	-6.690816116	-9.578591822	-72.380307424
C	-6.699699044	-10.809070587	-71.733813695
C	-6.707749841	-10.823031976	-70.334490187
C	-6.706082351	-9.622654930	-69.636773689
C	-9.181267710	-4.809398582	-72.994909756
C	-10.610791576	-4.548952743	-73.082982313
C	-11.516222633	-5.549746981	-72.836203149
C	-11.111197140	-6.871253546	-72.478413711
C	-9.699779498	-7.122012652	-72.375145829
C	-8.166439258	-3.899125410	-73.237816401
C	-5.724201691	-3.542164695	-73.324404087
C	-5.904870107	-2.179240861	-73.706374809
C	-7.255043685	-1.701666792	-73.832795783
C	-8.337531259	-2.503495453	-73.610898533
H	-1.229224937	-6.522381538	-72.138055900
H	-3.482215247	-6.048244438	-70.876279317
H	-8.450373544	-6.997912173	-75.180366814
H	-8.055435546	-7.605352885	-77.583590894
H	-5.678078444	-7.892992206	-78.359657376
H	-3.826878555	-7.563998742	-76.734493189
H	-6.667847707	-3.759124541	-70.251645901
H	-6.681506989	-9.504769214	-73.462532578
H	-6.699604745	-11.725988812	-72.311521261
H	-6.713977993	-11.764764222	-69.794647371
H	-6.709517611	-9.610684993	-68.552233384
H	-6.670256787	-4.252240266	-67.666116026
H	-12.573429293	-5.319794648	-72.915328377
H	-9.378954889	-8.119125520	-72.085272586
H	-4.719005599	-3.925068002	-73.205872617
H	-7.423083338	-0.665158662	-74.112397695
H	-9.339646439	-2.096871771	-73.709242420
H	-10.966036095	-3.557437830	-73.348022855
N	-6.450721043	-6.951445543	-74.700064376
N	-6.694647042	-8.416256164	-71.712581517
S	-2.437782238	-7.016796287	-74.215869839
S	-6.687365775	-6.672005664	-68.075445741
Pt	-6.670219056	-6.340252488	-72.551979403
C	-4.738025594	-1.226518444	-73.983279505
C	-6.783154054	-4.392014668	-73.103270969
C	-4.828285394	-0.705596710	-75.440771764
H	-4.008835353	-0.007106132	-75.647096915
H	-4.757764223	-1.532741856	-76.155120832
H	-5.769080579	-0.179351456	-75.628238625
C	-4.810423768	-0.020056634	-73.012194802
H	-3.990098710	0.679175763	-73.212225919
H	-5.749738410	0.531466369	-73.115342560
H	-4.727951758	-0.351716608	-71.971698448
C	-3.365879852	-1.903365166	-73.802360153
H	-3.222179658	-2.266376600	-72.779472702
H	-3.236220117	-2.749294433	-74.485164437
H	-2.569238392	-1.182054490	-74.012816062
C	-12.105442873	-8.003390064	-72.201503194
C	-13.571660206	-7.557802605	-72.365002559
H	-14.238508261	-8.401754538	-72.159564309
H	-13.833078371	-6.753531399	-71.669428170
H	-13.781037123	-7.210938984	-73.382389742
C	-11.918810630	-8.515922836	-70.750237764
H	-10.903312186	-8.883579843	-70.576286618
H	-12.115189577	-7.717360606	-70.026981583
H	-12.612921791	-9.339352957	-70.544675157
C	-11.847821502	-9.173601202	-73.185145802
H	-11.993543634	-8.850999934	-74.221725715
H	-10.829872386	-9.563942873	-73.094231034
H	-12.541337180	-9.999012087	-72.985970894
C	-8.750431068	-6.162208844	-72.619198672

2cb (S_0)

C	-4.574546449	-6.484223308	-72.816044671
C	-4.204627146	-6.819442913	-74.105749641
C	-2.235053090	-6.554775970	-72.628553996
C	-3.425792908	-6.338454873	-71.979597477
C	-5.186051411	-7.022748208	-75.149690938
C	-7.489364535	-7.033387211	-75.604938421
C	-7.278109675	-7.351625783	-76.941115738
C	-5.961088945	-7.508223248	-77.384861024
C	-4.912091428	-7.343923449	-76.489938157
C	-6.661764444	-6.022097367	-70.606883647
C	-6.644035525	-7.173974313	-69.837345625
C	-6.627162920	-5.113402672	-68.459308271
C	-6.653295386	-4.843119725	-69.803345986
C	-6.647392519	-8.483243389	-70.447134031
C	-6.675179670	-9.586234094	-72.514698336
C	-6.656308098	-10.836162081	-71.907381716
C	-6.629821877	-10.894332154	-70.509542550
C	-6.624162908	-9.716473981	-69.774414808
C	-9.210362352	-4.865546998	-72.970176011
C	-10.583537624	-4.596404977	-73.073224814
C	-11.519473634	-5.601962382	-72.823654240
C	-11.087303412	-6.881776871	-72.469456327
C	-9.715794888	-7.153815570	-72.365712186
C	-8.135367557	-3.884002133	-73.209165157
C	-5.734579810	-3.505920895	-73.261322984
C	-5.951770293	-2.162741485	-73.597236235
C	-7.253038580	-1.679941076	-73.742723465
C	-8.336748711	-2.537505252	-73.549530376
H	-1.231164250	-6.505794160	-72.226574554
H	-3.472284590	-6.078437810	-70.927289888
H	-8.485136097	-6.895809328	-75.198310686
H	-8.122393931	-7.470299813	-77.610062986
H	-5.755995348	-7.754918167	-78.421969585
H	-3.883688193	-7.458619125	-76.814888443
H	-6.665636117	-3.837001213	-70.203493947

H	-6.693486768	-9.479262924	-73.594038946
H	-6.661356131	-11.734314728	-72.513792385
H	-6.612995151	-11.852586425	-69.999905171
H	-6.602126486	-9.738669951	-68.690216351
H	-6.616207416	-4.411442887	-67.636027007
H	-12.581366316	-5.385406594	-72.904422563
H	-9.399189304	-8.156065426	-72.086937907
H	-4.719053166	-3.869698308	-73.148956428
H	-7.425617780	-0.639371812	-74.003685638
H	-9.346151139	-2.151005011	-73.661620172
H	-10.932461756	-3.604253342	-73.348279506
N	-6.479584487	-6.876496952	-74.734805392
N	-6.673140062	-8.445416529	-71.810538576
S	-2.459493037	-6.951595935	-74.303473545
S	-6.613954391	-6.816745749	-68.121256086
Pt	-6.673538426	-6.346571287	-72.586234104
C	-6.812241181	-4.371877045	-73.068733687
C	-8.763952658	-6.161396663	-72.614749879
H	-11.813806412	-7.666601501	-72.272572757
H	-5.102737375	-1.499783861	-73.742646734

2cb (T_1)

$\langle S^2 \rangle = 2.03374$

C	-4.581372163	-6.466103485	-72.775575841
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C	-2.227484855	-6.545611149	-72.643276237
C	-3.456791720	-6.331636424	-71.987926198
C	-5.155473147	-7.023257541	-75.151381660
C	-7.476848329	-7.038467683	-75.584777297
C	-7.269896897	-7.360662860	-76.930603103
C	-5.944040071	-7.521503957	-77.396798205
C	-4.897885194	-7.354568855	-76.519803333
C	-6.664622372	-6.021602533	-70.597345756
C	-6.648868871	-7.176681425	-69.832804755
C	-6.637354926	-5.121724493	-68.445423718
C	-6.658857409	-4.846312018	-69.788552307
C	-6.651878143	-8.486183974	-70.444156351
C	-6.681798195	-9.589560820	-72.511284085
C	-6.664575645	-10.839848753	-71.904024616
C	-6.638397247	-10.897409267	-70.506241013
C	-6.631513233	-9.719307778	-69.771072524
C	-9.208781540	-4.860448782	-72.967284058
C	-10.582354120	-4.592888267	-73.068708815
C	-11.516500345	-5.600588479	-72.821474559
C	-11.081874106	-6.880654009	-72.471180916
C	-9.709943722	-7.150865989	-72.368662349
C	-8.135411320	-3.877489824	-73.205429166
C	-5.734706071	-3.497510856	-73.259320048
C	-5.952794145	-2.155703554	-73.599867304
C	-7.254487731	-1.674160963	-73.745231236
C	-8.337496121	-2.531913801	-73.548972624
H	-1.227588219	-6.497458189	-72.233349081
H	-3.485372514	-6.075022712	-70.933475970
H	-8.477826625	-6.904955310	-75.187394817
H	-8.121353092	-7.480651790	-77.589702362
H	-5.755011396	-7.771158617	-78.435748302
H	-3.870290039	-7.467247096	-76.849408791
H	-6.669967591	-3.838454889	-70.184592794
H	-6.701547514	-9.481131237	-73.590713596
H	-6.671110826	-11.738302978	-72.510034697
H	-6.623361046	-11.855539764	-69.996267607
H	-6.611256910	-9.741860096	-68.686812154
H	-6.629509927	-4.423188918	-67.619193350
H	-12.578792927	-5.385607099	-72.901059642
H	-9.391736689	-8.153346990	-72.092967353
H	-4.719207316	-3.860397652	-73.142394101
H	-7.427959283	-0.634530163	-74.009227182
H	-9.347213039	-2.146705519	-73.662444630
H	-10.932805457	-3.600441287	-73.340704863
N	-6.483471241	-6.878822950	-74.714082811
N	-6.676483615	-8.449387899	-71.807042301
S	-2.436037911	-6.945398158	-74.370456272
S	-6.625000331	-6.826403816	-68.114783190
Pt	-6.668745456	-6.336866388	-72.581385782
C	-6.811847738	-4.363103455	-73.063378942
C	-8.759707016	-6.156303385	-72.615459505
H	-11.806940496	-7.667313720	-72.276379129
H	-5.104171921	-1.492971096	-73.748424291

2cb (T_2)

$\langle S^2 \rangle = 2.035867$

C	-4.560327361	-6.463913167	-72.822878995
C	-4.196725678	-6.811543725	-74.110653527
C	-2.220354430	-6.521486858	-72.647049800
C	-3.408399926	-6.302163262	-71.994162023
C	-5.182966006	-7.026354445	-75.147586400
C	-7.488318616	-7.044536499	-75.591644960
C	-7.282714258	-7.373718510	-76.925996085
C	-5.967654130	-7.532240063	-77.374708759
C	-4.914755015	-7.358733744	-76.486157715
C	-6.644597352	-5.974663400	-70.624160226
C	-6.653540659	-7.227443387	-69.820626269
C	-6.618685818	-5.130850339	-68.440051511
C	-6.627761155	-4.856017891	-69.817040035
C	-6.667718852	-8.478694529	-70.428585310
C	-6.669034175	-9.566144938	-72.517796669
C	-6.668748367	-10.831292486	-71.912822717
C	-6.673655322	-10.906282670	-70.502747385
C	-6.673069787	-9.744854551	-69.762650668
C	-9.204031434	-4.861302425	-72.968949908
C	-10.578447627	-4.599046477	-73.073761400
C	-11.509784980	-5.609488447	-72.826308593
C	-11.072734897	-6.888161235	-72.474096153
C	-9.700001593	-7.154383695	-72.369937137
C	-8.133080295	-3.875278963	-73.208811138
C	-5.733921884	-3.486116352	-73.265566985
C	-5.957815508	-2.144735525	-73.604191211
C	-7.261604689	-1.668417569	-73.748421645
C	-8.341132416	-2.530392162	-73.551544954
H	-1.214575586	-6.464806524	-72.250863260
H	-3.450779510	-6.027827616	-70.945263922
H	-8.482451899	-6.905651284	-75.181700870
H	-8.130020592	-7.499331059	-77.589812960
H	-5.767112251	-7.787580469	-78.410598095
H	-3.887686709	-7.474755274	-76.814768319
H	-6.622311052	-3.839824262	-70.192927335
H	-6.667614816	-9.467536938	-73.599051313
H	-6.666216359	-11.722093909	-72.529288282

H	-6.676795512	-11.871287761	-70.006348433
H	-6.675820344	-9.773423825	-68.678112480
H	-6.602666194	-4.432763618	-67.614853038
H	-12.572524664	-5.397571162	-72.907934713
H	-9.377302798	-8.155522649	-72.094365968
H	-4.716640589	-3.845127095	-73.153419509
H	-7.439437508	-0.629213334	-74.011217417
H	-9.352375798	-2.148572399	-73.662748907
H	-10.931913317	-3.608710078	-73.349399245
N	-6.474664091	-6.878593764	-74.727497983
N	-6.673114608	-8.433930049	-71.827236764
S	-2.452222803	-6.938501708	-74.315927203
S	-6.635640921	-6.886975296	-68.087244806
Pt	-6.660895535	-6.330415188	-72.582300201
C	-6.807419900	-4.356152717	-73.069937036
C	-8.754598497	-6.156012867	-72.614965783
H	-11.796021770	-7.676355825	-72.279129792
H	-5.112177569	-1.478111063	-73.752407408

2cb (T_3)

$\langle S^2 \rangle = 2.038017$

C	-4.567797682	-6.494299477	-72.821155465
C	-4.195209468	-6.829445527	-74.110197376
C	-2.228019012	-6.559806541	-72.629172605
C	-3.420537966	-6.345570878	-71.983014375
C	-5.171013104	-7.037321326	-75.159951156
C	-7.472025566	-7.070032153	-75.622144620
C	-7.254145089	-7.378173071	-76.960142835
C	-5.934079103	-7.519338775	-77.399758422
C	-4.888881942	-7.350771003	-76.500304210
C	-6.655129302	-6.024333935	-70.607354615
C	-6.643469146	-7.173965793	-69.834768002
C	-6.626358623	-5.107939976	-68.463886183
C	-6.647705104	-4.842158580	-69.809023529
C	-6.648667889	-8.485193407	-70.440716699
C	-6.670629380	-9.594255363	-72.505020743
C	-6.655959687	-10.842391185	-71.893647450
C	-6.634879647	-10.896324983	-70.495596084
C	-6.629664235	-9.716225903	-69.763989487
C	-9.191707372	-4.817031250	-72.959923731
C	-10.624161609	-4.544944601	-73.029180862
C	-11.524908866	-5.552042023	-72.806658125
C	-11.086921028	-6.871984499	-72.496558669
C	-9.696445205	-7.156384620	-72.405548649
C	-8.182821845	-3.896281982	-73.185582902
C	-5.744461507	-3.528462576	-73.276382310
C	-5.970375953	-2.165643244	-73.610339192
C	-7.300490644	-1.667720161	-73.722217317
C	-8.376430337	-2.487916978	-73.517535262
H	-1.225031568	-6.508982135	-72.225203985
H	-3.469896726	-6.084677445	-70.931018470
H	-8.470365332	-6.952013509	-75.213611317
H	-8.094661656	-7.502179938	-77.633022929
H	-5.723103596	-7.758394068	-78.437526867
H	-3.858610594	-7.456457225	-76.822627660
H	-6.656733080	-3.837623091	-70.213125502
H	-6.684274374	-9.490095870	-73.584626470
H	-6.660302486	-11.742414262	-72.497283113
H	-6.621607564	-11.853046016	-69.982976791
H	-6.611266806	-9.735085463	-68.679671436
H	-6.615668767	-4.403231453	-67.642992038
H	-12.591039094	-5.346482485	-72.863327187
H	-9.392663755	-8.169049689	-72.150428593
H	-4.723225565	-3.882002404	-73.182324229
H	-7.456850615	-0.621033767	-73.970681382
H	-9.384500826	-2.093564603	-73.596839881
H	-10.974363916	-3.543608412	-73.260019091
N	-6.466434115	-6.905565663	-74.750426704
N	-6.670118354	-8.451388877	-71.804265708
S	-2.449100075	-6.958058618	-74.304129725
S	-6.616626524	-6.810346621	-68.120059616
Pt	-6.668095997	-6.354644257	-72.584966196
C	-6.794392350	-4.393253530	-73.074095840
C	-8.746920559	-6.184551449	-72.628269299
H	-11.817173884	-7.657249245	-72.324793555
H	-5.126659033	-1.503945047	-73.780145821

2cc (S_0)

C	-4.578526745	-6.477650662	-72.813132079
C	-4.203366042	-6.811416035	-74.101767053
C	-2.240727373	-6.529107222	-72.619065848
C	-3.434573895	-6.320865603	-71.972974824
C	-5.181697542	-7.021883321	-75.147219151
C	-7.484627235	-7.046564306	-75.605803097
C	-7.269282099	-7.365330203	-76.941040065
C	-5.950668704	-7.514662753	-77.382592441
C	-4.903883889	-7.343053429	-76.486442412
C	-6.657603576	-6.022960455	-70.606961436
C	-6.642903350	-7.175515065	-69.839028408
C	-6.616829887	-5.116215101	-68.460101508
C	-6.643799512	-4.844307040	-69.804015925
C	-6.651383204	-8.483199467	-70.452034213
C	-6.684705707	-9.579747863	-72.524018735
C	-6.671046001	-10.831180459	-71.920106842
C	-6.644324191	-10.893845734	-70.522530147
C	-6.633394088	-9.718418655	-69.783534648
C	-9.210595930	-4.866312527	-72.963771379
C	-10.583414379	-4.595952430	-73.058570837
C	-11.525785660	-5.595238867	-72.807074058
C	-11.065632227	-6.859153379	-72.461446701
C	-9.708705977	-7.160555648	-72.358545009
C	-8.135256113	-3.887087120	-73.207821576
C	-5.729409166	-3.521304078	-73.272265311
C	-5.973104126	-2.190715011	-73.606656119
C	-7.255227574	-1.679204773	-73.751167017
C	-8.334041123	-2.541131190	-73.548715973
H	-1.238295496	-6.471510459	-72.214768609
H	-3.486363160	-6.059263972	-70.921459413
H	-8.482186728	-6.914689790	-75.201819660
H	-8.111815413	-7.490051513	-77.611030322
H	-5.742669501	-7.761507853	-78.419034239
H	-3.874379007	-7.452101620	-76.809706739
H	-6.652736627	-3.837569941	-70.202670018
H	-6.703090700	-9.469413718	-73.602849218
H	-6.680415296	-11.727352661	-72.529285636
H	-6.631702255	-11.853749134	-70.016006447
H	-6.611647390	-9.744058351	-68.699461078
H	-6.601987153	-4.414975102	-67.636306413

H	-12.591671038	-5.405197294	-72.874390696
H	-9.419996448	-8.170015385	-72.081266185
H	-4.705562099	-3.861118598	-73.171974580
H	-7.398681811	-0.636408854	-74.012883267
H	-9.340945305	-2.148645055	-73.657260810
H	-10.936711208	-3.604833156	-73.329821274
N	-6.476745504	-6.882622919	-74.734450843
N	-6.677212821	-8.441184805	-71.815586926
S	-2.457793923	-6.930357670	-74.293564701
S	-6.609195130	-6.819525464	-68.123486568
Pt	-6.673449842	-6.350022158	-72.587553343
C	-6.811628499	-4.378417961	-73.072847510
C	-8.763942339	-6.164082449	-72.611693880
F	-11.973954974	-7.840009922	-72.214565934
F	-4.911756993	-1.365195264	-73.795957109

2cc (T_1)

$\langle S^2 \rangle = 2.03353$

C	-4.584961308	-6.459563701	-72.773932745
C	-4.195446027	-6.817749334	-74.159959088
C	-2.232281265	-6.520251864	-72.636735606
C	-3.464201545	-6.309943861	-71.984482842
C	-5.152215575	-7.026621045	-75.148095998
C	-7.473374386	-7.050246480	-75.584815398
C	-7.263267576	-7.374820362	-76.929337840
C	-5.936213699	-7.532169207	-77.393394537
C	-4.891801386	-7.359910053	-76.515437092
C	-6.660091662	-6.021933481	-70.596728206
C	-6.647113378	-7.177934516	-69.834135635
C	-6.626230033	-5.124715598	-68.445179239
C	-6.648918031	-4.847234390	-69.788080810
C	-6.655145019	-8.485573092	-70.449218990
C	-6.690811407	-9.581484358	-72.521337923
C	-6.678560107	-10.833555883	-71.918095968
C	-6.651844487	-10.896298154	-70.520600238
C	-6.639678279	-9.721008554	-69.780972901
C	-9.208847582	-4.861164733	-72.962977084
C	-10.582074979	-4.593282922	-73.058400442
C	-11.522484440	-5.594962849	-72.809466998
C	-11.059744601	-6.858446874	-72.465668477
C	-9.702317485	-7.157231727	-72.362001066
C	-8.135257965	-3.880043834	-73.204811087
C	-5.729733975	-3.510265901	-73.263892139
C	-5.974494328	-2.180937811	-73.602596800
C	-7.257092448	-1.671839330	-73.750860094
C	-8.334972740	-2.535018013	-73.548808049
H	-1.233613568	-6.461097785	-72.225382317
H	-3.496886030	-6.045677981	-70.932180015
H	-8.475774105	-6.919575790	-75.190217449
H	-8.113416915	-7.499409801	-77.589211815
H	-5.745036352	-7.783284978	-78.431542930
H	-3.863401363	-7.469587700	-76.843420622
H	-6.656808329	-3.838642318	-70.182287168
H	-6.710792610	-9.469061921	-73.600180577
H	-6.689446341	-11.729729037	-72.527307043
H	-6.640780132	-11.856323793	-70.014223649
H	-6.619456406	-9.747536051	-68.696856467
H	-6.614401228	-4.427173718	-67.618195851
H	-12.588722568	-5.407155726	-72.877335567
H	-9.411809441	-8.166541442	-72.086456356
H	-4.705908949	-3.847946995	-73.155225062
H	-7.401677695	-0.629947107	-74.015486290
H	-9.342250044	-2.144559023	-73.660948117
H	-10.937042791	-3.602348881	-73.328100390
N	-6.481499738	-6.885375170	-74.712995351
N	-6.680081121	-8.443950338	-71.812241468
S	-2.434681566	-6.935319025	-74.360617280
S	-6.619251508	-6.829471404	-68.116554875
Pt	-6.668647188	-6.339363787	-72.582043021
C	-6.811187271	-4.368371341	-73.065548569
C	-8.759385911	-6.158390248	-72.612668625
F	-11.966066952	-7.841732182	-72.221388617
F	-4.913850223	-1.354677782	-73.791463864

2cc (T_2)

$\langle S^2 \rangle = 2.035676$

C	-4.565551039	-6.458354001	-72.819371079
C	-4.196176069	-6.804470583	-74.106021638
C	-2.227330727	-6.497152960	-72.636320731
C	-3.418714840	-6.285836186	-71.986662523
C	-5.179023398	-7.025929357	-75.144773294
C	-7.483928297	-7.056958194	-75.592849896
C	-7.273948701	-7.386719707	-76.926207756
C	-5.957209441	-7.538632366	-77.372349157
C	-4.906726963	-7.358390467	-76.482278316
C	-6.641972951	-5.976846785	-70.624289874
C	-6.653212305	-7.229766952	-69.822014301
C	-6.609992811	-5.134830901	-68.440752671
C	-6.620101102	-4.858600832	-69.818317998
C	-6.670828298	-8.478807032	-70.433151581
C	-6.678114963	-9.559759832	-72.527017053
C	-6.680260089	-10.826214501	-71.925663732
C	-6.682958046	-10.906057717	-70.515750858
C	-6.678185502	-9.747295064	-69.771809139
C	-9.204904841	-4.861186667	-72.963162296
C	-10.578879065	-4.597004075	-73.059678935
C	-11.517123716	-5.600611286	-72.809794558
C	-11.052736019	-6.863369705	-72.465440401
C	-9.694596312	-7.159546454	-72.362128598
C	-8.133119718	-3.878047846	-73.208313182
C	-5.728705148	-3.502227931	-73.276914133
C	-5.978376213	-2.173373010	-73.613839171
C	-7.262939010	-1.667711144	-73.757404958
C	-8.337923220	-2.533557383	-73.551548129
H	-1.223170658	-6.431995206	-72.237505239
H	-3.466767822	-6.010041757	-70.938531200
H	-8.479897190	-6.923239654	-75.185792469
H	-8.119338990	-7.517920845	-77.591320057
H	-5.753547374	-7.794195131	-78.407523046
H	-3.878507558	-7.469305331	-76.808914032
H	-6.611354120	-3.841885381	-70.192727836
H	-6.678254084	-9.457925756	-73.607800200
H	-6.681619492	-11.714913979	-72.545070994
H	-6.687873362	-11.872725536	-70.022771449
H	-6.679263066	-9.779285998	-68.687410124
H	-6.589927998	-4.436737215	-67.615648391
H	-12.583681784	-5.414793923	-72.878133037
H	-9.399891893	-8.168012661	-72.087583503

H	-4.703394992	-3.837752263	-73.176713363
H	-7.411160446	-0.626049664	-74.020956925
H	-9.346511667	-2.145280334	-73.659326718
H	-10.936275907	-3.607663911	-73.331949625
N	-6.472358519	-6.884512664	-74.727207465
N	-6.678145761	-8.429552219	-71.832279823
S	-2.451177323	-6.918391862	-74.304909203
S	-6.632304035	-6.890368381	-68.088480435
Pt	-6.661935739	-6.334340519	-72.584371400
C	-6.807185474	-4.363023227	-73.074729794
C	-8.755615259	-6.157800692	-72.611992336
F	-11.957409189	-7.847687649	-72.220394822
F	-4.920943600	-1.343798823	-73.806232143

2cc (T_3)

$\langle S^2 \rangle = 2.036341$

C	-4.570525834	-6.489509471	-72.819365787
C	-4.191850389	-6.824958898	-74.106611671
C	-2.232286467	-6.535640497	-72.619398172
C	-3.428306966	-6.328666681	-71.977239463
C	-5.163499406	-7.040441461	-75.158836709
C	-7.463183861	-7.087308044	-75.626792384
C	-7.239790998	-7.393540008	-76.964249250
C	-5.917777798	-7.526410488	-77.400506679
C	-4.875855333	-7.351738815	-76.498268465
C	-6.650597270	-6.025946232	-70.608124567
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C	-6.619244153	-5.110726565	-68.465252519
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C	-6.668969827	-10.839640786	-71.903727747
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C	-7.307168702	-1.663837132	-73.725001319
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H	-3.483634670	-6.064964428	-70.926367532
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H	-6.641367254	-11.854809182	-69.995459553
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N	-6.460692594	-6.917105855	-74.752384660
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Pt	-6.666837666	-6.359941321	-72.586639983
C	-6.793659386	-4.401747174	-73.082475361
C	-8.746101287	-6.187657984	-72.625844080
F	-11.978128701	-7.820107777	-72.277111510
F	-4.949729964	-1.372258516	-73.856425134

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