Supplementary Information

Easy access to strongly fluorescent higher homologues of BODIPY

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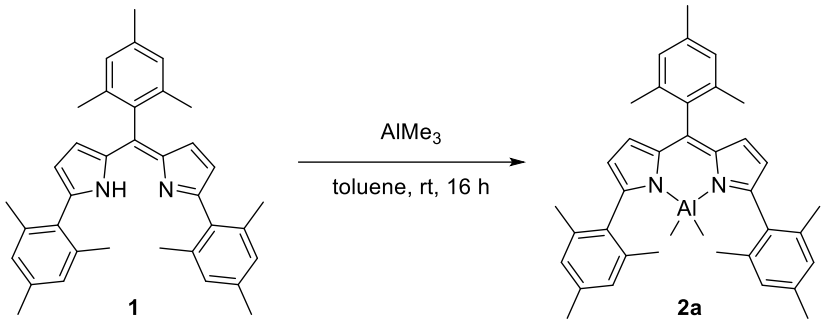
Content

1. Synthesis and characterization of ^{Mes}DPM triel dialkyls:

General procedure:

At room temperature 0.15 g (^{Mes}DPM)H (**1**, 0.30 mmol, 1.00 eq.) were suspended in 10 mL toluene under stirring. To this suspension MR_3 (M = Al-In; R = Me, Et) (0.30 mmol, 1.00 eq.) was added dropwise. The reaction mixture was stirred at room temperature for 16 h. Evaporation of the solvent and drying under reduced pressure at 85 °C afforded the desired products ((^{Mes}DPM)MR_2 (M = Al–In; R = Me, Et)) as red/orange solids in almost quantitative yield between 95 and 98%.

1.1 (^{Mes}DPM)$AlMe_2$ (**2a**):



^{1}H-NMR (300.19 MHz, C_6D_6) δ = 6.80 (s, 2 H, -C*H*(Mes)), 6.75 (s, 4 H, -C*H*(Mes)), 6.72 (d, $^{3}J_{AB}$ = 4.0 Hz, 2 H, -C*H*(py)), 6.08 (d, $^{3}J_{AB}$ = 4.0 Hz, 2 H, -C*H*(py)), 2.21 (s, 3 H, -*Me*), 2.20 (s, 6 H, -*Me*), 2.19 (s, 12 H, -*Me*), 2.07 (s, 6 H, -*Me*), -0.72 (s, 6 H, -Al*Me*) ppm.

^{13}C{^{1}H}-NMR (75.48 MHz, C_6D_6) δ = 162.22 (s, 2 C, C_{quart} (pyr)), 146.37 (s, 1 C, C_{quart}), 138.97 (s, 2 C, C_{quart} (Mes)), 138.69 (s, 2 C, C_{quart} (Mes)), 137.83 (s, 1 C, C_{quart} (Mes)), 137.70 (s, 4 C, C_{quart} (Mes)), 136.82 (s, 2 C, C_{quart} (Mes)), 134.64 (s, 1 C, C_{quart} (Mes)), 132.55 (s, 2 C, -*C*H (pyr)), 131.70 (s, 2 C, C_{quart} (pyr)), 128.25 (s, 6 C, -*C*H(Mes)), 120.09 (s, 2 C, -*C*H (pyr)), 21.20 (s, 1 C, -*Me*), 21.19 (s, 2 C, -*Me*), 20.71 (s, 4 C, -*Me*), 19.91 (s, 2 C, -*Me*), -8.54 (s, 2 C, -Al*Me*) ppm.

IR (cm^{-1}) ν = 2920.63 (m, br), 1611.02 (m), 1551.26 (s), 1460.66 (m), 1378.87 (m), 1331.79 (m), 1313.59 (w), 247.56 (s), 1211.65 (m), 1178.35 (m), 1078.57 (m), 1051.83 (m), 1009.81 (s), 917.85 (m), 889.75 (w), 866.07 (m), 854.07 (m), 841.95 (m), 793.08 (m), 737.46 (m), 727.29 (m), 698.13 (m), 669.49 (m), 620.62 (m), 580.41 (m), 467.74 (w), 449.40 (w), 426.32 (m).

MS (HR-CI^{+}) (m/z (%)) calculated for $[C_{38}H_{44}N_2Al_1]^{+}$: 555.33199.; found: 555.33318 (25.24); calculated for $[C_{37}H_{40}N_2Al_1]^{+}$: 539.30069.; found: 539.30072 (100.0).

CHNS calculated: C = 82.27%, H = 7.81%, N = 5.05%; found: C = 81.47%, H = 7.573%, N = 5.07%.

SS-UV/Vis ($BaSO_4$): $\lambda_{max,ss}$ = 509 nm (FWHM = 91 nm).

UV/Vis (toluene): λ_{max} = 504 nm (FWHM = 20 nm), ε_{max} (504 nm) = $1.27 \cdot 10^5$ L mol^{-1} cm^{-1}.

Excitation/Emission (toluene): λ_{Ex} = 339 nm; λ_{Em} = 521 nm.

SS-PL (λ_{Ex} = 325 nm): $\lambda_{F,ss}$ = 562 nm; $\varphi_{F,ss}$ = 34%.

PL (toluene, λ_{Ex} = 405 nm): λ_{F} = 540 nm; φ_{F} = 44%.

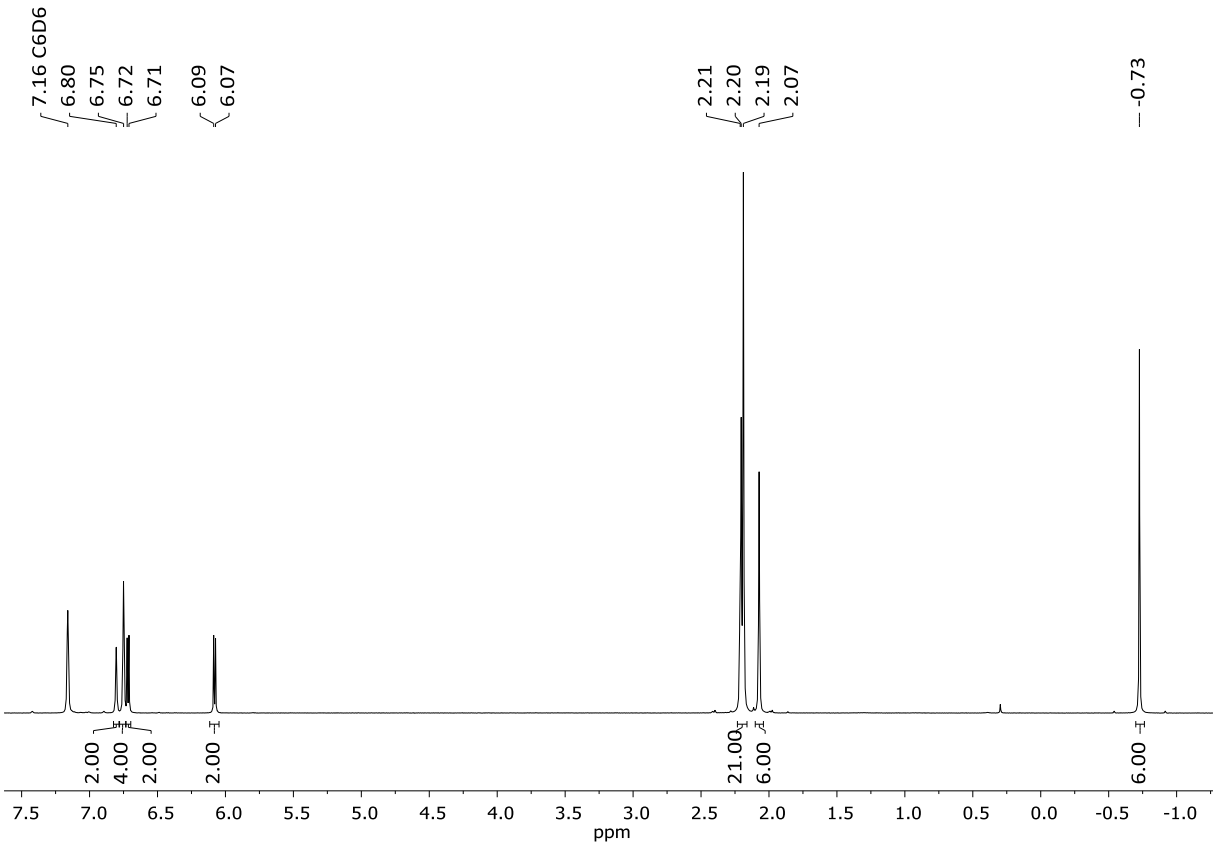


Figure 1: ^{1}H NMR spectrum of compound 2a in C_6D_6 at 300 K.

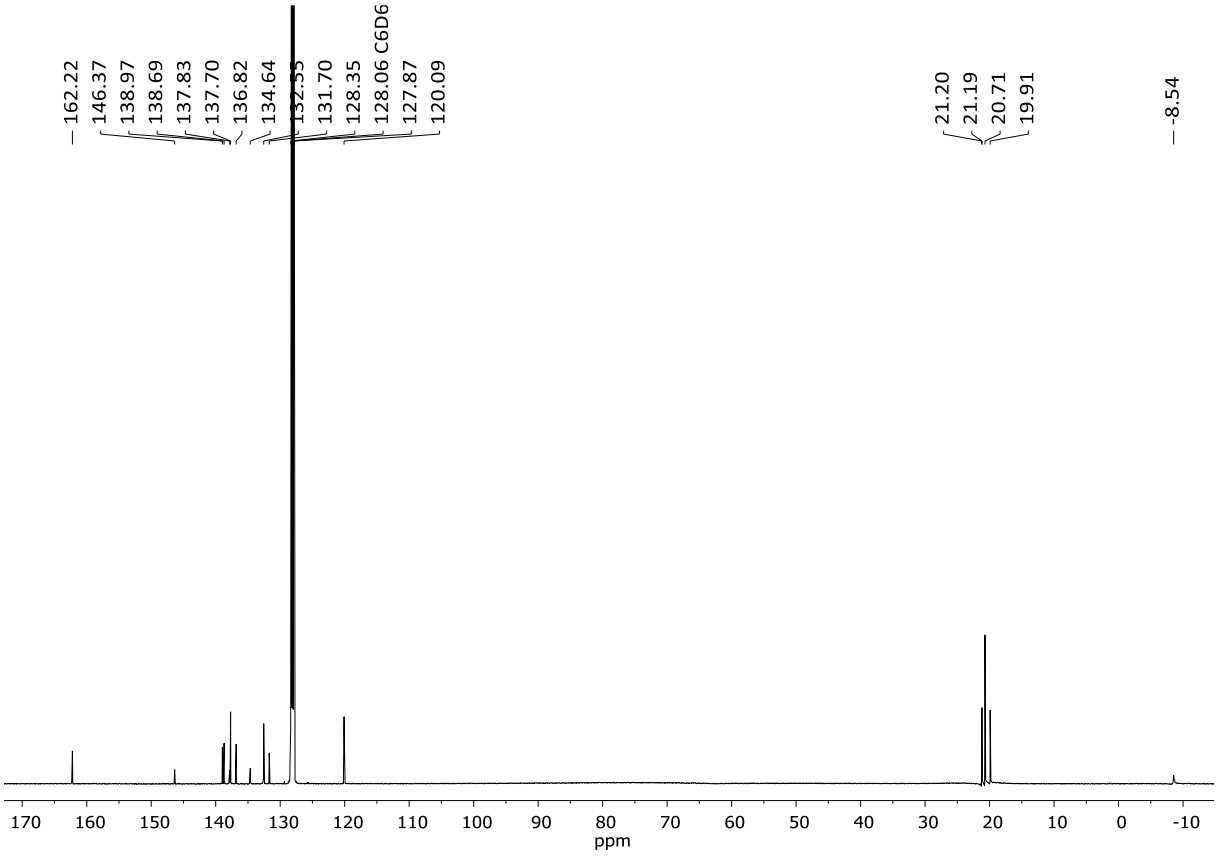


Figure 2: ^{13}C NMR spectrum of compound 2a in C_6D_6 at 300 K.

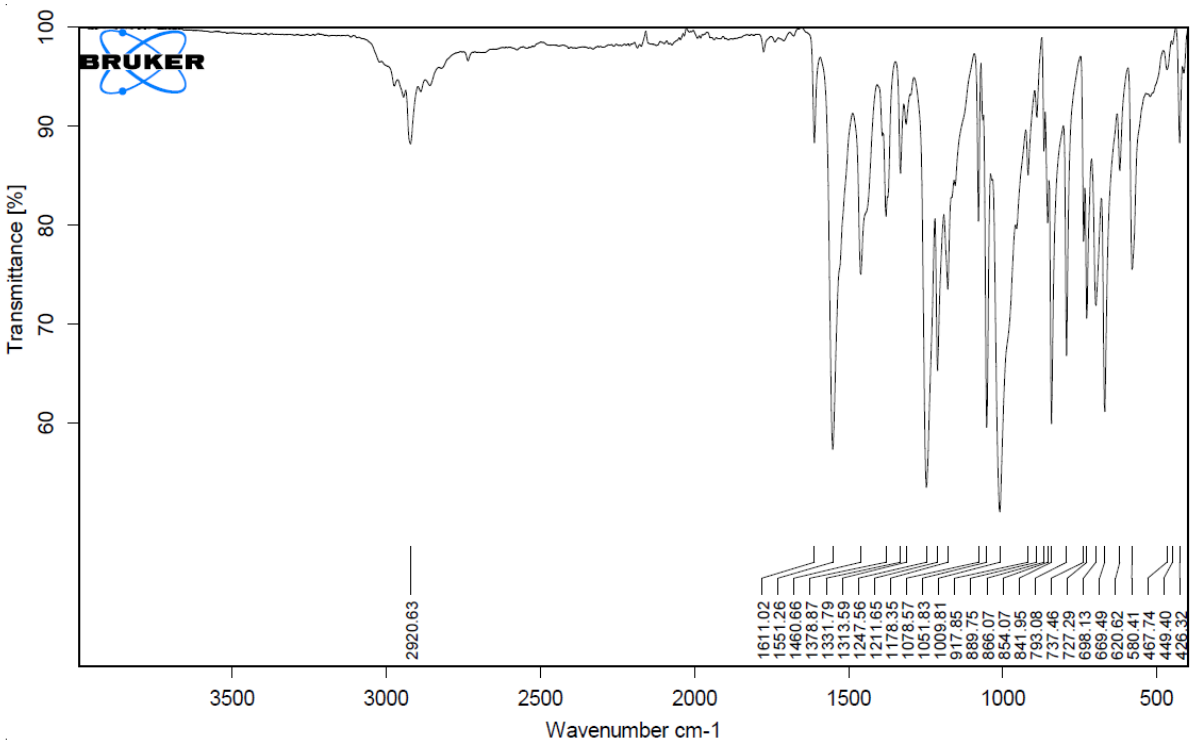


Figure 3: IR spectrum of compound 2a.

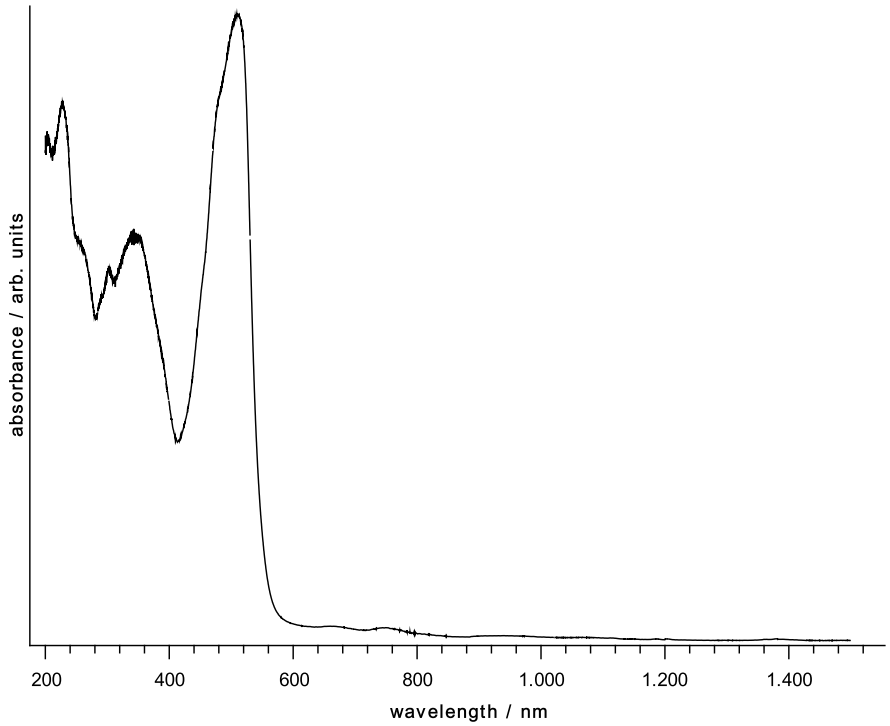


Figure 4: Solid-state UV/VIS spectrum of compound 2a.

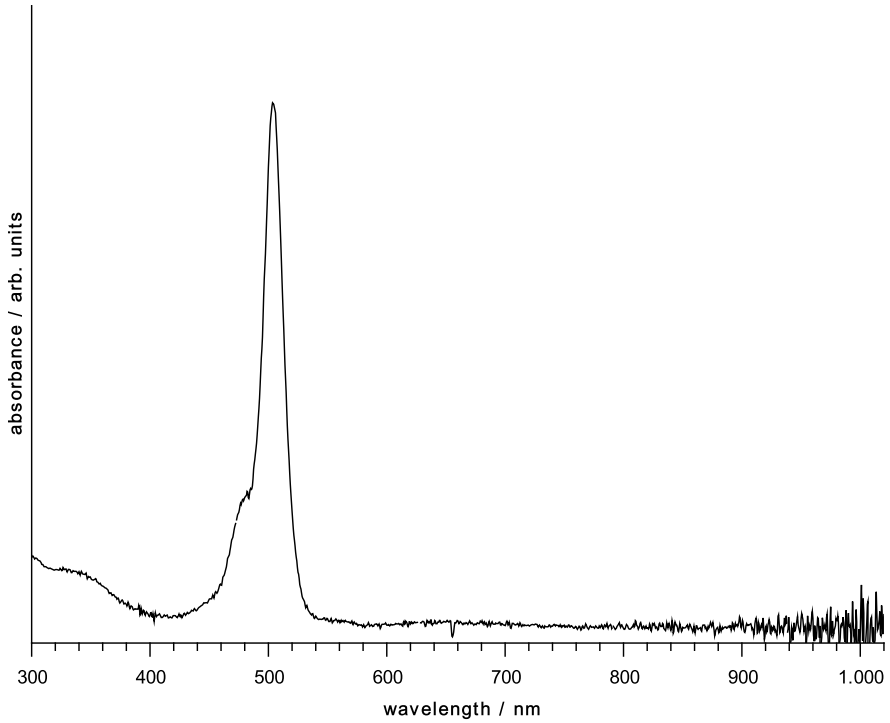


Figure 5: Solution-state UV/VIS spectrum of compound 2a (2 µM in toluene).

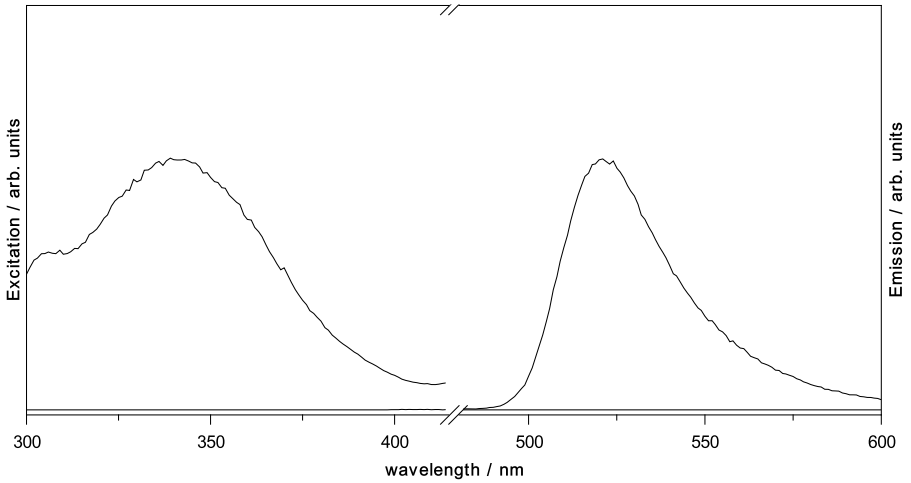


Figure 6: Excitation spectrum of 2a in toluene with emission detected at λ_F (left); emission spectra obtained with excitation detected at λ_{Ex} (right).

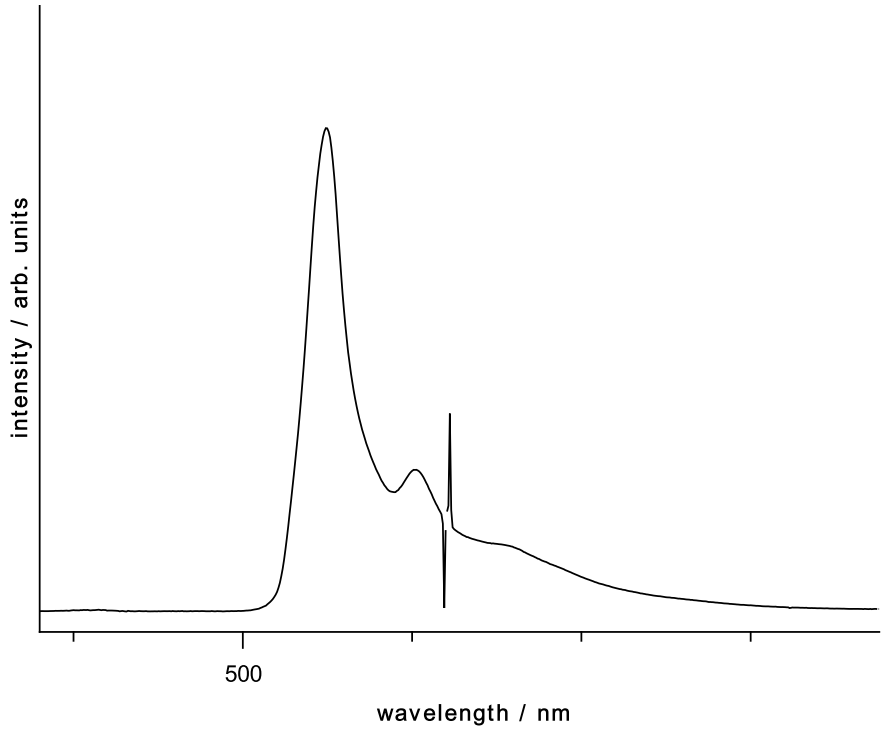


Figure 7: Solid-state PL spectrum of compound 2a. Excitation with 325 nm He-Cd continuous wave laser (the signal at 650 nm is the second diffraction order of the laser).

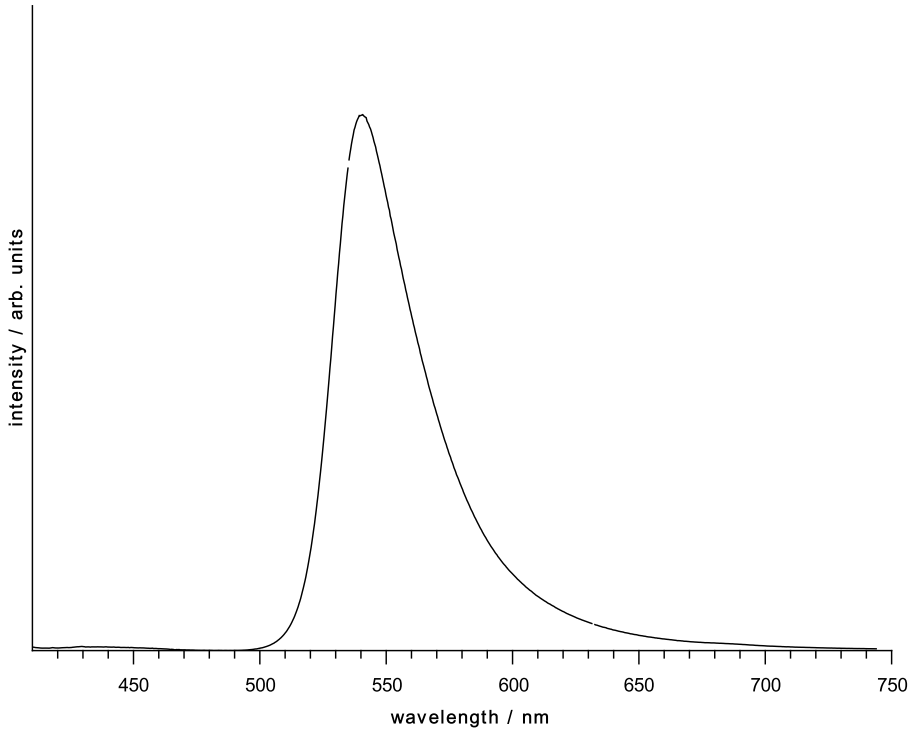
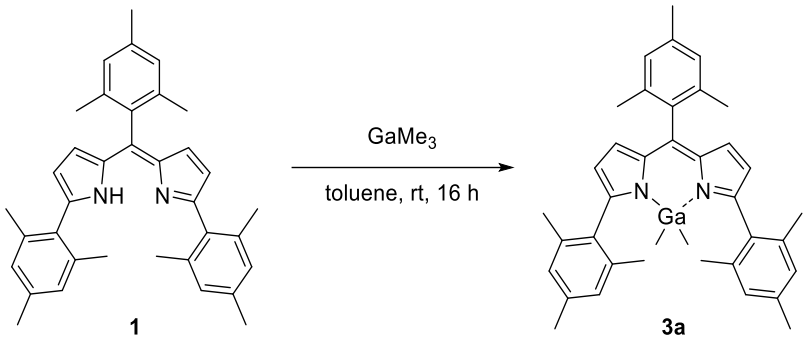


Figure 8: Solution-state PL spectrum of compound 2a in toluene. Excitation with 405 nm continuous wave diode laser.

1.2 (^{Mes}DPM)$GaMe_2$ (**3a**):



^{1}H-NMR (300.19 MHz, C_6D_6) δ = 6.82 (s, 2 H, -C*H*(Mes)), 6.77 (d, $^3J_{AB}$ = 4.0 Hz, 2 H, -C*H*(py)), 6.75 (s, 4 H, -C*H*(Mes)), 6.12 (d, $^3J_{AB}$ = 4.1 Hz, 2 H, -C*H*(py)), 2.24 (s, 6 H, -*Me*), 2.22 (s, 3 H, -*Me*), 2.16 (s, 12 H, -*Me*), 2.08 (s, 6 H, -*Me*), -0.38 (s, 6 H, -Al*Me*) ppm.

^{13}C{^{1}H}-NMR (75.48 MHz, C_6D_6) δ = 161.03 (s, 2 C, C_{quart} (pyr)), 148.53 (s, 1 C, C_{quart}), 138.44 (s, 2 C, C_{quart} (Mes)), 138.28 (s, 2 C, C_{quart} (Mes)), 137.64 (s, 1 C, C_{quart} (Mes)), 137.61 (s, 4 C, C_{quart} (Mes)), 136.88 (s, 2 C, C_{quart} (Mes)), 135.29 (s, 1 C, C_{quart} (Mes)), 132.22 (s, 2 C, C_{quart} (pyr)), 131.92 (s, 2 C, -*C*H (pyr)), 128.20 (s, 6 C, -*C*H (Mes)), 119.29 (s, 2 C, -*C*H (pyr)), 21.21 (s, 1 C, -*Me*), 21.18 (s, 2 C, -*Me*), 20.67 (s, 4 C, -*Me*), 19.96 (s, 2 C, -*Me*), -5.85 (s, 2 C, -Ga*Me*) ppm.

IR (cm^{-1}) ν = 2952.06 (w), 2919.98 (m), 2857.41 (w), 1610.78 (m), 1549.48 (s), 1461.36 (m), 1374.92 (m), 1335.52 (m), 1312.51 (w), 1252.05 (s), 1216.93 (m), 1187.15 (m), 1076.84 (w), 1050.61 (m), 1004.73 (s), 916.50 (m), 887.28 (w), 865.45 (m), 853.60 (m), 839.65 (s), 789.05 (m), 750.42 (m), 730.45 (m), 676.32 (m), 620.15 (w), 582.83 (w), 566.09 (m), 536.48 (m), 468.24 (w), 412.12 (m).

MS (HR-CI$^+$) (m/z (%)) calculated for $[C_{38}H_{44}N_2Ga_1]^+$: 597.27603; found: 597.27602 (13.54); calculated for $[C_{37}H_{40}N_2Ga_1]^+$: 581.24473.; found: 581.24546 (32.17).

CHNS: calculated: C = 76.39%, H = 7.25%, N = 4.69%; found: C = 76.48%, H = 6.923%, N = 4.77%.

UV/Vis ($BaSO_4$): $\lambda_{max,ss}$ = 502 nm (FWHM = 110 nm).

UV/Vis (toluene): λ_{max} = 500 nm (FWHM = 21 nm), ε_{max} (500 nm) = $1.30 \cdot 10^5$ L mol^{-1} cm^{-1}.

Excitation/Emission (toluene): λ_{Ex} = 337 nm; λ_{Em} = 517 nm.

SS-PL (λ_{Ex} = 325 nm): $\lambda_{F,ss}$ = 562 nm; $\varphi_{F,ss}$ = 33%.

PL (toluene, λ_{Ex} = 405 nm): λ_F = 539 nm; φ_F = 51%.

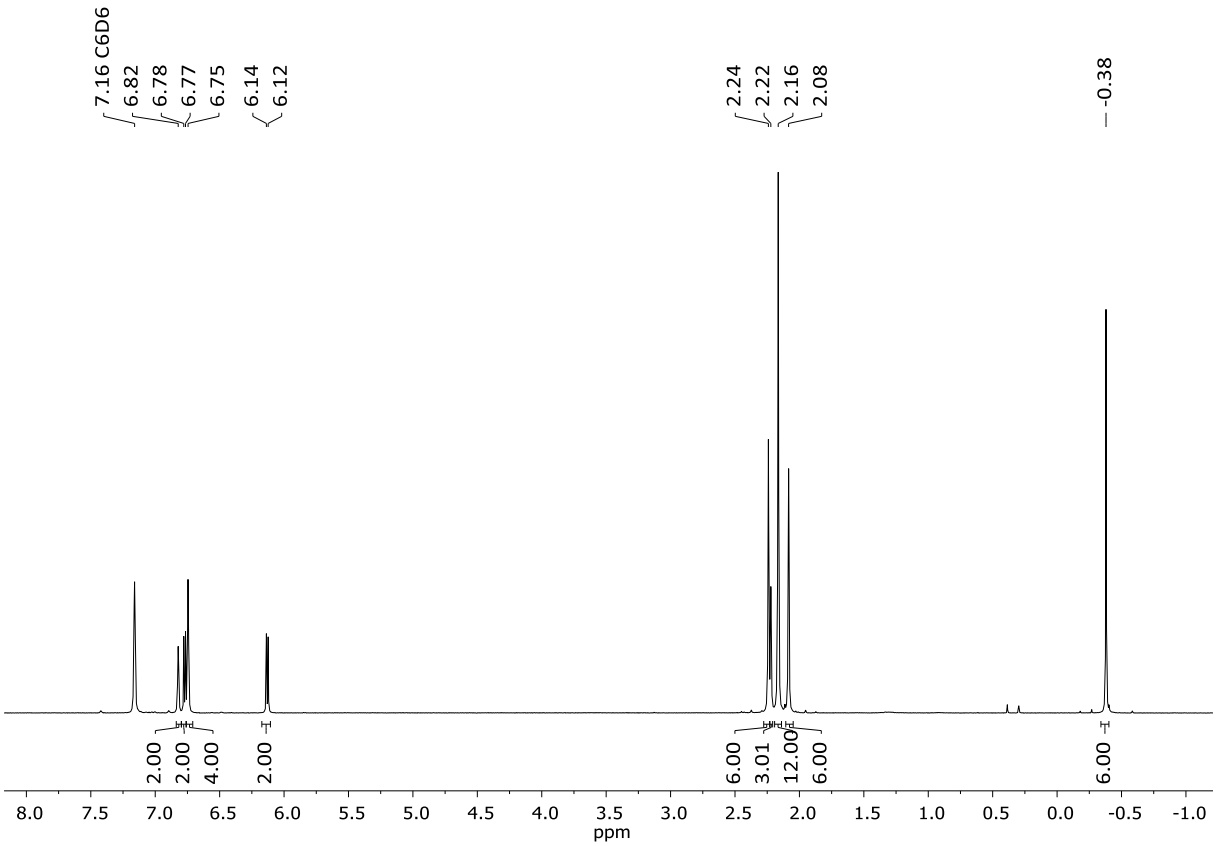


Figure 9: ^{1}H NMR spectrum of compound 3a in C_6D_6 at 300 K.

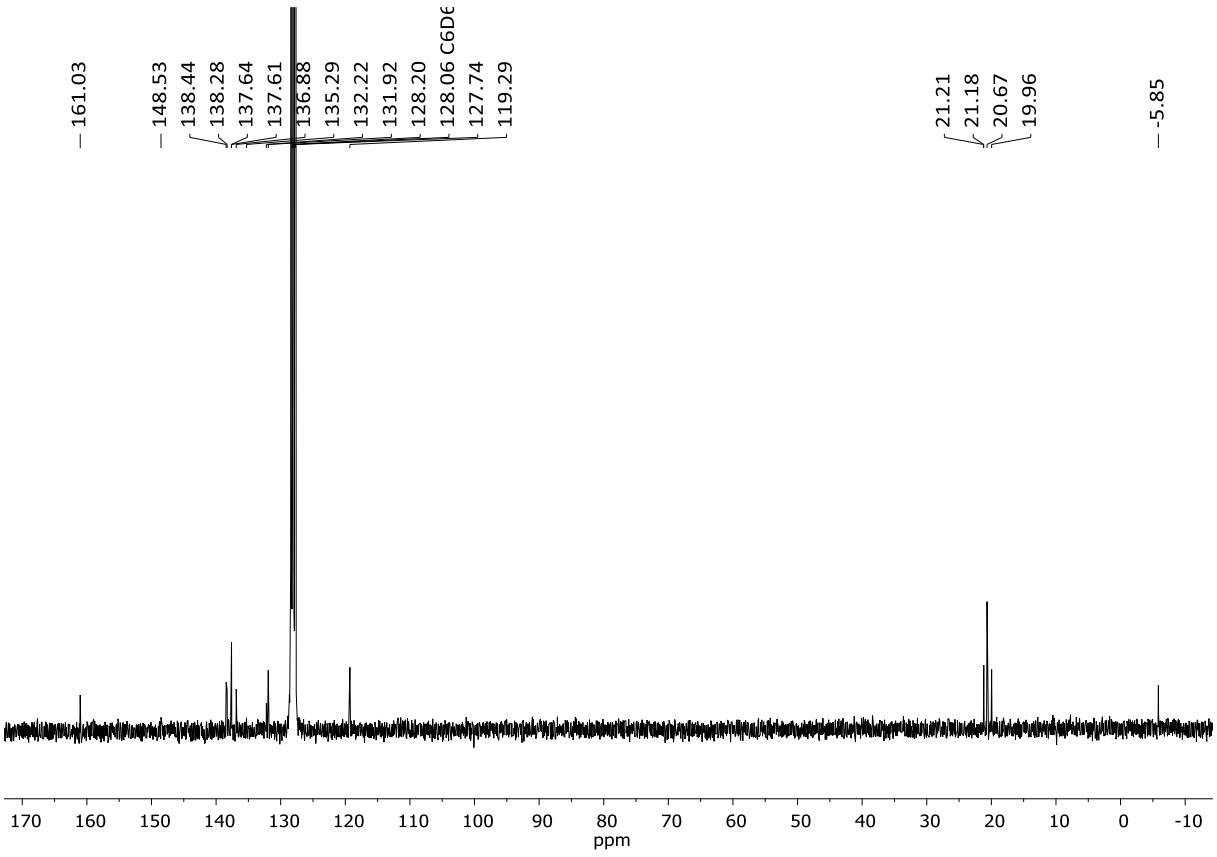


Figure 10: ^{13}C NMR spectrum of compound 3a in C_6D_6 at 300 K.

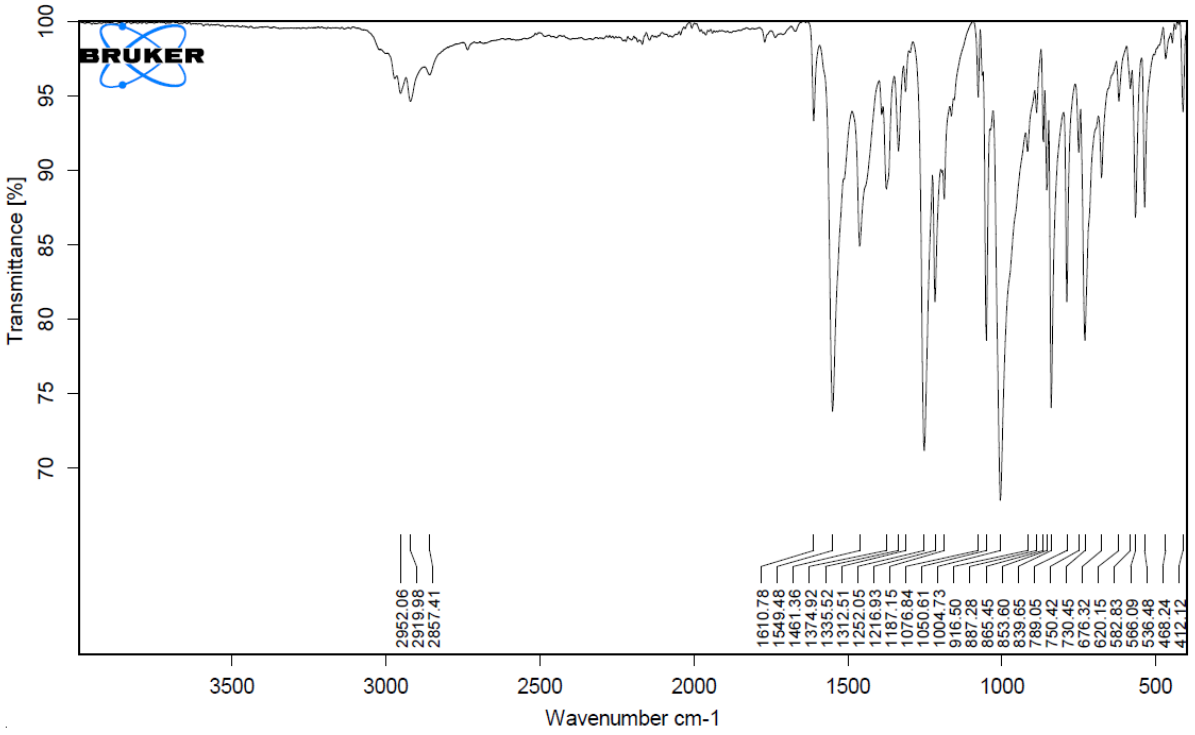


Figure 11: IR spectrum of compound 3a.

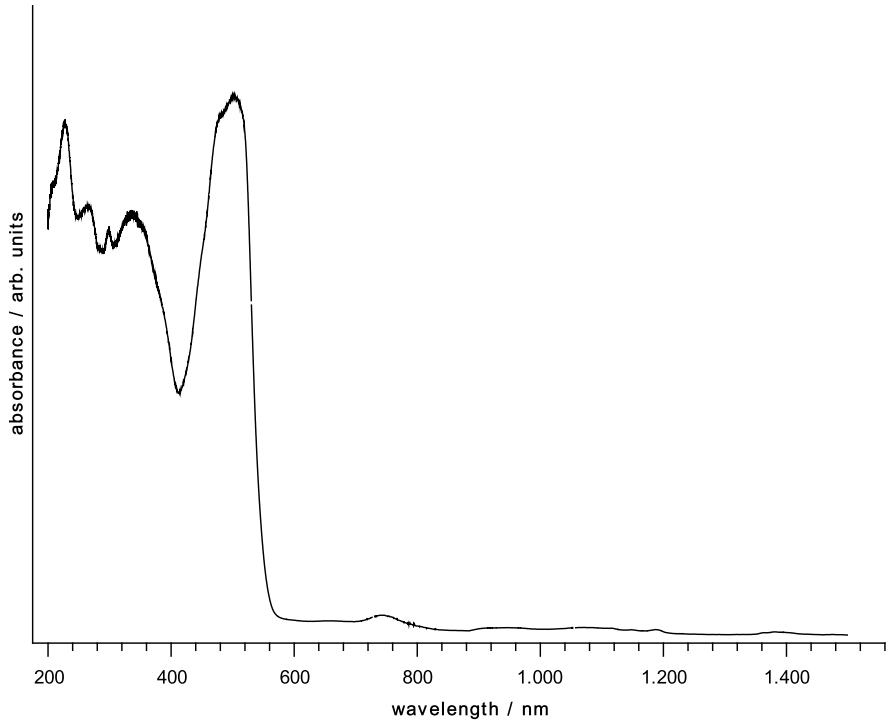


Figure 12: Solid-state UV/VIS spectrum of compound 3a.

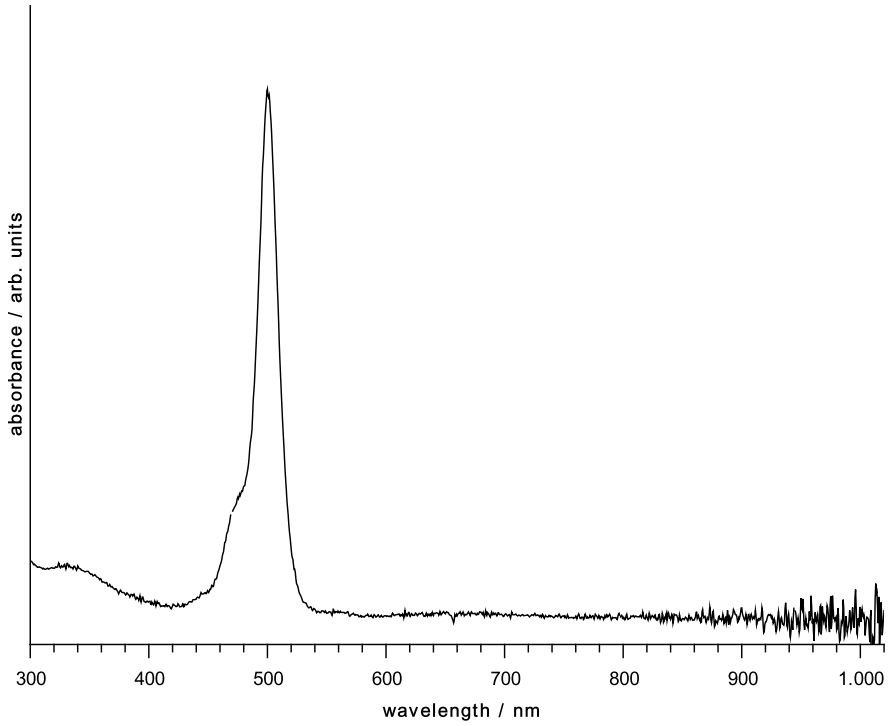


Figure 13: Solution-state UV/VIS spectrum of compound 3a (2 µM in toluene).

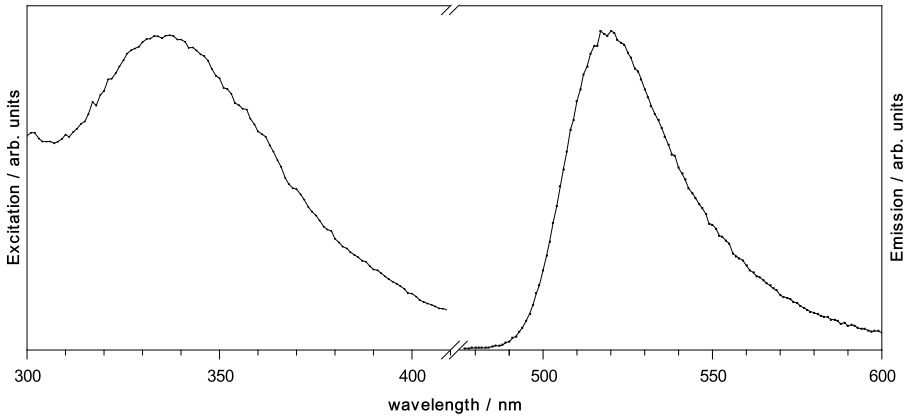


Figure 14: Excitation spectrum of 3a in toluene with emission detected at λ_F (left); emission spectra obtained with excitation detected at λ_{Ex} (right).

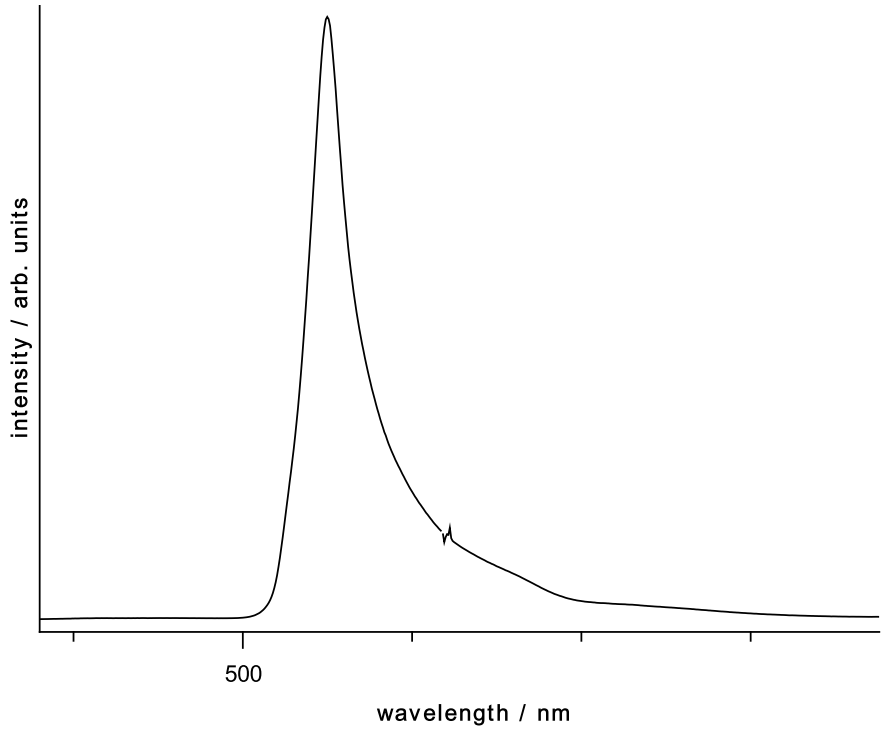


Figure 15: Solid-state PL spectrum of compound 3a. Excitation with 325 nm He-Cd continuous wave laser (the signal at 650 nm is the second diffraction order of the laser).

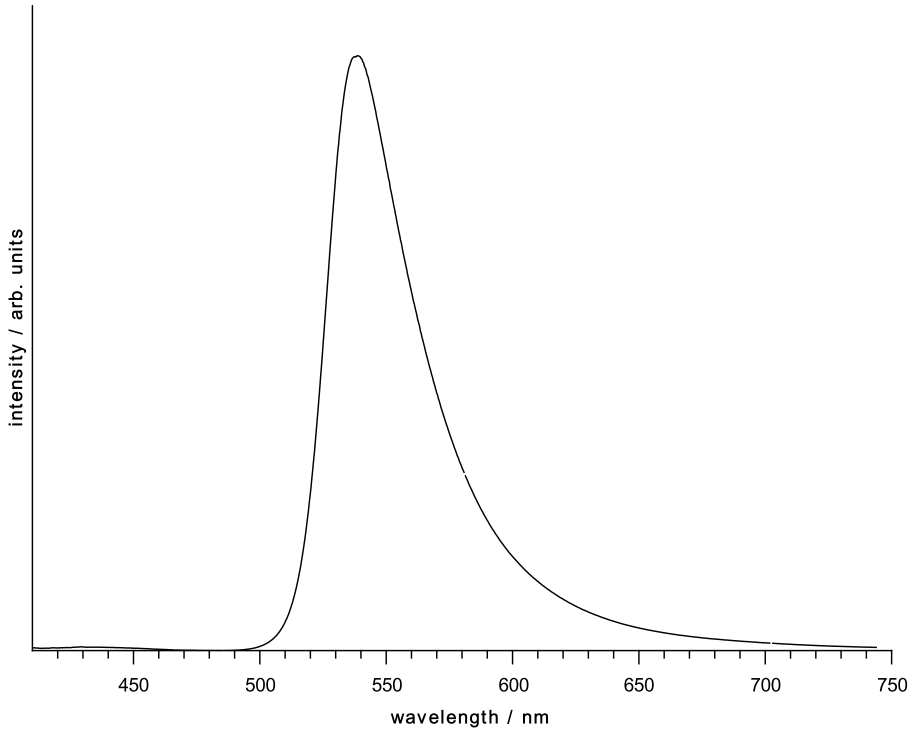
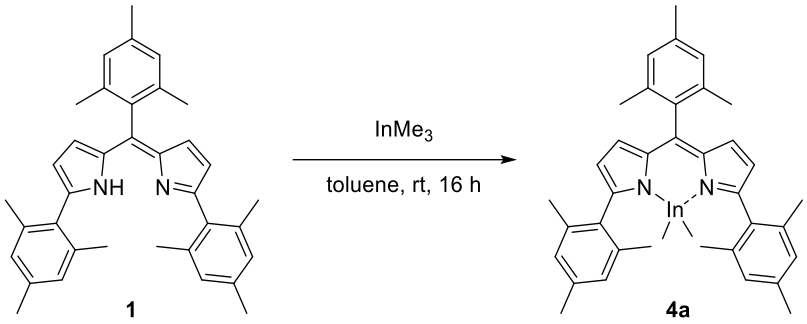


Figure 16: Solution-state PL spectrum of compound 3a in toluene. Excitation with 405 nm continuous wave diode laser.

1.3 (^{Mes}DPM)InMe$_2$ (**4a**):



^{1}H-NMR (300.19 MHz, C_6D_6) δ = 6.83 (s, 2 H, -C*H*(Mes)), 6.83 (d, $^3J_{AB}$ = 43.9 Hz, 2 H, -C*H*(py)), 6.74 (s, 4 H, -C*H*(Mes)), 6.18 (d, $^3J_{AB}$ = 4.0 Hz, 2 H, -C*H*(py)), 2.27 (s, 6 H, -*Me*), 2.23 (s, 3 H, -*Me*), 2.15 (s, 12 H, -*Me*), 2.07 (s, 6 H, -*Me*), -0.29 (s, 6 H, -In*Me*) ppm.

^{13}C{^{1}H}-NMR (75.48 MHz, C_6D_6) δ = 161.36 (s, 2 C, C_{quart} (pyr)), 146.48 (s, 1 C, C_{quart}), 139.37 (s, 2 C, C_{quart} (Mes)), 138.49 (s, 2 C, C_{quart} (Mes)), 137.66 (s, 4 C, C_{quart} (Mes)), 137.37 (s, 1 C, C_{quart} (Mes)), 136.91 (s, 2 C, C_{quart} (Mes)), 136.53 (s, 1 C, C_{quart} (Mes)), 132.94 (s, 2 C, -*C*H (pyr)), 132.89 (s, 2 C, C_{quart} (pyr)), 128.23 (s, 4 C, -*C*H (Mes)), 127.92 (s, 2 C, -*C*H (Mes)), 118.64 (s, 2 C, -*C*H (pyr)), 21.23 (s, 1 C, -*Me*), 21.17 (s, 2 C, -*Me*), 20.55 (s, 4 C, -*Me*), 20.01 (s, 2 C, -*Me*), -7.35 (s, 2 C, -In*Me*) ppm.

IR (cm^{-1}) ν = 2968.70 (w), 2916.43 (m), 2855.30 (w), 2163.36 (w), 1610.75 (m), 1544.28 (s), 1461.60 (m), 1363.12 (m), 1334.37 (m), 1307.93 (w), 1248.87 (s), 1219.00 (m), 1148.72 (m), 1076.43 (w), 1049.10 (m), 1000.18 (s), 13.97 (m), 886.70 (w), 864.45 (m), 851.89 (m), 838.79 (s), 786.71 (m), 727.24 (m), 662.11 (m), 618.95 (w), 572.27 (w), 502.58 (m), 481.82 (m), 407.90 (w).

MS (HR-CI$^+$) (m/z (%)) calculated for $[C_{38}H_{44}N_2In_1]^+$: 643.25433; found: 643.25263 (39.58); calculated for $[C_{37}H_{40}N_2In_1]^+$: 627.22303; found: 627.22203 (100.0).

CHNS: calculated: C = 71.03%, H = 6.75%, N = 4.36%; found: C = 71.20%, H = 6.556%, N = 4.43%.

UV/Vis ($BaSO_4$): $\lambda_{max,ss}$ = 509 nm (FWHM = 95 nm).

UV/Vis (toluene): λ_{max} = 499 nm (FWHM = 26 nm), ε_{max} (499 nm) = 1.43·10^5 L mol^{-1} cm^{-1}.

Excitation/Emission (toluene): λ_{Ex} = 327 nm; λ_{Em} = 529 nm.

SS-PL (λ_{Ex} = 325 nm): $\lambda_{F,ss}$ = 557 nm; $\varphi_{F,ss}$ = 3 %.

PL (toluene, λ_{Ex} = 405 nm): λ_F = 540 nm; φ_F = 2 %.

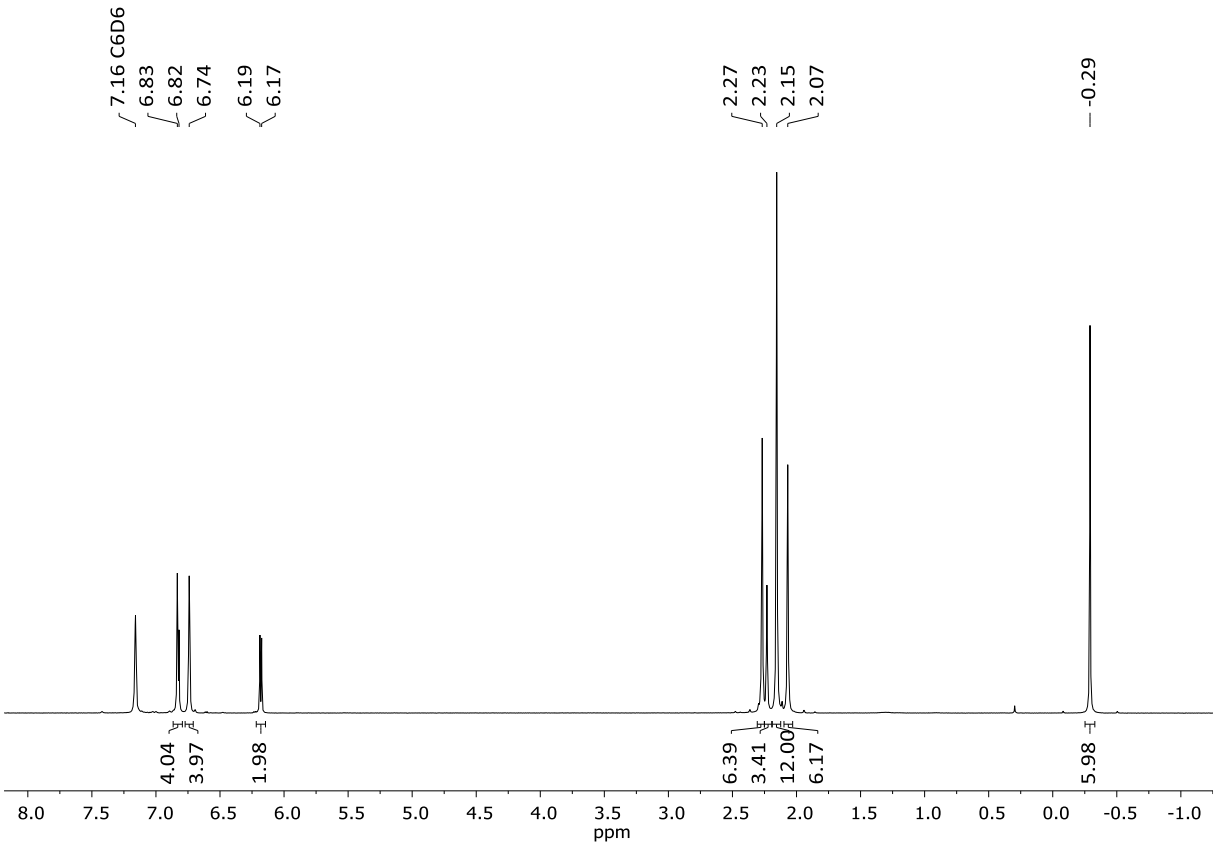


Figure 17: ^{1}H NMR spectrum of compound 4a in C_6D_6 at 300 K.

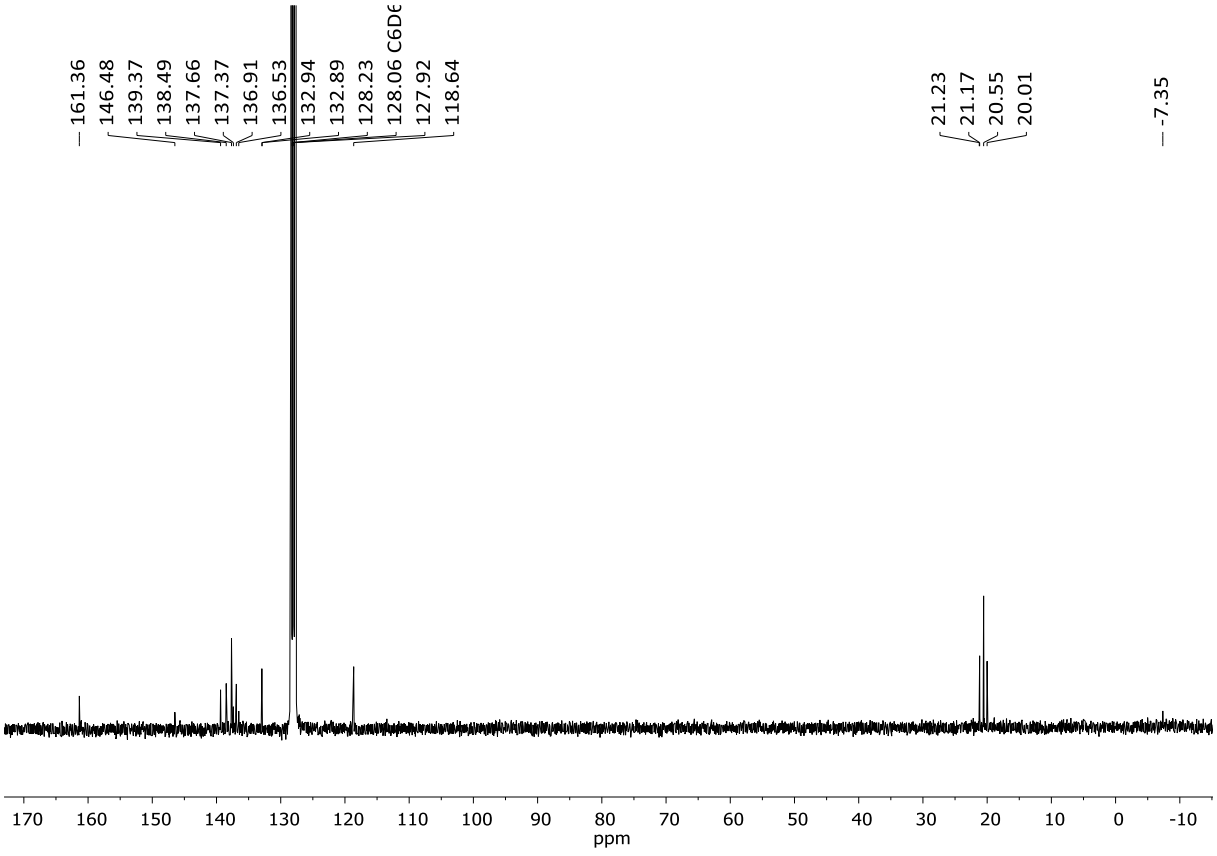


Figure 18: ^{13}C NMR spectrum of compound 4a in C_6D_6 at 300 K.

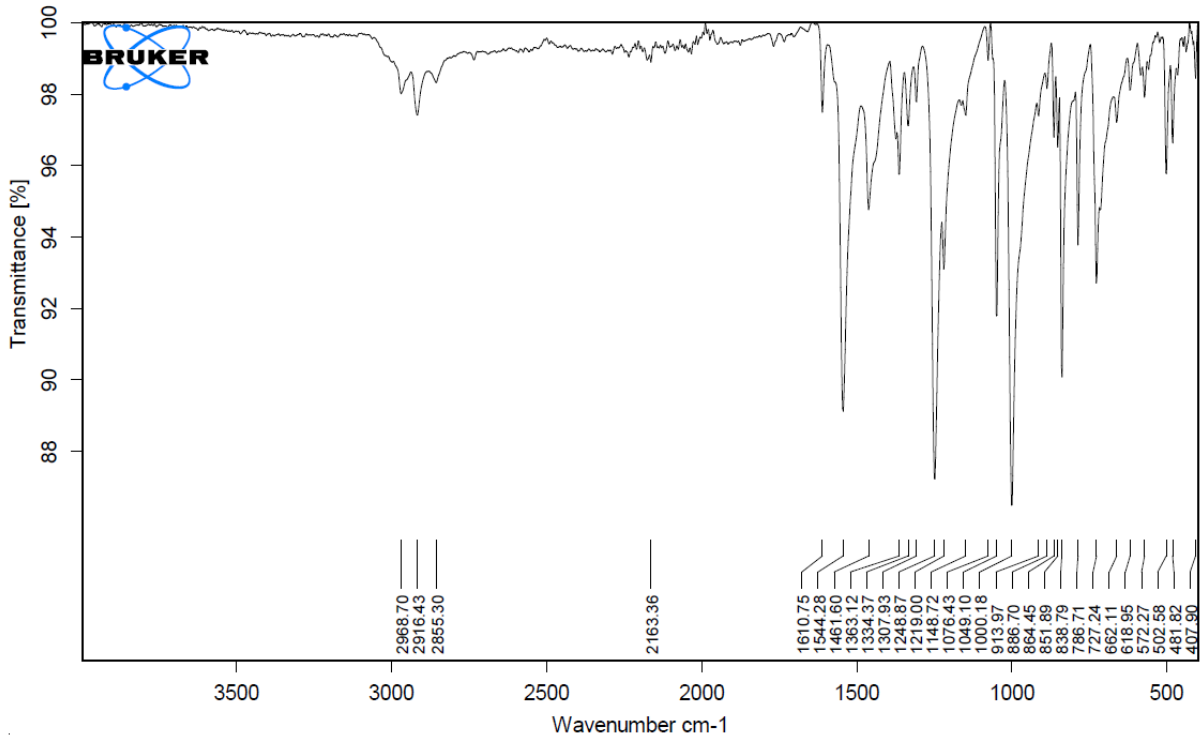


Figure 19: IR spectrum of compound 4a.

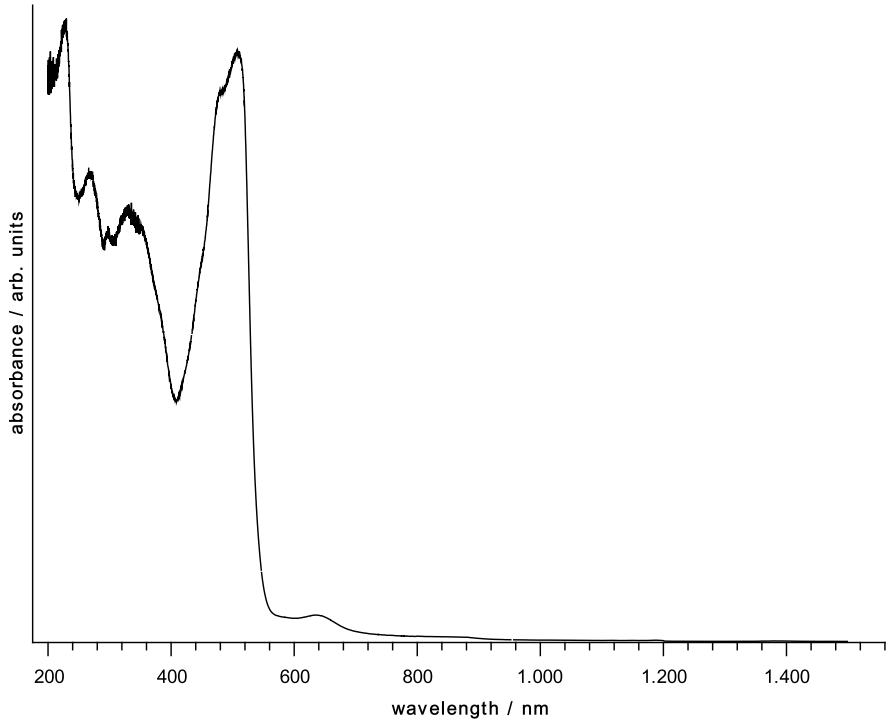


Figure 20: Solid state UV/VIS spectrum of compound 4a.

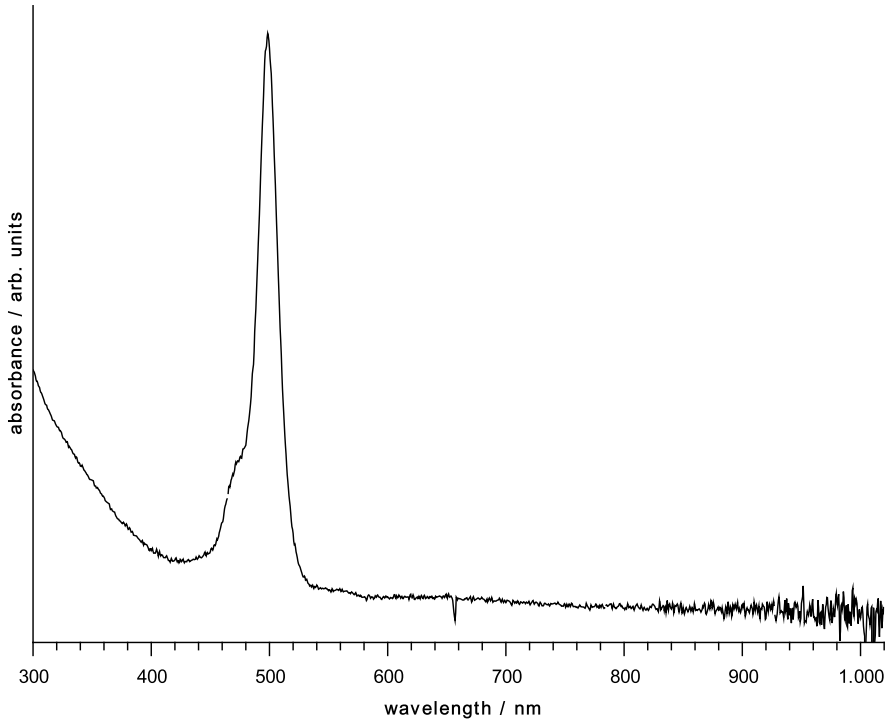


Figure 21: Solution-state UV/VIS spectrum of compound 4a (2 µM in toluene).

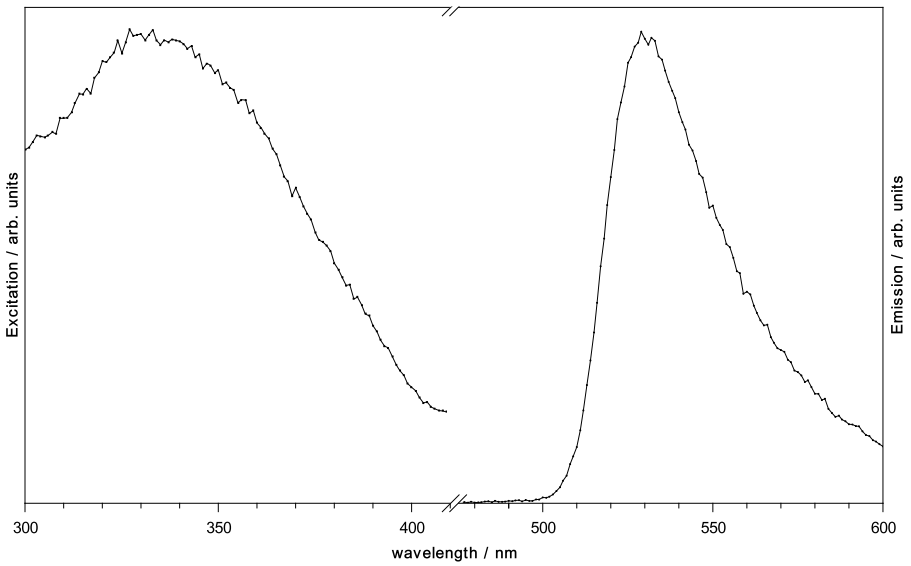


Figure 22: Excitation spectrum of 4a in toluene with emission detected at λ_F (left); emission spectra obtained with excitation detected at λ_{Ex} (right).

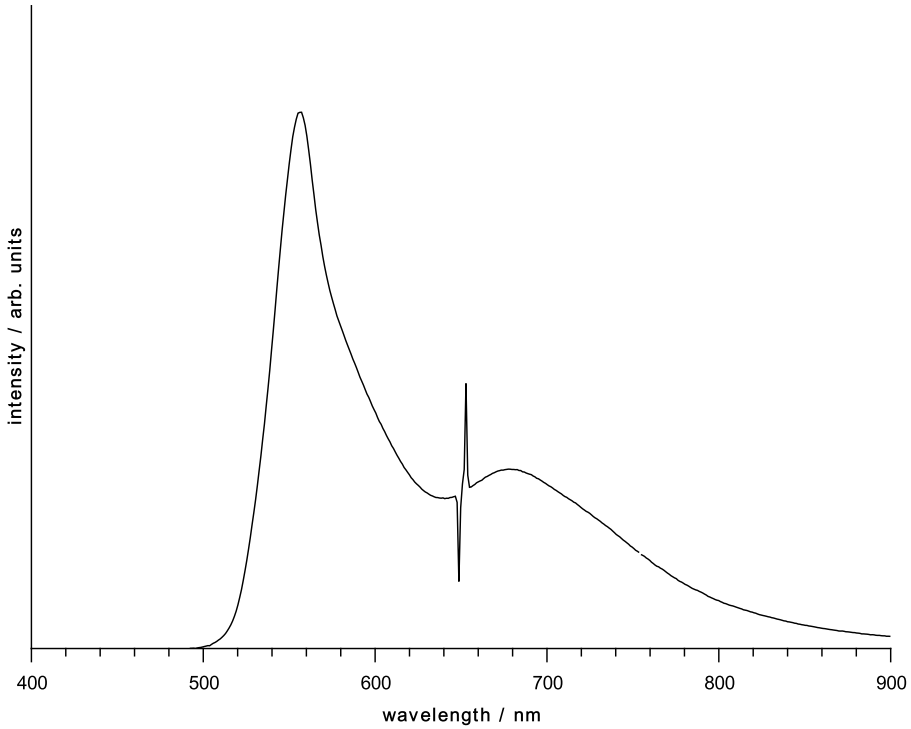


Figure 23: Solid state PL spectrum of compound 4a. Excitation with 325 nm He-Cd continuous wave laser (the signal at 650 nm is the second diffraction order of the laser).

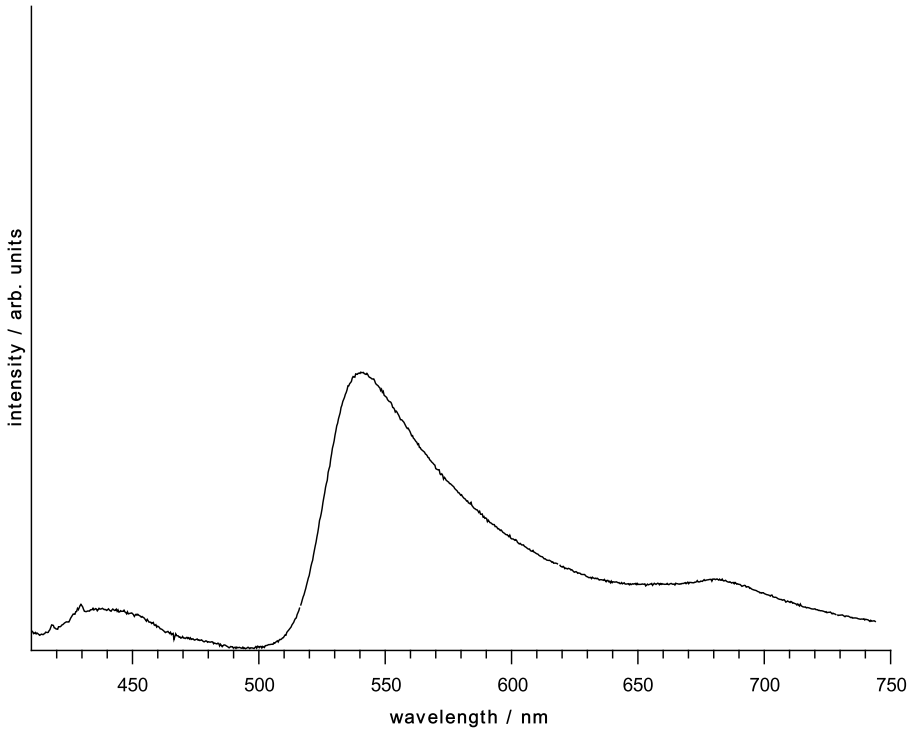
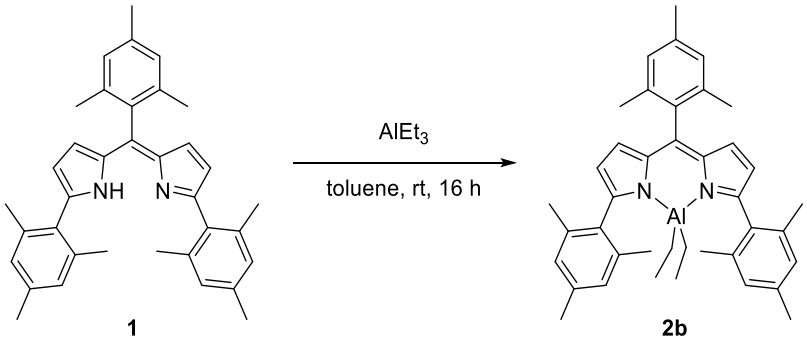


Figure 24: Solution-state PL spectrum of compound 4a in toluene. Excitation with 405 nm continuous wave diode laser.

1.4 (^{Mes}DPM)AlEt$_2$ (**2b**):



^{1}H-NMR (300.19 MHz, C_6D_6) δ = 6.81 (s, 2 H, -C*H*(Mes)), 6.78 (s, 4 H, -C*H*(Mes)), 6.72 (d, $^3J_{AB}$ = 3.8 Hz, 2 H, -C*H*(py)), 6.07 (d, $^3J_{AB}$ = 3.8 Hz, 2 H, -C*H*(py)), 2.23 (m, 21 H, -*Me*), 2.07 (s, 6 H, -*Me*), 0.81 (t, $^3J_{AB}$ = 8.0 Hz, 6 H, -Al*Me*), 0.05 (q, $^3J_{AB}$ = 8.1 Hz, 4 H, -AlCH_2) ppm.

^{13}C{^{1}H}-NMR (75.48 MHz, C_6D_6) δ = 162.29 (s, 2 C, C_{quart} (pyr)), 146.52 (s, 1 C, C_{quart}), 139.66 (s, 2 C, C_{quart} (Mes)), 138.68 (s, 2 C, C_{quart} (Mes)), 137.86 (s, 1 C, C_{quart} (Mes)), 137.54 (s, 4 C, C_{quart} (Mes)), 136.94 (s, 2 C, C_{quart} (Mes)), 134.84 (s, 1 C, C_{quart} (Mes)), 132.63 (s, 4 C, -*C*H (Mes)), 132.04 (s, 2 C, C_{quart} (pyr)), 128.46 (s, 2 C, -*C*H (Mes)), 128.26 (s, 2 C, -*C*H (Im)), 120.47 (s, 2 C, -*C*H (Im)), 21.20 (s, 1 C, -*Me*), 21.16 (s, 2 C, -*Me*), 20.65 (s, 4 C, -*Me*), 20.04 (s, 2 C, -*M*), 9.14 (s, 2 C, -AlCH$_2$*C*H$_3$), 0.77 (s, 2 C, -Al*C*H$_2$) ppm.

IR (cm^{-1}) ν = 2920.20 (w), 2859.56 (m), 1609.42 (w), 1546.52 (s), 1459.97 (m), 1370.77 (m), 330.35 (m), 1247.48 (s), 1212.14 (m), 1077.42 (m), 1051.17 (s), 1010.26 (s), 917.52 (m), 889.91 (w), 865.89 (m), 841.13 (s),793.36 (m), 737.47 (m), 725.27 (m), 642.43 (m), 621.31 (m), 571.53 (m), 429.58 (w), 410.68 (w).

MS (HR-CI$^+$) (m/z (%)) calculated for $[C_{40}H_{48}N_2Al_1]^+$: 583.36329; found: 583.36552 (20.55). calculated for $[C_{38}H_{42}N_2Al_1]^+$: 553.31634; found: 553.31903 (100.0).

CHNS: calculated: C = 82.43%, H = 8.13%, N = 4.81%; found: C = 82.58%, H = 7.757%, N = 4.89%.

UV/Vis ($BaSO_4$): $\lambda_{max,ss}$ = 513 nm.

UV/Vis (toluene): λ_{max} = 505 nm (FWHM = 21 nm), ε_{max} (505 nm) = 1.30·10^5 L mol^{-1} cm^{-1}.

SS-PL (λ_{Ex} = 325 nm): $\lambda_{F,ss}$ = 564 nm; $\varphi_{F,ss}$ < 1 %.

PL (toluene, λ_{Ex} = 405 nm): λ_F = 551 nm; φ_F < 1 %.

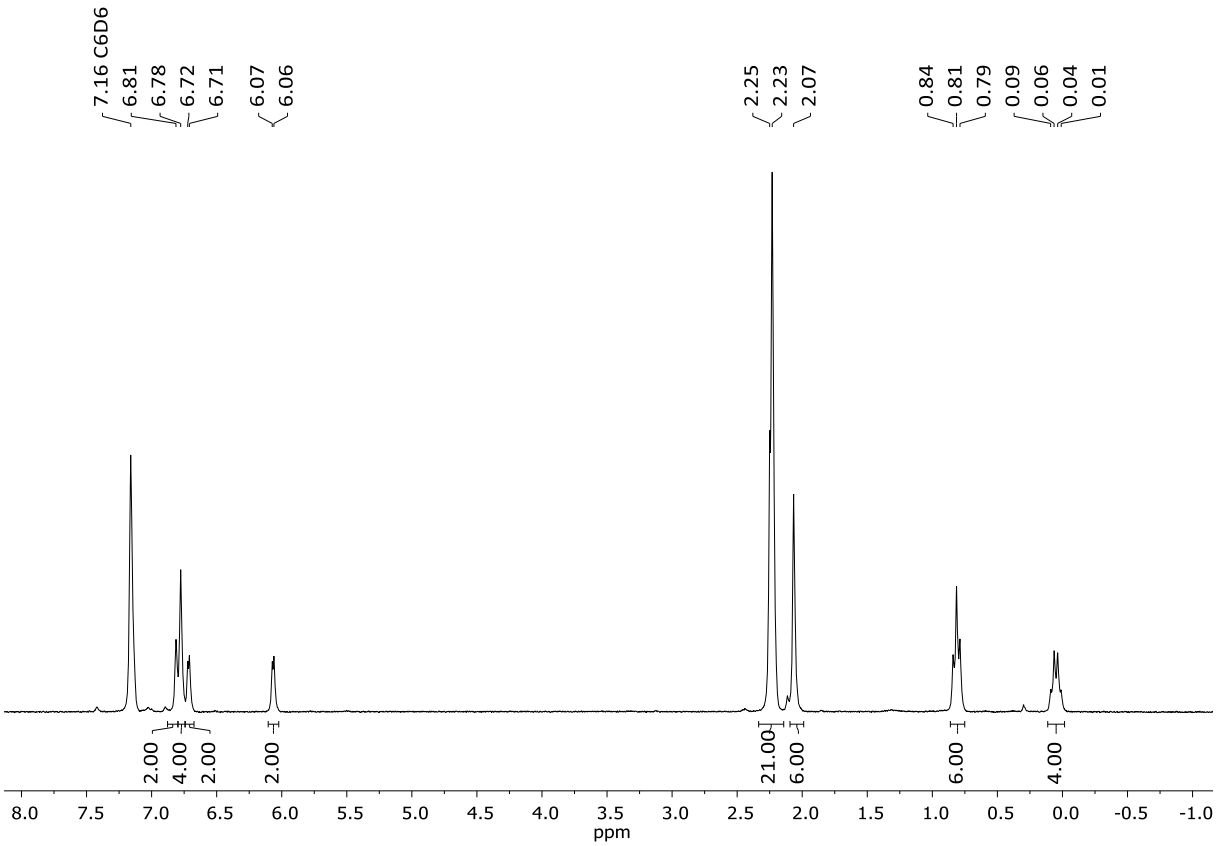


Figure 25: ^{1}H NMR spectrum of compound 2b in C_6D_6 at 300 K.

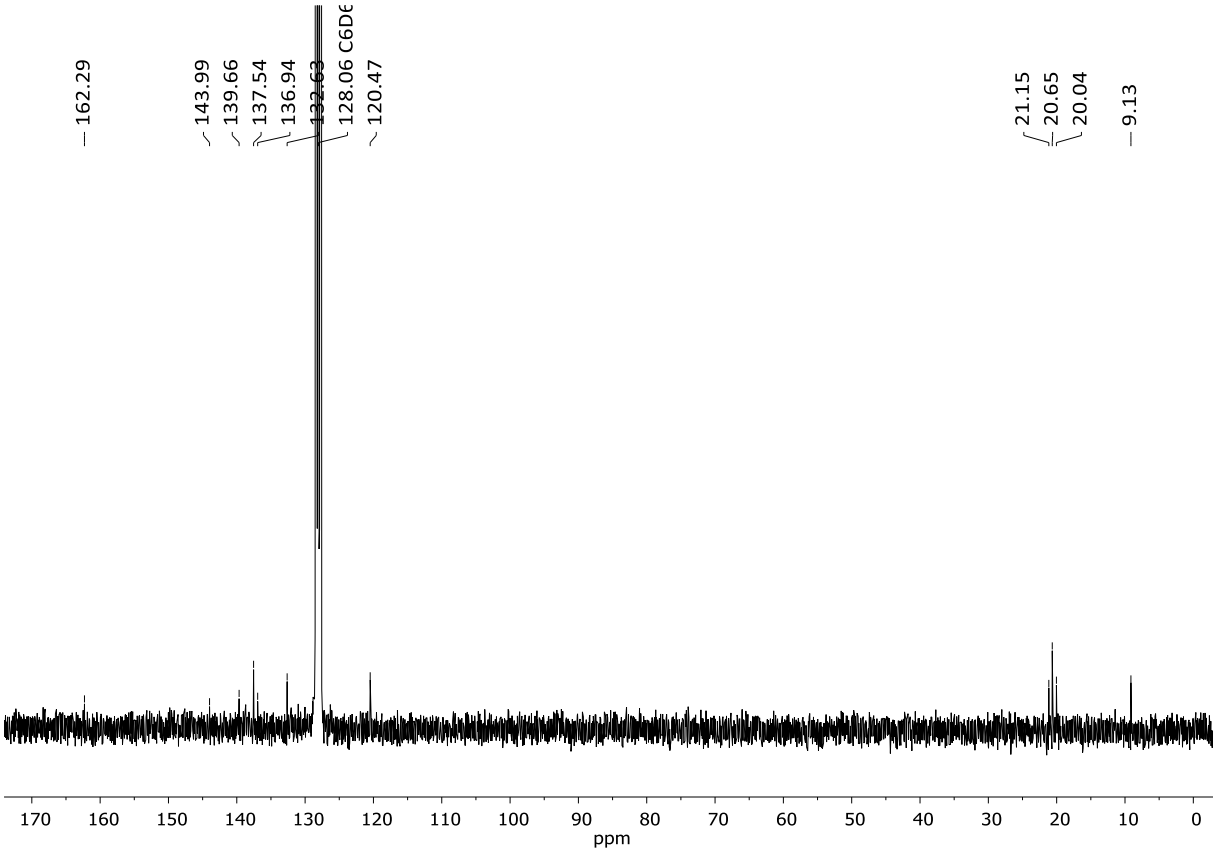


Figure 26: ^{13}C NMR spectrum of compound 2b in C_6D_6 at 300 K.

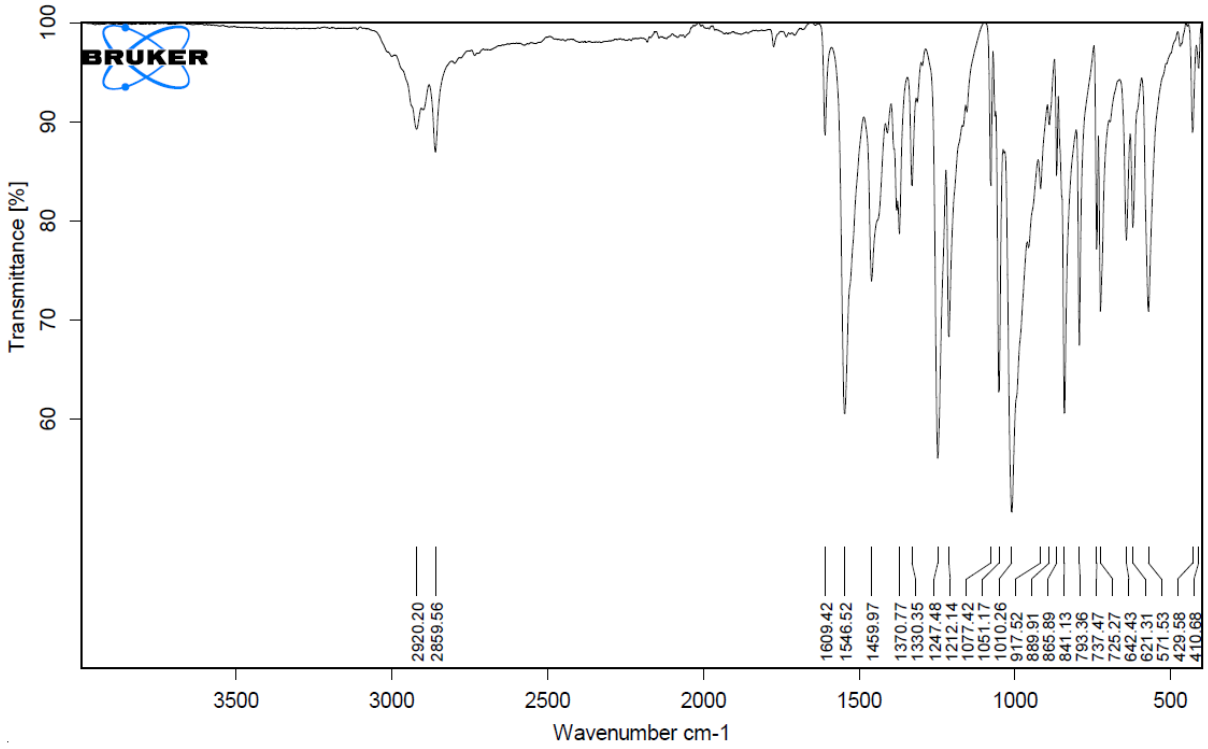


Figure 27: IR spectrum of compound 2b.

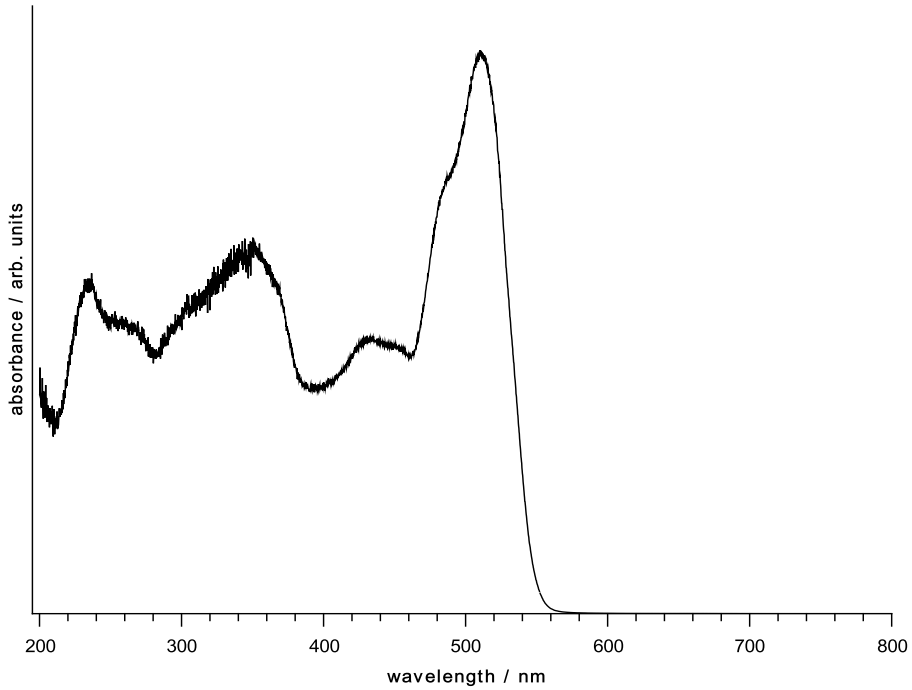


Figure 28: Solid state UV/VIS spectrum of compound 2b.

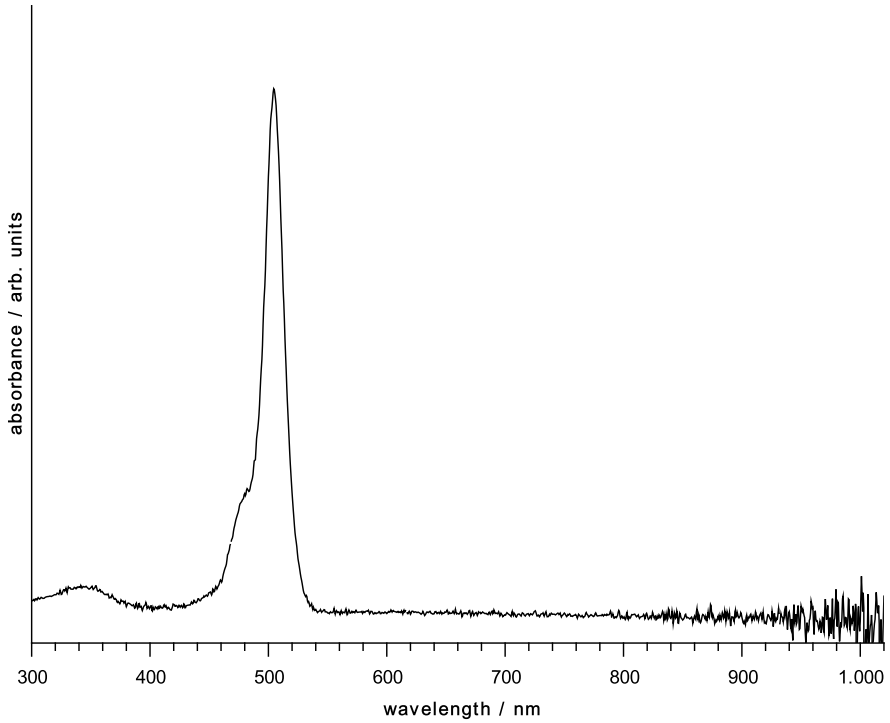


Figure 29: Solution-state UV/VIS spectrum of compound 2b (2 µM in toluene).

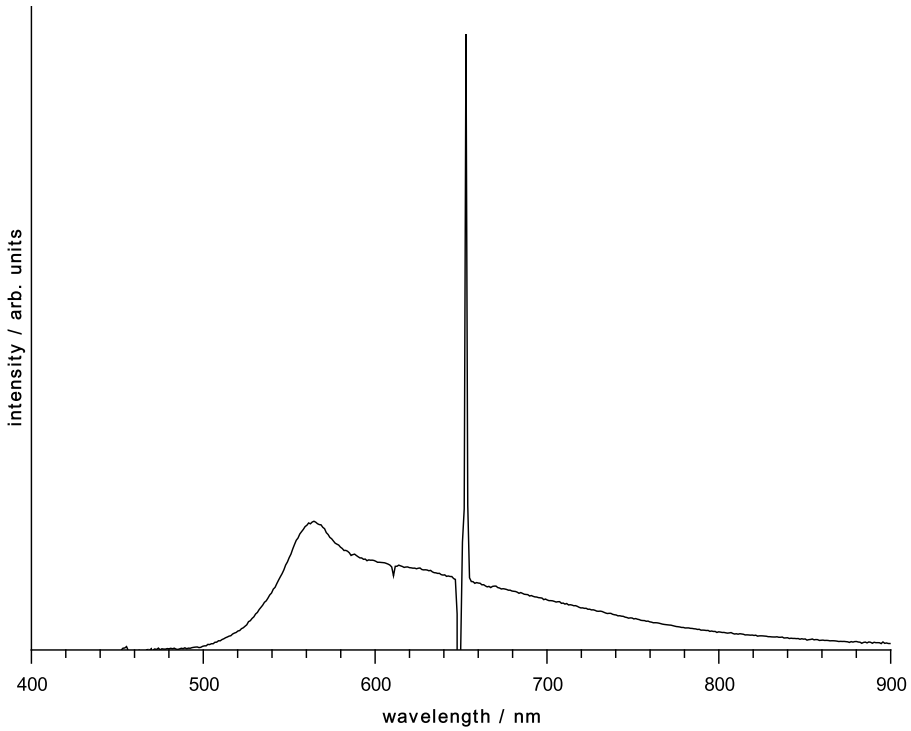


Figure 30: Solid state PL spectrum of compound 2b. Excitation with 325 nm He-Cd continuous wave laser (the signal at 650 nm is the second diffraction order of the laser).

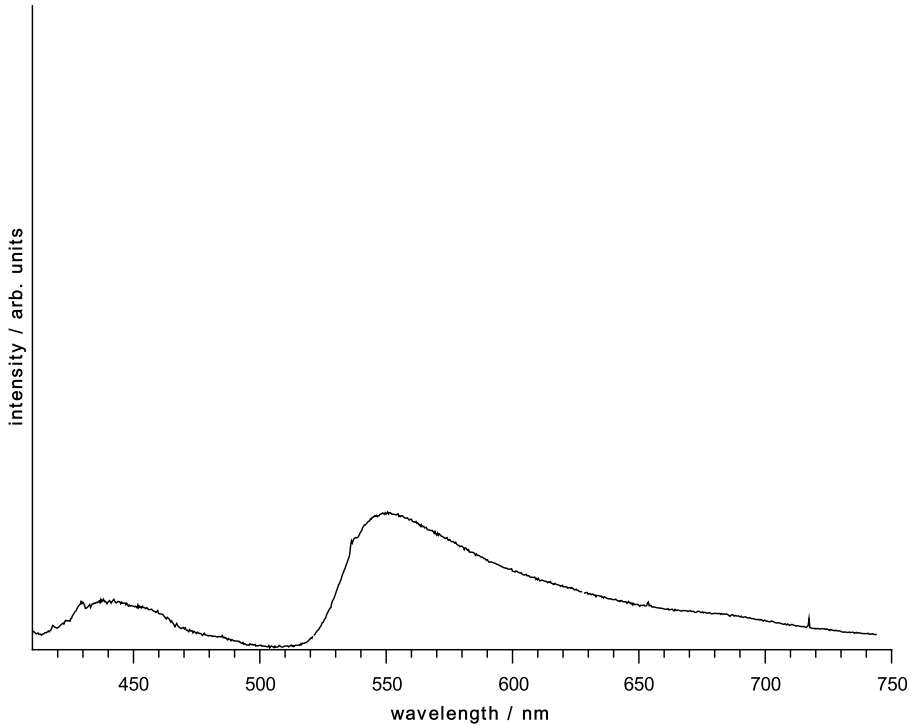
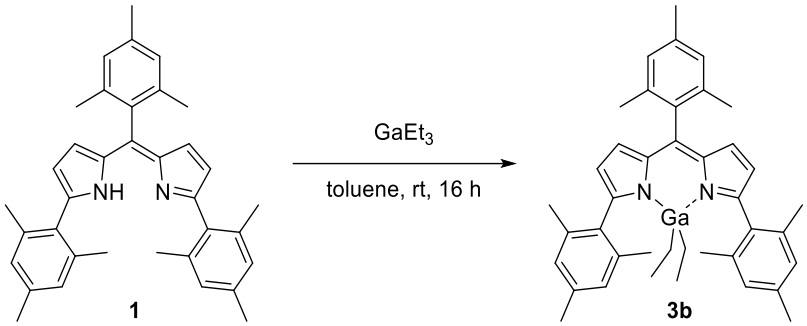


Figure 31: Solution-state PL spectrum of compound 2b in toluene. Excitation with 405 nm continuous wave diode laser.

1.5 (^{Mes}DPM)GaEt$_2$ (**3b**):



^{1}H-NMR (300.19 MHz, C_6D_6) δ = 6.83 (s, 2 H, -C*H*(Mes)), 6.77 (s, 4 H, -C*H*(Mes)), 6.77 (d, $^3J_{AB}$ = 4.0 Hz, 2 H, -C*H*(py)), 6.12 (d, $^3J_{AB}$ = 4.1 Hz, 2 H, -C*H*(py)), 2.28 (s, 6 H, -*Me*), 2.23 (s, 3 H, -*Me*), 2.21 (s, 12 H, -*Me*), 2.07 (s, 6 H, -*Me*), 0.83 (t, $^3J_{AB}$ = 7.9 Hz, 6 H, -Ga*Me*), 0.44 (q, $^3J_{AB}$ = 8.0 Hz, 4 H, -GaCH_2) ppm.

^{13}C{^{1}H}-NMR (75.48 MHz, C_6D_6) δ = 161.12 (s, 2 C, C_{quart} (pyr)), 146.04 (s, 1 C, C_{quart}), 139.01 (s, 2 C, C_{quart} (Mes)), 138.45 (s, 2 C, C_{quart} (Mes)), 137.64 (s, 1 C, C_{quart} (Mes)), 137.53 (s, 4 C, C_{quart} (Mes)), 136.97 (s, 2 C, C_{quart} (Mes)), 135.49 (s, 1 C, C_{quart} (Mes)), 132.51 (s, 2 C, C_{quart} (pyr)), 131.92 (s, 4 C, -*C*H (Mes)), 128.40 (s, 2 C, -*C*H (Mes)), 128.22 (s, 2 C, -*C*H (Im)), 119.63 (s, 2 C, -*C*H (Im)), 21.22 (s, 1 C, -*Me*), 21.15 (s, 2 C, -*Me*), 20.61 (s, 4 C, -*Me*), 20.10 (s, 2 C, -*Me*), 9.94 (s, 2 C, -GaCH$_2$*C*H$_3$), 4.18 (s, 2 C, -Ga*C*H$_2$) ppm.

IR (cm^{-1}) ν = 2999.17 (w),2920.33 (m), 2861.84 (m), 2815.19 (w), 1609.48 (m), 1545.87 (s), 1461.50 (m), 1366.97 (m), 1334.91 (m), 1311.03 (w), 1251.58 (s), 1217.50 (m), 1075.96 (w), 1050.15 (m), 1004.35 (s), 916.25 (m), 886.64 (w), 865.25 (m), 850.19 (m), 838.88 (s), 789.18 (m), 734.68 (m), 724.86 (m), 650.87 (w), 620.37 (w), 582.01 (w), 571.22 (w), 558.01 (m), 522.86 (m), 467.45 (w), 411.55 (m).

MS (HR-CI$^+$) (m/z (%)) calculated for $[C_{40}H_{48}N_2Ga_1]^+$: 625.30733; found: 625.30431(2.80); calculated for $[C_{38}H_{42}N_2Ga_1]^+$: 595.26038; found: 595.25720 (8.57).

CHNS: calculated: C = 76.80%, H = 7.57%, N = 4.48%; found: C = 77.08%, H = 7.501%, N = 4.47%.

UV/Vis ($BaSO_4$): $\lambda_{max,ss}$ = 505 nm (FWHM = 86 nm).

UV/Vis (toluene): λ_{max} = 502 nm (FWHM = 22 nm), ε_{max} (502 nm) = 1.10·10^5 L mol^{-1} cm^{-1}.

Excitation/Emission (toluene): λ_{Ex} = 344 nm; λ_{Em} = 536 nm.

SS-PL (λ_{Ex} = 325 nm): $\lambda_{F,ss}$ = 563 nm; $\varphi_{F,ss}$ < 1 %.

PL (toluene, λ_{Ex} = 405 nm): λ_F = 545 nm; φ_F = 2 %.

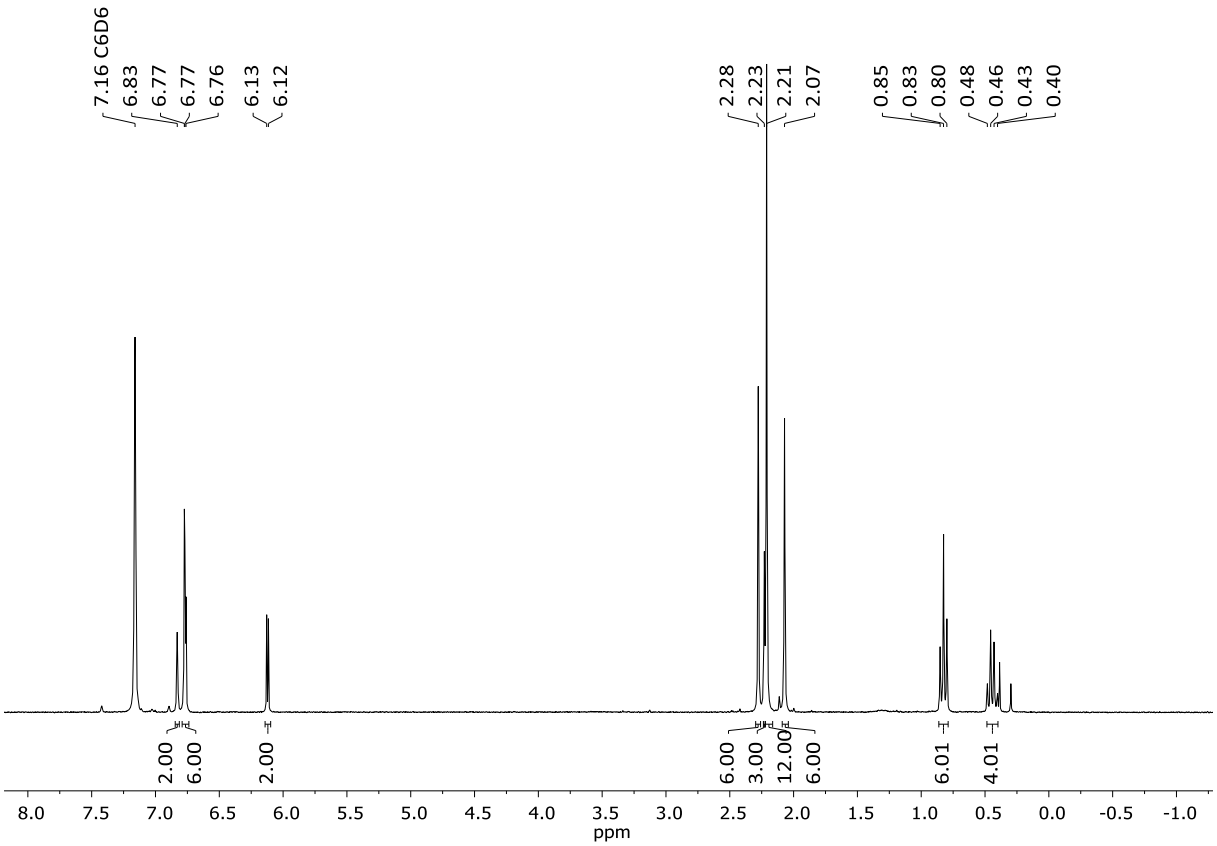


Figure 32: ^{1}H NMR spectrum of compound 3b in C_6D_6 at 300 K.

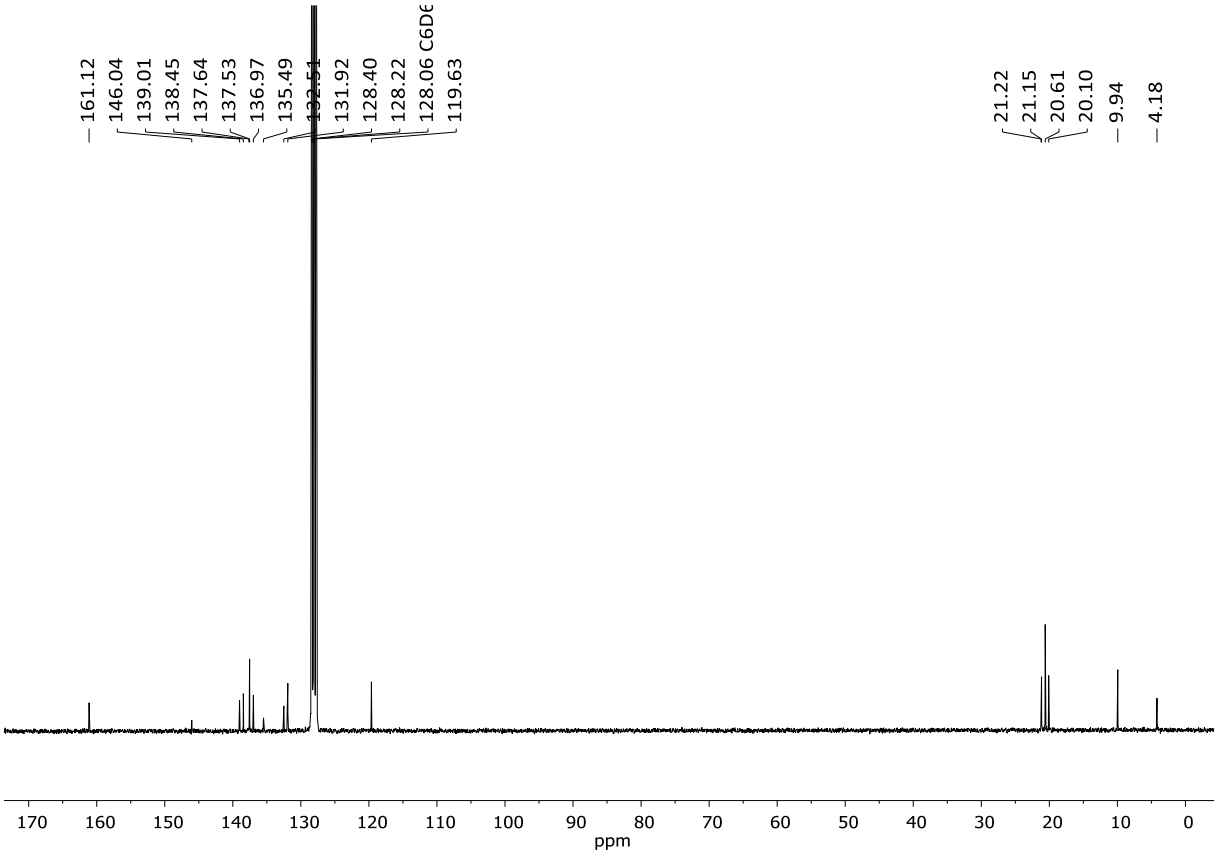


Figure 33: ^{13}C NMR spectrum of compound 3b in C_6D_6 at 300 K.

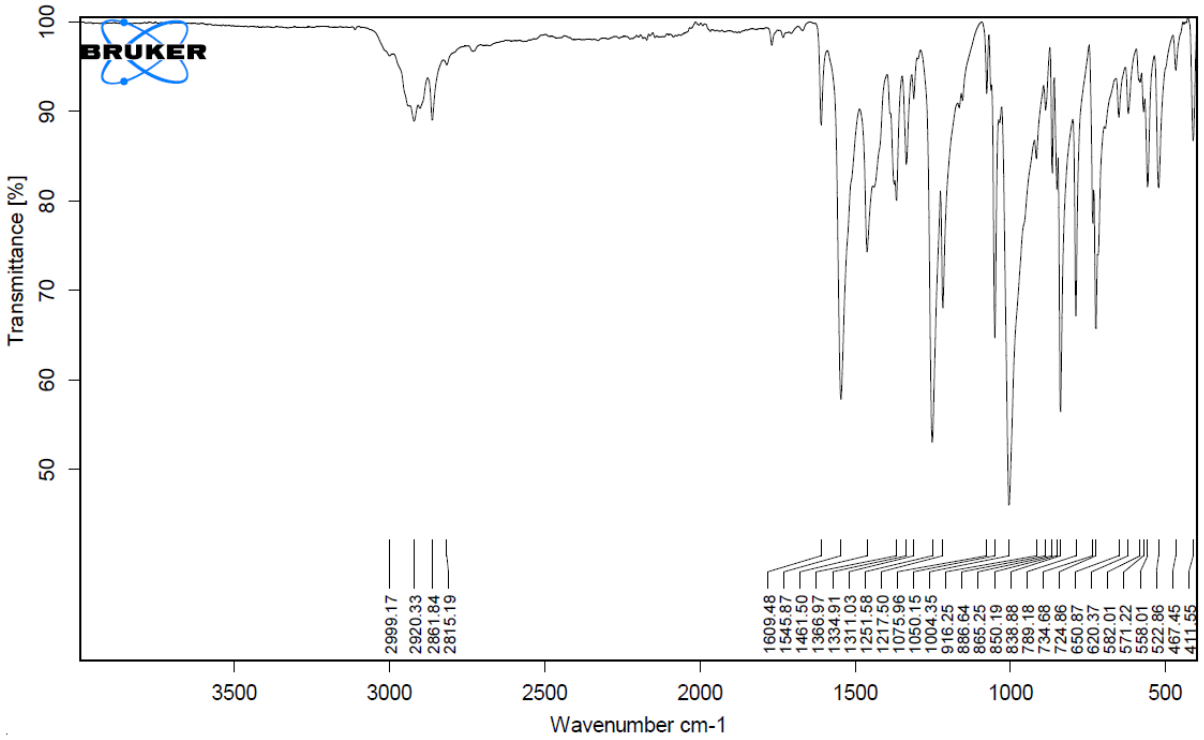


Figure 34: IR spectrum of compound 3b.

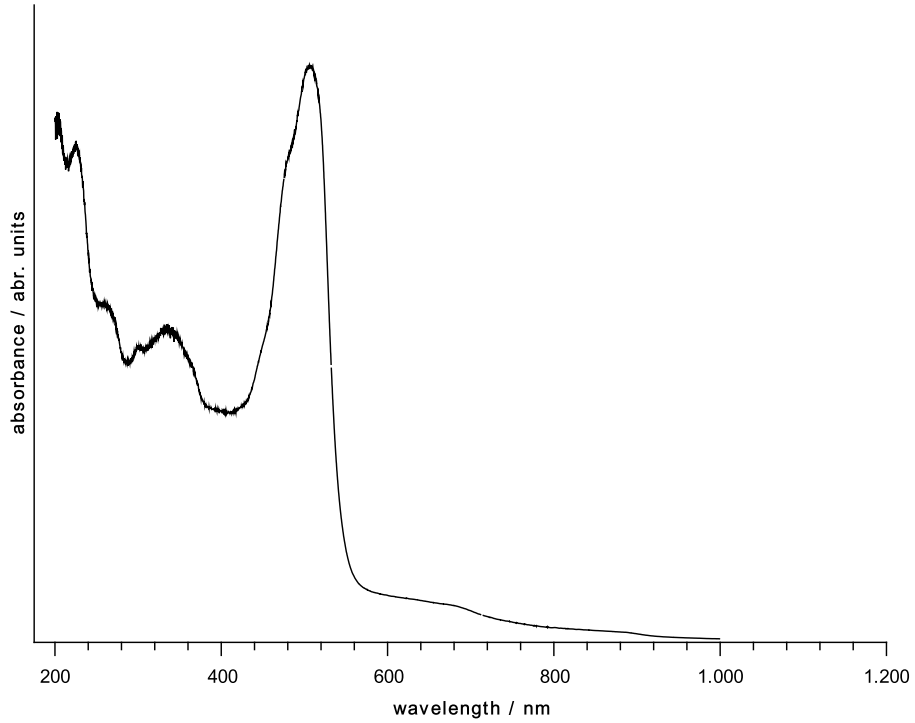


Figure 35: Solid state UV/VIS spectrum of compound 3b.

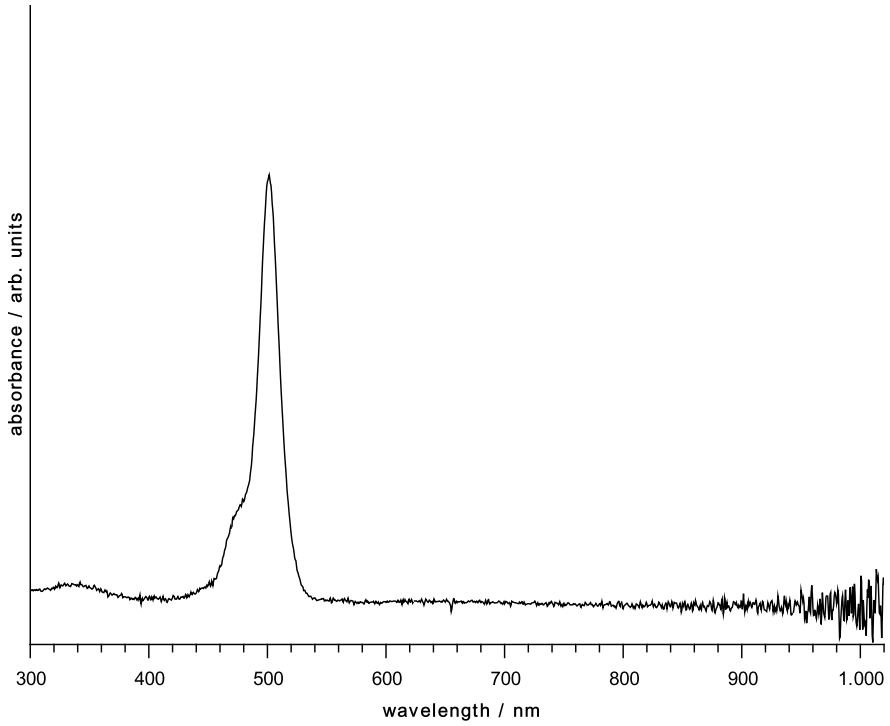


Figure 36: Solution-state UV/VIS spectrum of compound 3b (2 µM in toluene).

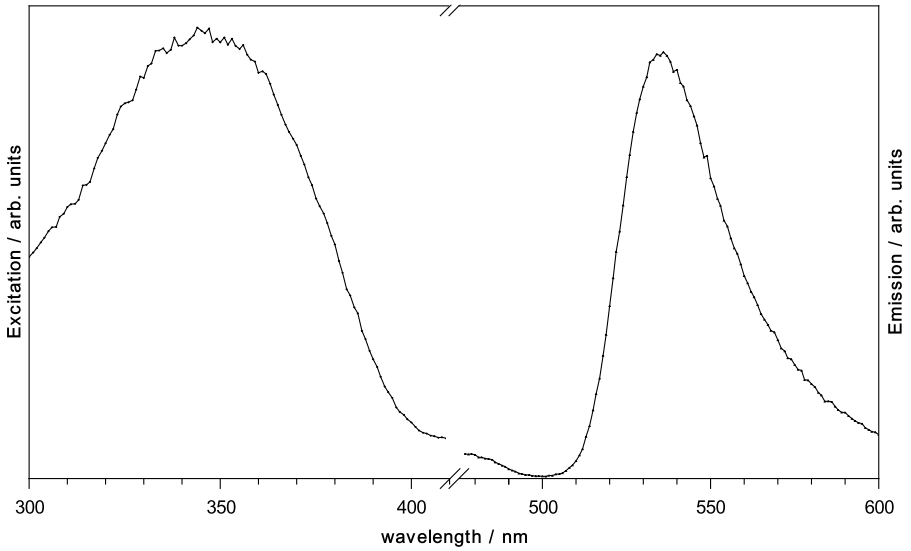


Figure 37: Excitation spectrum of 3b in toluene with emission detected at λ_F (left); emission spectra obtained with excitation detected at λ_{Ex} (right).

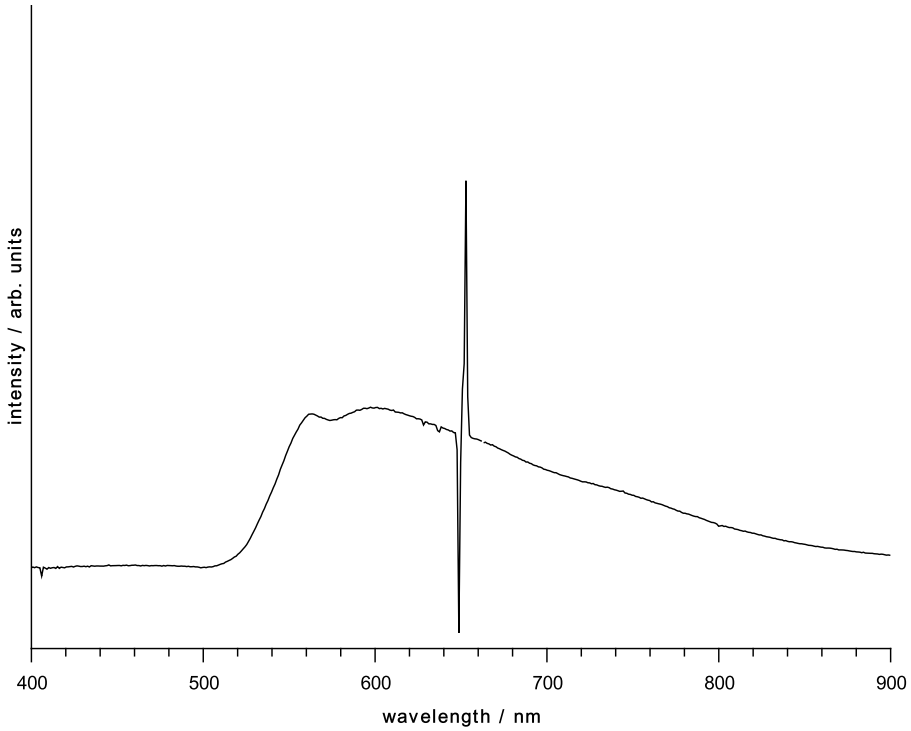


Figure 38: Solid state PL spectrum of compound 3b. Excitation with 325 nm He-Cd continuous wave laser (the signal at 650 nm is the second diffraction order of the laser).

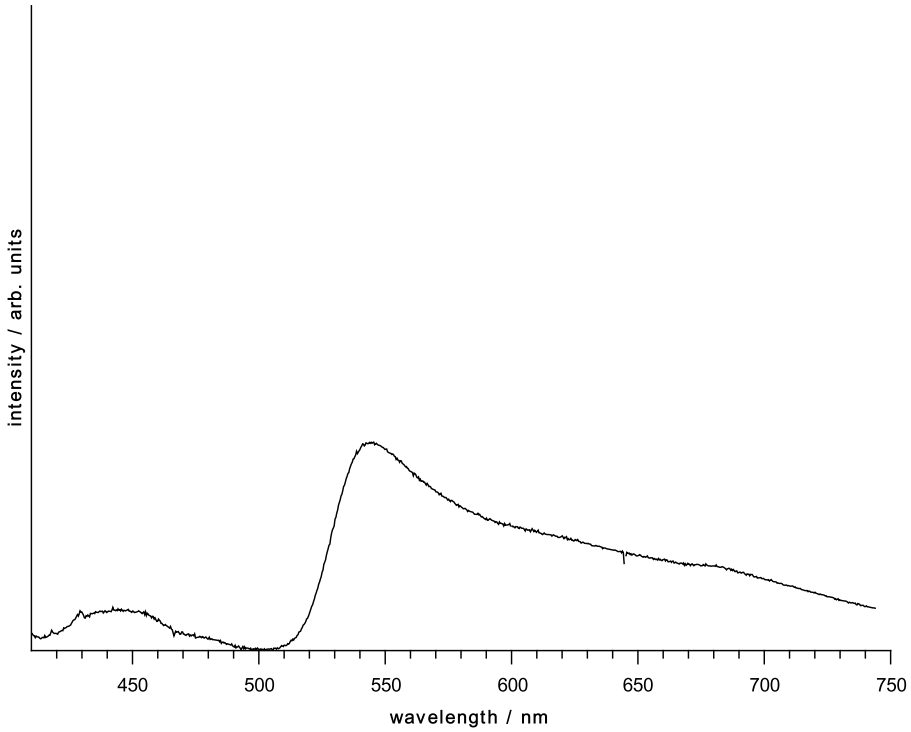
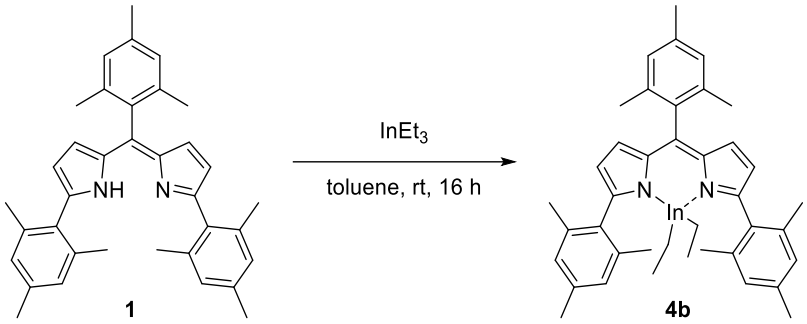


Figure 39: Solution-state PL spectrum of compound 3b in toluene. Excitation with 405 nm continuous wave diode laser.

1.6 (^{Mes}DPM)InEt$_2$ (**4b**):



^{1}H-NMR (300.19 MHz, C_6D_6) δ = 6.81 (s, 2 H, -C*H*(Mes)), 6.78 (s, 4 H, -C*H*(Mes)), 6.71 (d, $^3J_{AB}$ = 4.0 Hz, 2 H, -C*H*(py)), 6.06 (d, $^3J_{AB}$ = 4.0 Hz, 2 H, -C*H*(py)), 2.25 (s, 6 H, -*Me*), 2.23 (s, 12 H, -*Me*), 2.22 (s, 3 H, -*Me*), 2.06 (s, 6 H, -*Me*), 0.81 (t, $^3J_{AB}$ = 8.0 Hz, 6 H, -In*Me*), 0.05 (q, $^3J_{AB}$ = 8.0 Hz, 4 H, -InCH_2) ppm.

^{13}C{^{1}H}-NMR (75.48 MHz, C_6D_6) δ = 162.28 (s, 2 C, C_{quart} (pyr)), 146.51 (s, 1 C, C_{quart}), 139.62 (s, 2 C, C_{quart} (Mes)), 138.68 (s, 2 C, C_{quart} (Mes)), 137.84 (s, 1 C, C_{quart} (Mes)), 137.53 (s, 4 C, C_{quart} (Mes)), 136.91 (s, 2 C, C_{quart} (Mes)), 134.80 (s, 1 C, C_{quart} (Mes)), 132.62 (s, 2 C, C_{quart} (pyr)), 132.00 (s, 4 C, -*C*H (Mes)), 128.45 (s, 2 C, -*C*H (Mes)), 128.35 (s, 2 C, -*C*H (Im)), 120.46 (s, 2 C, -*C*H (Im)), 21.20 (s, 1 C, -*Me*), 21.16 (s, 2 C, -*Me*), 20.66 (s, 4 C, -*Me*), 20.05 (s, 2 C, -*Me*), 9.16 (s, 2 C, -InCH$_2$*C*H$_3$), 0.74 (s, 2 C, -In*C*H$_2$) ppm.

IR (cm^{-1}) ν = 2920.94 (w), 2859.93 (w), 1609.74 (w), 1547.15 (s), 1460.58 (m), 1409.57 (w), 1379.55 (m), 1371.25 (m), 1330.84 (w), 1248.10 (s), 1212.64 (m), 1153.76 (w), 1077.64 (m), 1051.55 (s), 1010.85 (s), 956.22 (m), 918.00 (w), 890.19 (w), 866.05 (w), 841.45 (s), 793.59 (m), 737.53 (m), 725.60 (m), 642.66 (m), 621.51 (m), 572.47 (m), 429.83 (w), 411.66 (w).

MS (HR-CI$^+$) (m/z (%)) calculated for $[C_{40}H_{48}N_2In_1]^+$: 671.28563; found: 671.28396 (31.28); calculated for $[C_{38}H_{42}N_2In_1]^+$: 641.23868; found: 641.23735 (100.0); calculated for $[C_{36}H_{39}N_2]^+$: 499.31132; found: 499.30974 (52.60).

UV/Vis ($BaSO_4$): $\lambda_{max,ss}$ = 512 nm (FWHM = 59 nm).

UV/Vis (toluene): λ_{max} = 505 nm (FWHM = 21 nm), ε_{max} (505 nm) = 1.49·10^5 L mol^{-1} cm^{-1}.

SS-PL (λ_{Ex} = 325 nm): $\lambda_{F,ss}$ = 567 nm; $\varphi_{F,ss}$ < 1 %.

PL (toluene, λ_{Ex} = 405 nm): λ_F = 547 nm; φ_F < 1 %.

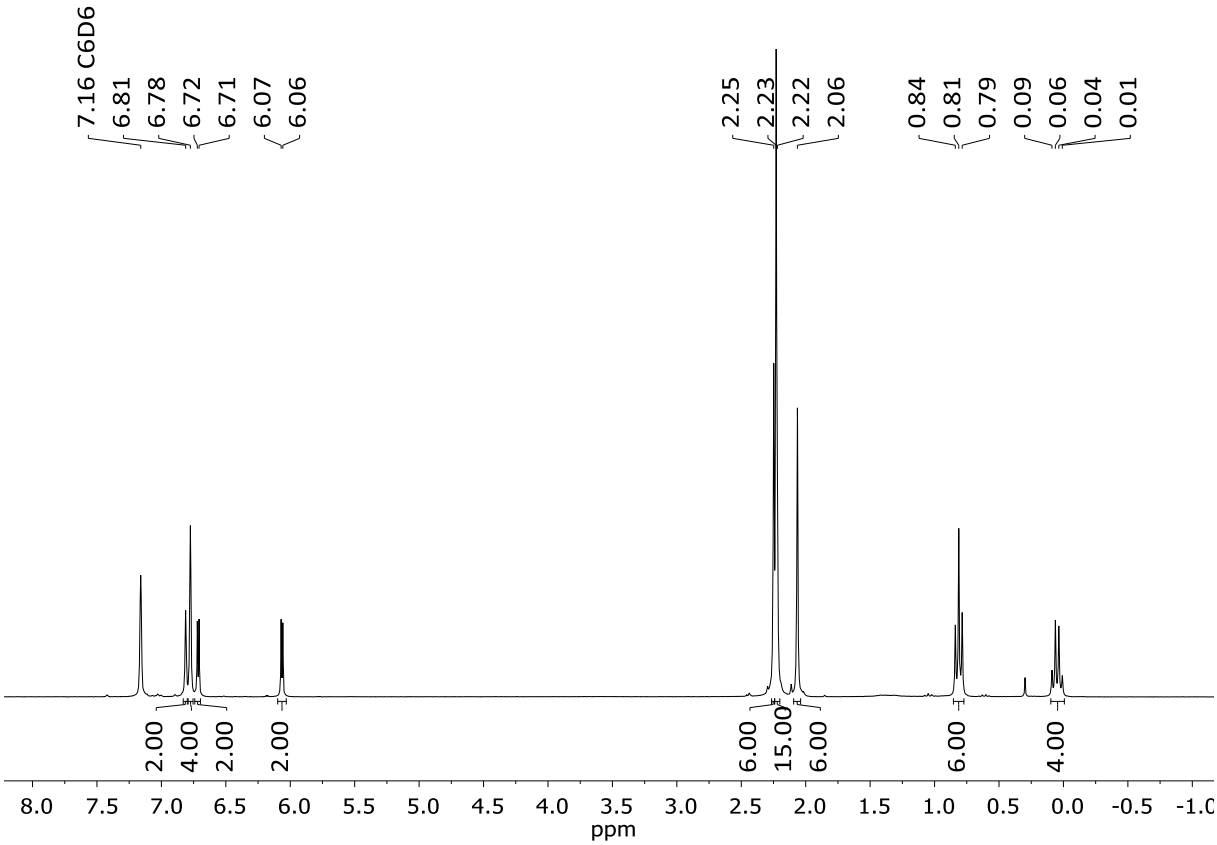


Figure 40: ^{1}H NMR spectrum of compound 4b in C_6D_6 at 300 K.

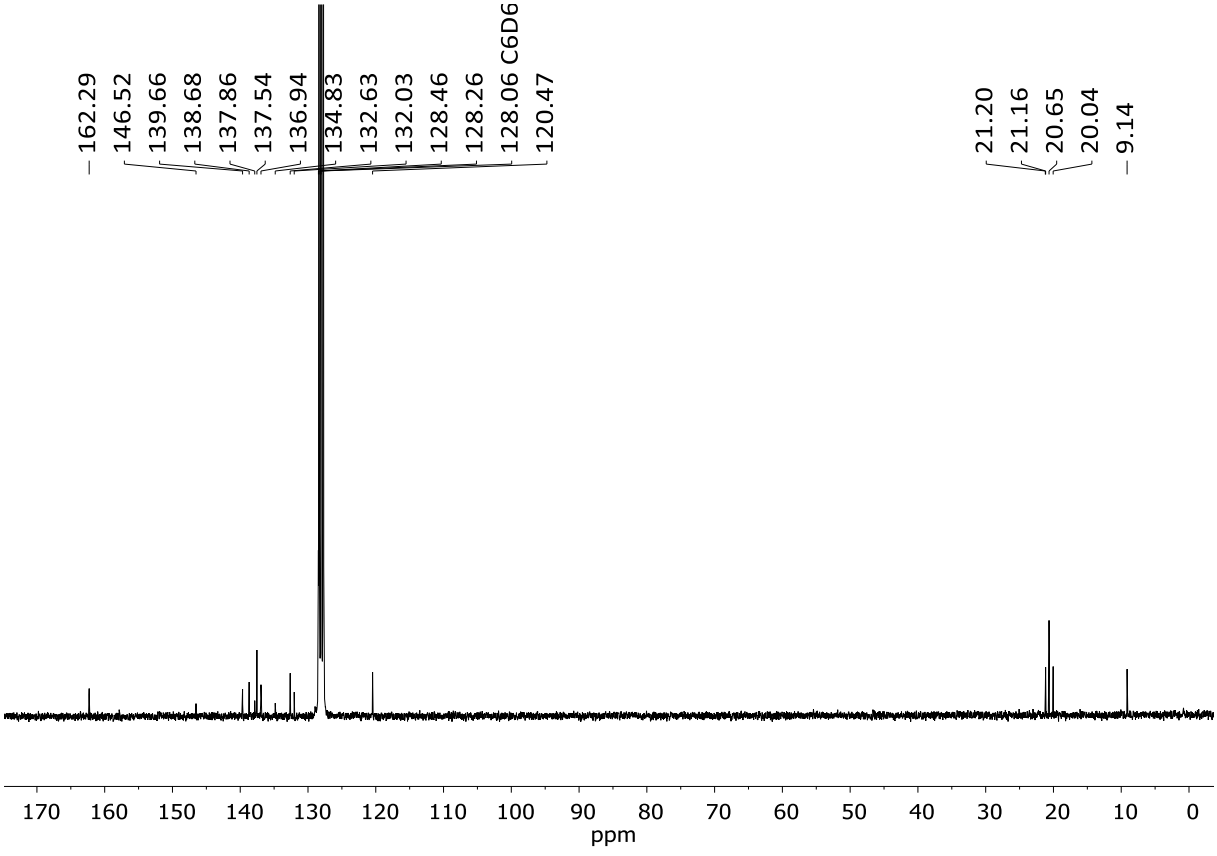


Figure 41: ^{13}C NMR spectrum of compound 4b in C_6D_6 at 300 K.

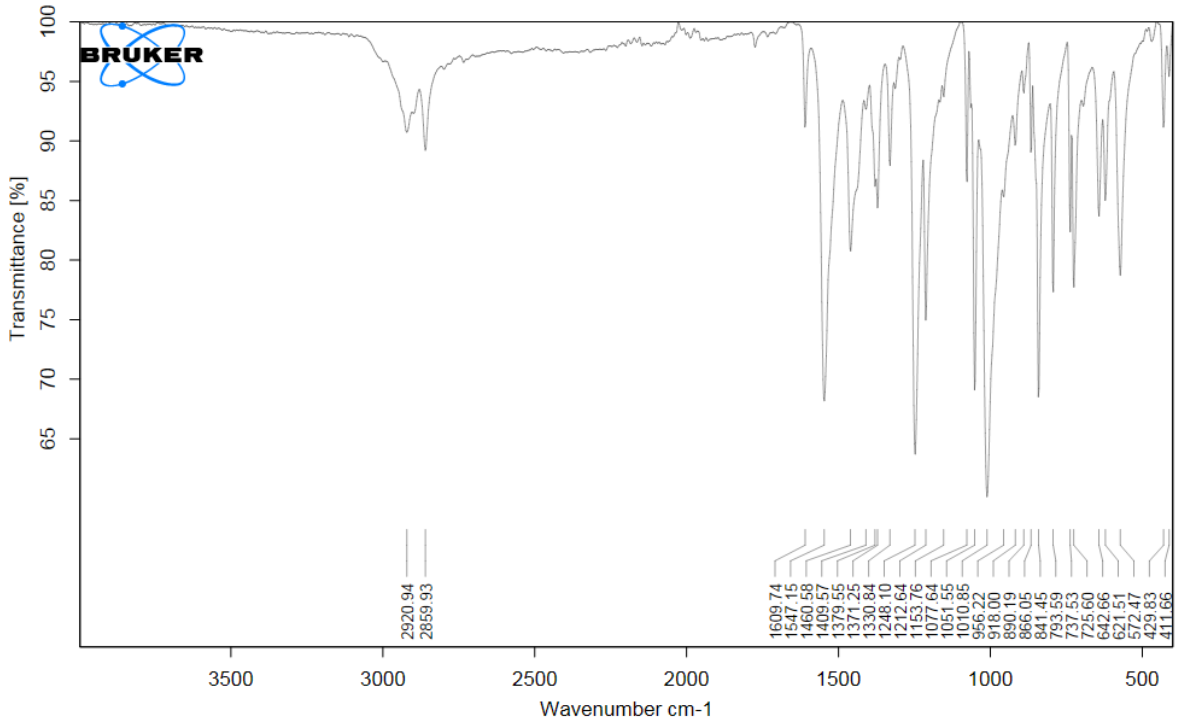


Figure 42: IR spectrum of compound 4b.

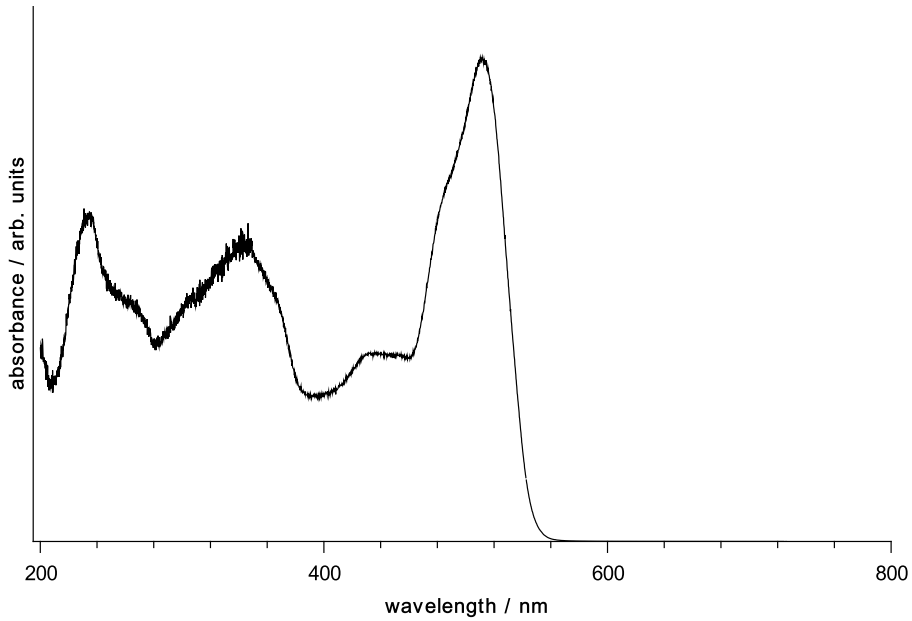


Figure 43: Solid state UV/VIS spectrum of compound 4b.

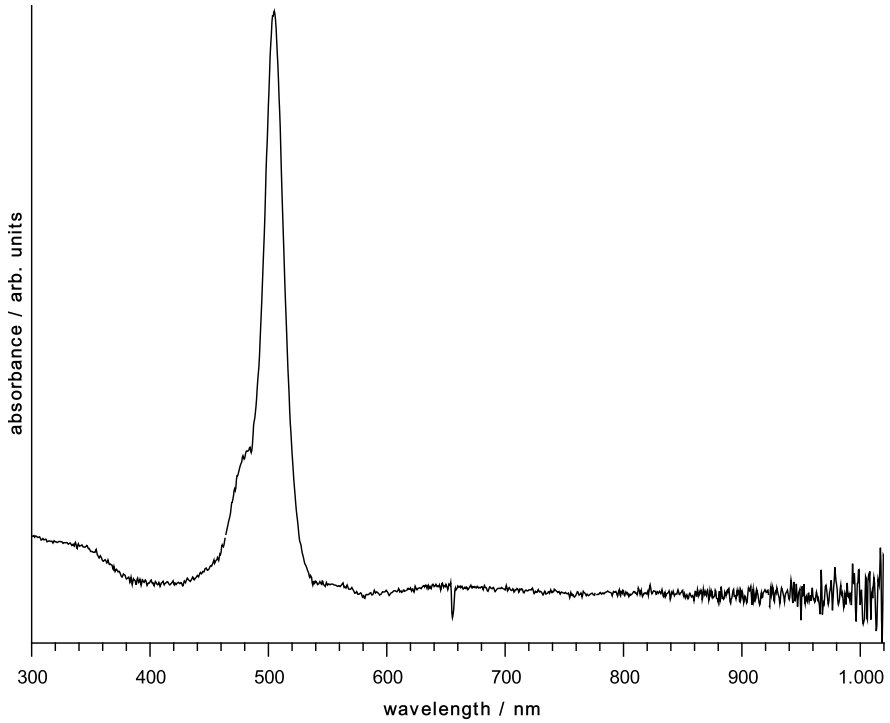


Figure 44: Solution-state UV/VIS spectrum of compound 4b (2 µM in toluene).

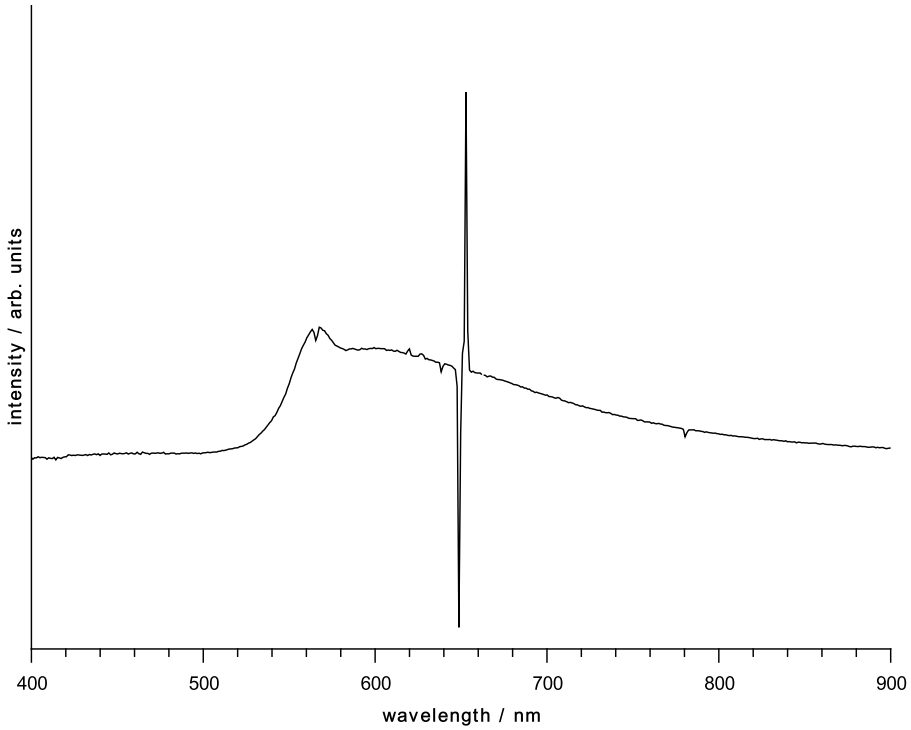


Figure 45: Solid state PL spectrum of compound 4b. Excitation with 325 nm He-Cd continuous wave laser (the signal at 650 nm is the second diffraction order of the laser).

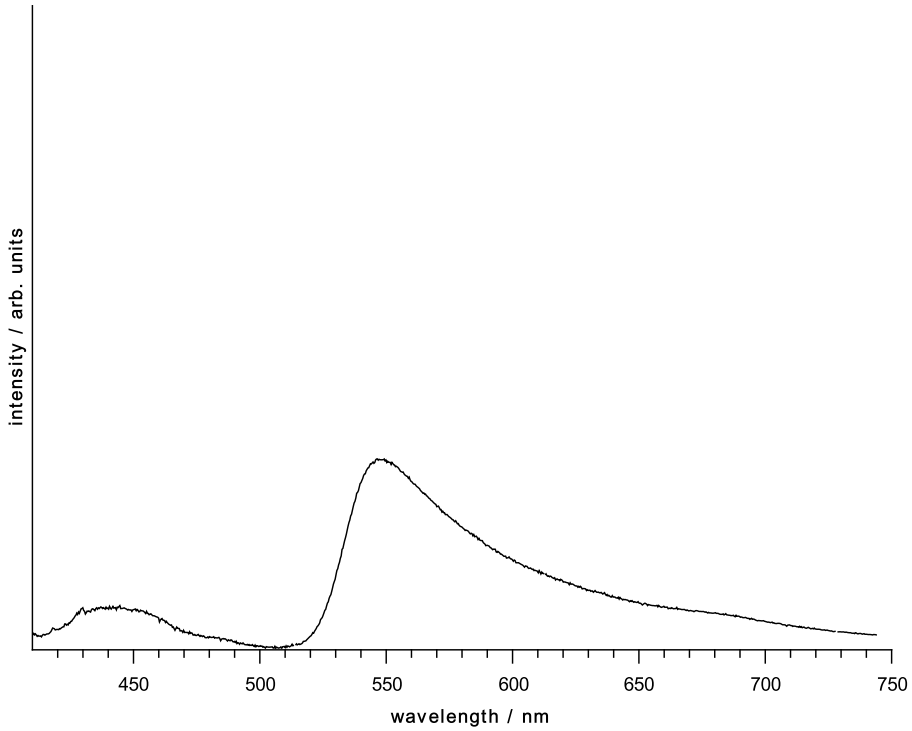


Figure 46: Solution-state PL spectrum of compound 4b in toluene. Excitation with 405 nm continuous wave diode laser.

2. UV/Vis and photoluminescence spectra in solution and solid-state:

2.1 Solid-state UV/Vis spectra:

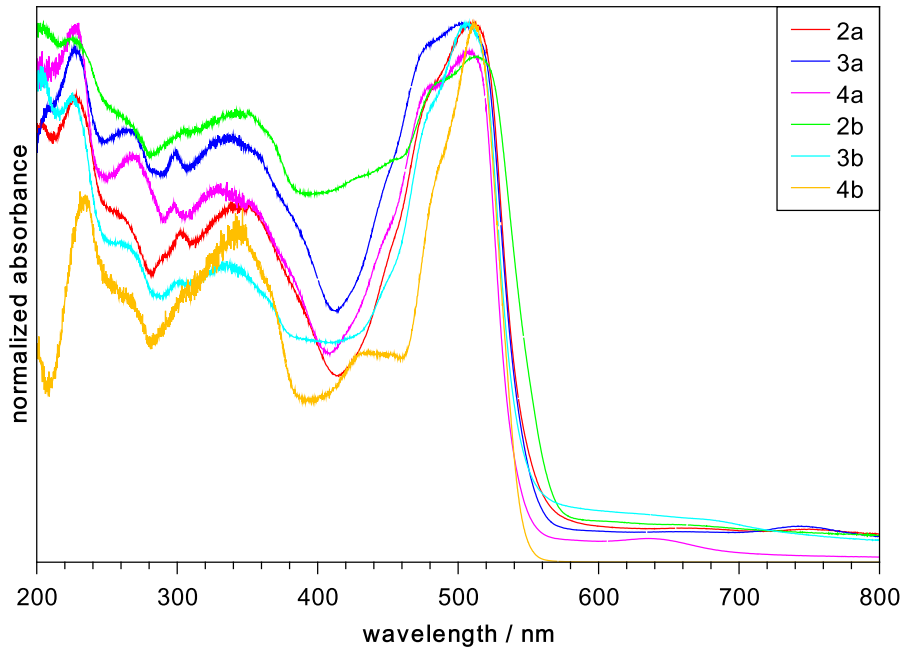


Figure 4. Normalized and stacked solid-state UV/Vis spectra of synthesized ^{Mes}DPM triel complexes (colour scheme: red = 2a; blue = 3a; violet = 4a; green = 2b; turquoise = 3b; yellow = 4b).

2.2 UV/Vis spectra in solution:

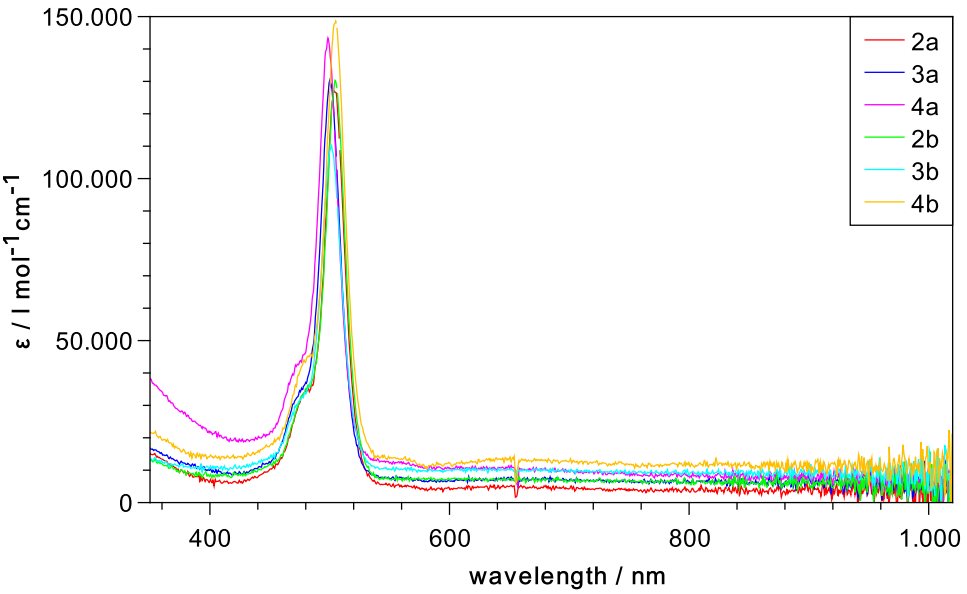


Figure 47: UV/Vis absoprtionen spectra of synthesized ^{Mes}DPM triel complexes in toluene solution (colour scheme: red = 2a; blue = 3a; violet = 4a; green = 2b; turquoise = 3b; yellow = 4b).

2.3 Comparison of extinction and emission spectra in the vicinity of the HOMO LUMO transition:

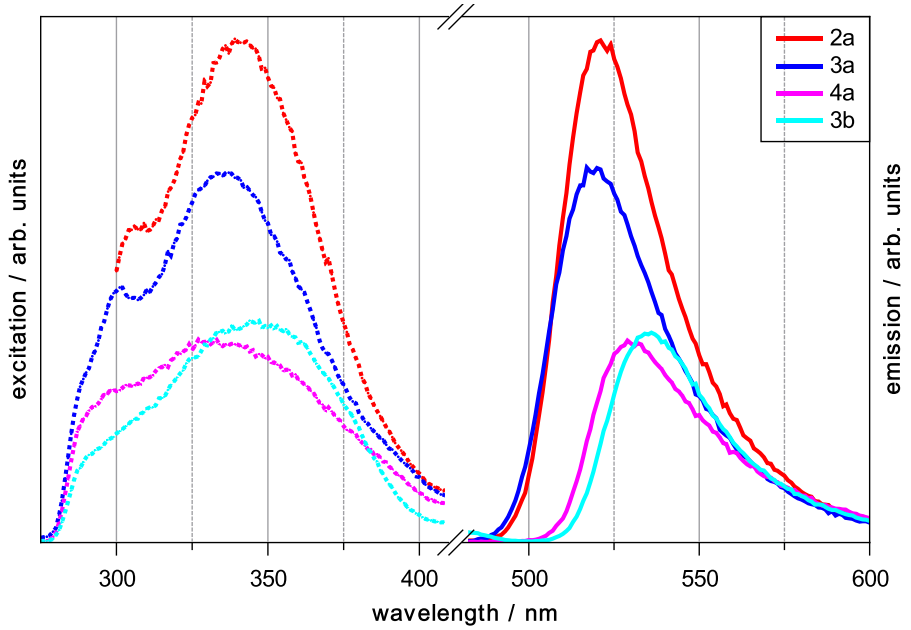


Figure 5. Extinction spectra obtained from samples of ^{Mes}DPM triel dialkyls (2a–4a & 3b) in toluene with emission detected at λ_F = dashed lines; emission spectra obtained with excitation detected at λ_{Ex} = solid lines.

2.4 Solid-state photoluminescence spectra:

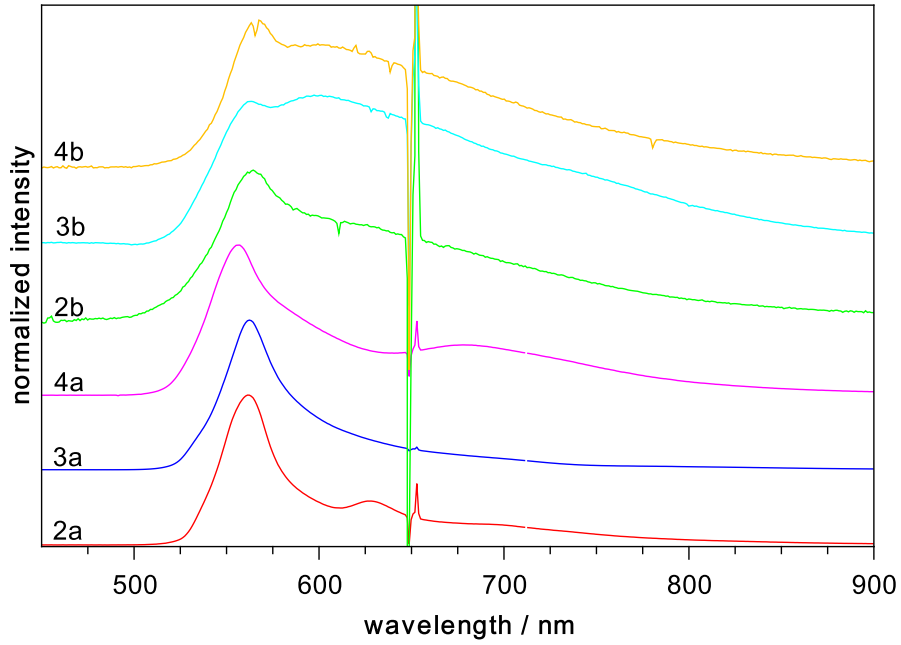


Figure 48: Normalized and vertically stacked solid-state photoluminescence spectra of synthesized ^{Mes}DPM triel complexes (colour scheme: red = 2a; blue = 3a; violet = 4a; green = 2b; turquoise = 3b; yellow = 4b). Excitation with 325 nm He-Cd continuous wave laser (the signal at 650 nm is the second diffraction order of the laser).

2.5 Photoluminescence spectra in toluene solution:

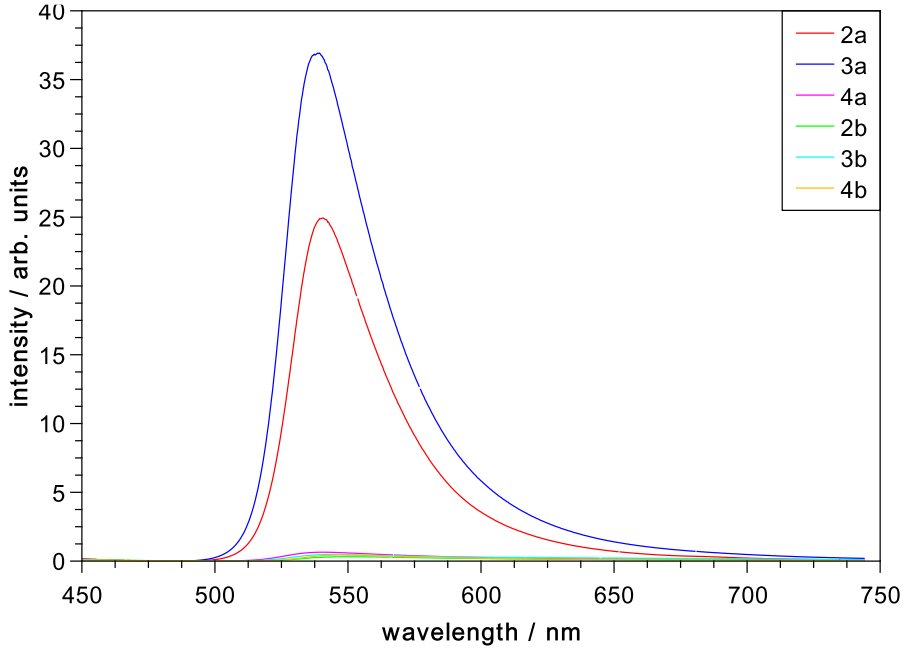


Figure 6. Photoluminescence spectra of synthesized ^{Mes}DPM triel complexes in toluene (colour scheme: red = 2a; blue = 3a; violet = 4a; green = 2b; turquoise = 3b; yellow = 4b). Excitation with 405 nm continuous wave diode laser.

2.6 Spectroscopic data:

Table 1: Spectroscopic data of (^{Mes}DPM)MX_2 (2–4a/b).

Compound	$\lambda_{max,ss}$ / nm	λ_{max} / nm	ε_{max} (λ_{max})/ L mol^{-1} cm^{-1}	λ_{Ex} / nm	λ_{Em} / nm	λ_F / nm	φ_F / %	$\lambda_{F,ss}$ / nm	$\varphi_{F,ss}$ / %
2a	509	504	$1.27 \cdot 10^5$	339	521	540	44	562	34
3a	502	500	$1.30 \cdot 10^5$	337	517	539	51	562	33
4a	509	499	$1.43 \cdot 10^5$	327	529	540	2	557	3
2b	513	505	$1.30 \cdot 10^5$	-	-	551	< 1	564	< 1
3b	505	502	$1.10 \cdot 10^5$	344	536	545	2	563	< 1
4b	512	505	$1.49 \cdot 10^5$	-	-	547	< 1	567	< 1

$\lambda_{max,ss}$ = absorption maximum (solid-state), λ_{max} = absorption maximum (toluene solution), ε_{max} (λ_{max}) = *molar absorption coefficient at* λ_{max}, λ_{Ex} = excitation maximum (in toluene solution), λ_{Em} = emission maximum (in toluene solution), λ_F = fluorescence maximum (in toluene solution), φ_F = fluorescence quantum yield (in toluene solution), $\lambda_{F,ss}$ = fluorescence maximum (solid-state), $\varphi_{F,ss}$ = fluorescence quantum yield (solid-state).

3. Crystallographic data:

3.1 (^{Mes}DPM)H (**1**):

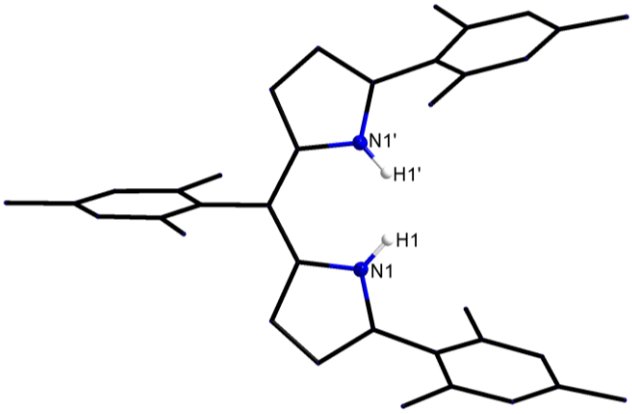


Figure 49: Solid-state molecular structure of (^{Mes}DPM)H (1) with thermal ellipsoids set at the 50% probability level (colour scheme: C = black; N = blue). C atoms are depicted as wireframe. Carbon-bound H atoms are omitted for clarity (H1' is generated by symmetry; total occupancy of H1 and H1' = 1).

Table 2: Crystal data and structure refinement of (^{Mes}DPM)H (1).

Empirical formula	$C_{36}H_{38}N_2$
Formular weight	498.68
Temperature / K	100.0
Crystal system	monoclinic
Space group	C2/c
a / Å	8.9174(7)
b / Å	15.1027(10)
c / Å	20.9603(17)
α / °	90
β / °	102.160(3)
γ / °	90
Volume / Å^3	2759.5(4)
Z	4
Density (calculated) / g/cm^3	1.200
Absorption coefficient / mm^{-1}	0.069
F(000)	1072.0
Crystal size / mm	0.235 × 0.231 × 0.151
Radiation / nm	MoKα (λ = 0.71073)
2Θ range for data collection / °	5.394 to 63.056
Index ranges	-12 ≤ h ≤ 13, -21 ≤ k ≤ 21, -30 ≤ l ≤ 30
Reflections collected	36656
Independent reflections	4534 [R_{int} = 0.0624, R_{sigma} = 0.0411]
Data/restraints/parameters	4534/0/180
Goodness-of-fit on F^2 (GooF)	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0513, wR_2 = 0.1227
Final R indexes [all data]	R_1 = 0.0594, wR_2 = 0.1284
Largest diff. peak/hole / e Å^{-3}	0.35/-0.25

3.2 (^{Mes}DPM)AlMe$_2$ (**2a**):

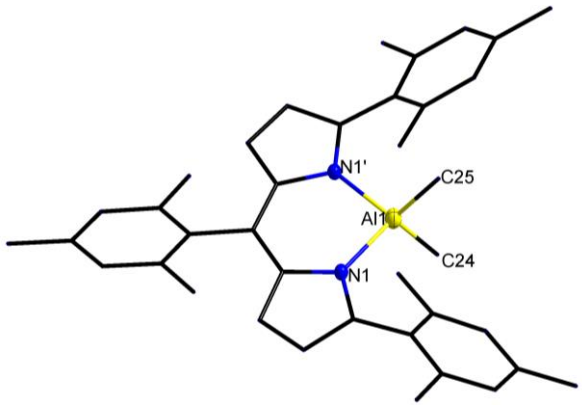


Figure 50: Solid-state molecular structure of (^{Mes}DPM)AlMe$_2$ (2a) with thermal ellipsoids set at the 50% probability level (colour scheme: C = black; N = blue, Al = yellow). C atoms are depicted as wireframe, carbon-bound H atoms are omitted for clarity.

Table 3: Crystal data and structure refinement of (^{Mes}DPM)AlMe$_2$ (2a).

Empirical formula	$C_{38}H_{43}AlN_2$
Formular weight	554.72
Temperature / K	100
Crystal system	monoclinic
Space group	$P2_1/m$
a / Å	8.0256(3)
b / Å	14.3869(7)
c / Å	14.5506(6)
α / °	90
β / °	103.338(2)
γ / °	90
Volume / Å^3	1634.74(12)
Z	2
Density (calculated) / g/cm^3	1.127
Absorption coefficient / mm^{-1}	0.090
F(000)	596.0
Crystal size / mm	0.367x0.11x0.1
Radiation / nm	MoKα (λ = 0.71073)
2Θ range for data collection / °	4.036 to 63.16
Index ranges	-10 ≤ h ≤ 11, -21 ≤ k ≤ 21, -21 ≤ l ≤ 20
Reflections collected	32186
Independent reflections	5610 [R_{int} = 0.0430, R_{sigma} = 0.0329]
Data/restraints/parameters	5610/0/213
Goodness-of-fit on F^2 (GooF)	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0447, wR_2 = 0.1121
Final R indexes [all data]	R_1 = 0.0622, wR_2 = 0.1221
Largest diff. peak/hole / e Å^{-3}	0.41/-0.30

3.3 (^{Mes}DPM)GaMe$_2$ (**3a**):

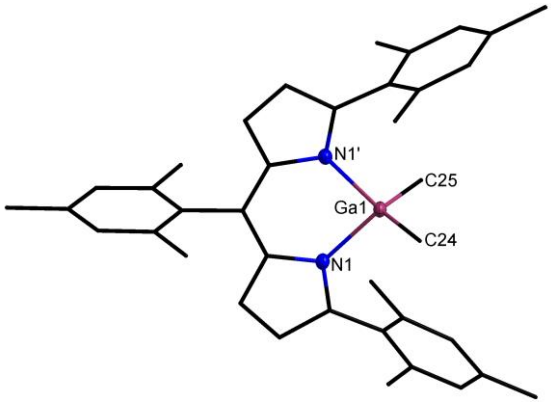


Figure 51: Solid-state molecular structure of (^{Mes}DPM)GaMe$_2$ (3a) with thermal ellipsoids set at the 50% probability level (colour scheme: C = black; N = blue, Ga = violet). C atoms are depicted as wireframe, carbon-bound H atoms are omitted for clarity.

Table 4: Crystal data and structure refinement of (^{Mes}DPM)GaMe$_2$ (3a).

Empirical formula	$C_{38}H_{43}GaN_2$
Formular weight	597.46
Temperature / K	100.0
Crystal system	monoclinic
Space group	$P2_1/m$
a / Å	8.0255(3)
b / Å	14.4109(5)
c / Å	14.5282(6)
α / °	90
β / °	103.255(2)
γ / °	90
Volume / Å^3	1635.49(11)
Z	2
Density (calculated) / g/cm^3	1.213
Absorption coefficient / mm^{-1}	0.869
F(000)	632.0
Crystal size / mm	0.282 × 0.131 × 0.104
Radiation / nm	MoKα (λ = 0.71073)
2Θ range for data collection / °	5.214 to 71.362
Index ranges	-12 ≤ h ≤ 13, -23 ≤ k ≤ 23, -23 ≤ l ≤ 23
Reflections collected	88361
Independent reflections	7725 [R_{int} = 0.0458, R_{sigma} = 0.0280]
Data/restraints/parameters	7725/0/213
Goodness-of-fit on F^2 (GooF)	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0367, wR_2 = 0.0833
Final R indexes [all data]	R_1 = 0.0502, wR_2 = 0.0883
Largest diff. peak/hole / e Å^{-3}	0.46/-0.50

3.4 (^{Mes}DPM)InMe$_2$ (**4a**):

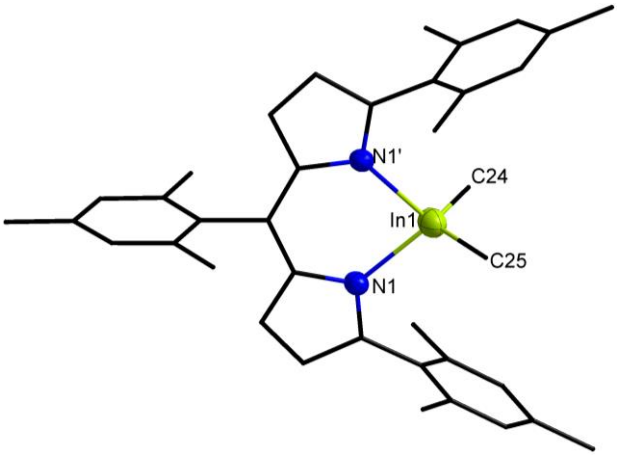


Figure 52: Solid-state molecular structure of (^{Mes}DPM)InMe$_2$ (4a) with thermal ellipsoids set at the 50% probability level (colour scheme: C = black; N = blue, In = green). C atoms are depicted as wireframe, carbon-bound H atoms are omitted for clarity.

Table 5: Crystal data and structure refinement of (^{Mes}DPM)InMe$_2$ (4a).

Empirical formula	$C_{38}H_{43}InN_2$
Formular weight	642.56
Temperature / K	100
Crystal system	Monoclinic
Space group	$P2_1/m$
a / Å	8.0070(2)
b / Å	14.4092(2)
c / Å	14.7134(3)
α / °	90
β / °	102.629(2)
γ / °	90
Volume / Å^3	1656.48(6)
Z	2
Density (calculated) / g/cm^3	1.288
Absorption coefficient / mm^{-1}	5.891
F(000)	668.0
Crystal radius / mm^3	0.0488
Radiation / nm	CuKα (λ = 1.54186)
2Θ range for data collection / °	6.156 to 151.916
Index ranges	-10 ≤ h ≤ 8, -11 ≤ k ≤ 18, -18 ≤ l ≤ 18
Reflections collected	29029
Independent reflections	3569 [R_{int} = 0.0497, R_{sigma} = 0.0348]
Data/restraints/parameters	3569/0/212
Goodness-of-fit on F^2 (GooF)	1.099
Final R indexes [I>=2σ (I)]	R_1 = 0.0446, wR_2 = 0.1185
Final R indexes [all data]	R_1 = 0.0539, wR_2 = 0.1241
Largest diff. peak/hole / e Å^{-3}	0.38/-1.08

3.5 (^{Mes}DPM)AlEt$_2$ (**2b**):

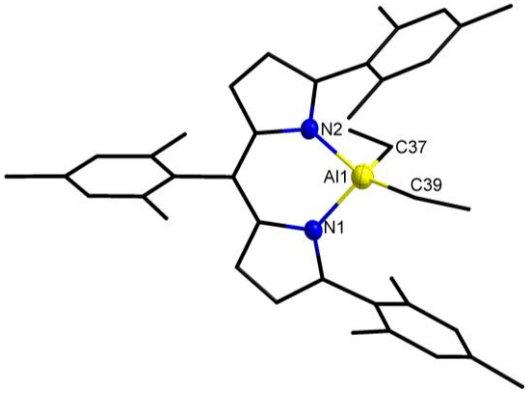


Figure 53: Solid-state molecular structure of (^{Mes}DPM)AlEt$_2$ (2b) with thermal ellipsoids set at the 50% probability level (colour scheme: C = black; N = blue, Al = yellow). C atoms are depicted as wireframe, carbon-bound H atoms are omitted for clarity.

Table 6: Crystal data and structure refinement of (^{Mes}DPM)AlEt$_2$ (2b).

Empirical formula	$C_{40}H_{47}AlN_2$
Formular weight	582.77
Temperature / K	100.0
Crystal system	triclinic
Space group	P-1
a / Å	8.259(3)
b / Å	14.610(6)
c / Å	14.774(6)
α / °	89.10(3)
β / °	73.44(3)
γ / °	87.79(3)
Volume / Å^3	1707.6(12)
Z	2
Density (calculated) / g/cm^3	1.133
Absorption coefficient / mm^{-1}	0.725
F(000)	628.0
Crystal radius / mm	0.0295
Radiation / nm	CuKα (λ = 1.54186)
2Θ range for data collection / °	8.678 to 152.6
Index ranges	-10 ≤ h ≤ 10, -15 ≤ k ≤ 18, -18 ≤ l ≤ 18
Reflections collected	59116
Independent reflections	59116 [R_{int} = 0.1119, R_{sigma} = 0.2117]
Data/restraints/parameters	59116/0/401
Goodness-of-fit on F^2 (GooF)	0.745
Final R indexes [I>=2σ (I)]	R_1 = 0.0609, wR_2 = 0.1163
Final R indexes [all data]	R_1 = 0.1487, wR_2 = 0.1422
Largest diff. peak/hole / e Å^{-3}	0.33/-0.35

3.6 (^{Mes}DPM)GaEt$_2$ (**3b**):

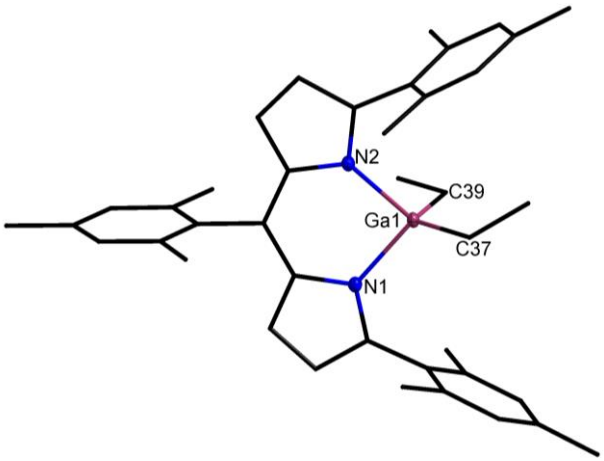


Figure 54: Solid-state molecular structure of (^{Mes}DPM)GaEt$_2$ (3b) with thermal ellipsoids set at the 50% probability level (colour scheme: C = black; N = blue, Ga = violet). C atoms are depicted as wireframe, carbon-bound H atoms are omitted for clarity.

Table 7: Crystal data and structure refinement of (^{Mes}DPM)GaEt$_2$ (3b).

Empirical formula	$C_{40}H_{47}GaN_2$
Formular weight	625.51
Temperature / K	100
Crystal system	triclinic
Space group	*P*-1
a / Å	8.254(4)
b / Å	14.620(6)
c / Å	14.709(7)
α / °	89.79(2)
β / °	74.07(2)
γ / °	87.68(2)
Volume / Å^3	1705.5(14)
Z	2
Density (calculated) / g/cm^3	1.218
Absorption coefficient / mm^{-1}	0.836
F(000)	664.0
Crystal size / mm	0.233 × 0.118 × 0.117
Radiation / nm	MoKα (λ = 0.71073)
2Θ range for data collection / °	5.578 to 56.774
Index ranges	-10 ≤ h ≤ 11, -19 ≤ k ≤ 19, 0 ≤ l ≤ 19
Reflections collected	8457
Independent reflections	8457 [R_{int} = 0.0308, R_{sigma} = 0.0284]
Data/restraints/parameters	8457/0/400
Goodness-of-fit on F^2 (GooF)	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0323, wR_2 = 0.0822
Final R indexes [all data]	R_1 = 0.0363, wR_2 = 0.0848
Largest diff. peak/hole / e Å^{-3}	0.44/-0.36

3.7 (^{Mes}DPM)InEt$_2$ (**4b**):

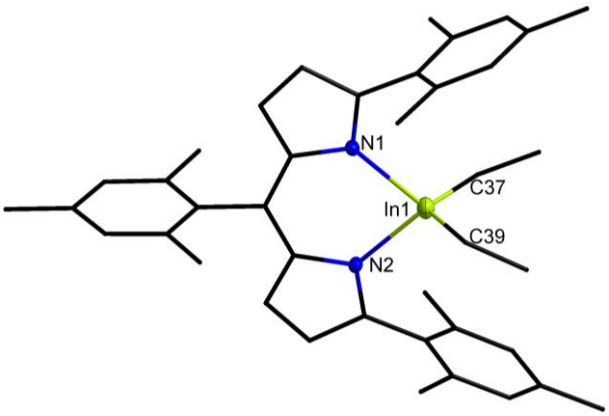


Figure 55: Solid-state molecular structure of (^{Mes}DPM)InEt$_2$ (4b) with thermal ellipsoids set at the 50% probability level (colour scheme: C = black; N = blue, In = green). C atoms are depicted as wireframe, carbon-bound H atoms are omitted for clarity.

Table 8: Crystal data and structure refinement of (^{Mes}DPM)InEt$_2$ (4b).

Empirical formula	$C_{40}H_{47}InN_2$
Formular weight	670.61
Temperature / K	100
Crystal system	monoclinic
Space group	$P2_1/c$
a / Å	15.6677(6)
b / Å	14.3638(5)
c / Å	16.0349(5)
α / °	90
β / °	105.4440(10)
γ / °	90
Volume / Å^3	3478.3(2)
Z	4
Density (calculated) / g/cm^3	1.281
Absorption coefficient / mm^{-1}	0.708
F(000)	1400.0
Crystal size / mm	0.1 × 0.1 × 0.1
Radiation / nm	MoKα (λ = 0.71073)
2Θ range for data collection / °	3.872 to 51.998
Index ranges	-19 ≤ h ≤ 19, -17 ≤ k ≤ 17, -19 ≤ l ≤ 19
Reflections collected	46401
Independent reflections	6842 [R_{int} = 0.0458, R_{sigma} = 0.0305]
Data/restraints/parameters	6842/0/399
Goodness-of-fit on F^2 (GooF)	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0362, wR_2 = 0.0955
Final R indexes [all data]	R_1 = 0.0471, wR_2 = 0.0998
Largest diff. peak/hole / e Å^{-3}	0.79/-0.74

4. XYZ coordinates of 2a, 3a and 4a obtained from geometry optimisation by the r2scan-3c method.

2a (Al)**:**

Al	-0.618176000	10.789520000	10.451423000
N	-0.047570000	12.206939000	9.250686000
N	-0.044931000	9.374644000	9.249035000
C	0.443199000	10.790175000	12.118378000
C	-2.580791000	10.787100000	10.684085000
C	-0.144664000	13.537479000	9.458109000
C	0.551892000	12.033435000	8.000722000
C	-0.141682000	8.043637000	9.453861000
C	0.552304000	9.550734000	7.998383000
H	1.528854000	10.791436000	11.960769000
H	0.200707000	9.906531000	12.723290000
H	0.198682000	11.672449000	12.724440000
H	-2.894280000	9.903734000	11.255811000
H	-2.895761000	11.669847000	11.256023000
H	-3.145489000	10.786855000	9.743620000
C	0.383715000	14.250211000	8.356889000
C	-0.730361000	14.102090000	10.692866000
C	0.820831000	13.310036000	7.443093000
C	0.831995000	10.792713000	7.420648000
C	0.384118000	7.333216000	8.349985000
C	-0.723942000	7.476611000	10.689133000
C	0.819504000	8.275323000	7.437285000
H	0.424274000	15.328151000	8.275586000
C	0.100003000	14.385368000	11.790005000
C	-2.106008000	14.380179000	10.747293000
H	1.283409000	13.481063000	6.480122000
C	1.486294000	10.793817000	6.079300000
H	0.424340000	6.255447000	8.266284000
C	0.109100000	7.195444000	11.784855000
C	-2.098566000	7.194169000	10.745626000
H	1.280183000	8.106358000	6.473086000
C	-0.472929000	14.904758000	12.950286000
C	1.585828000	14.163606000	11.707332000
C	-2.640870000	14.899769000	11.925620000
C	-2.984778000	14.153416000	9.547144000
C	2.886608000	10.789780000	5.992713000
C	0.695352000	10.805309000	4.920376000
C	-0.460472000	6.673678000	12.945702000
C	1.594153000	7.421294000	11.699977000
C	-2.630048000	6.672323000	11.924483000
C	-2.979771000	7.419349000	9.546925000
H	0.166481000	15.114185000	13.805892000
C	-1.841925000	15.157727000	13.039645000
H	1.822301000	13.193598000	11.260723000
H	2.043342000	14.209227000	12.699089000
H	2.055802000	14.931559000	11.080398000
H	-3.708539000	15.105817000	11.974108000
H	-2.801678000	14.920702000	8.784598000
H	-4.041405000	14.196086000	9.824025000
H	-2.787164000	13.183063000	9.082707000

C	3.480079000	10.795027000	4.729764000
C	3.736809000	10.785934000	7.234347000
C	1.327715000	10.810052000	3.676920000
C	-0.806791000	10.817945000	5.011912000
H	0.180960000	6.465736000	13.800172000
C	-1.828537000	6.416322000	13.037098000
H	1.827620000	8.392362000	11.254085000
H	2.053203000	7.375733000	12.691019000
H	2.065146000	6.655259000	11.071433000
H	-3.696988000	6.462929000	11.974549000
H	-2.795286000	6.653463000	8.783335000
H	-4.035934000	7.373151000	9.825060000
H	-2.785700000	8.390845000	9.083324000
C	-2.446748000	15.672952000	14.317050000
H	4.566157000	10.795504000	4.658706000
C	2.717872000	10.801843000	3.561987000
H	3.527541000	9.906019000	7.853502000
H	3.534108000	11.666961000	7.854241000
H	4.798906000	10.782170000	6.977988000
H	0.716865000	10.821884000	2.776098000
H	-1.257848000	10.808362000	4.016761000
H	-1.176086000	9.948052000	5.567171000
H	-1.162185000	11.708296000	5.543531000
C	-2.429504000	5.898474000	14.315251000
H	-2.748428000	14.839965000	14.964226000
H	-3.338986000	16.274541000	14.120221000
H	-1.731944000	16.281986000	14.878178000
C	3.377521000	10.771870000	2.209897000
H	-2.729596000	6.730128000	14.964874000
H	-3.322043000	5.296887000	14.119841000
H	-1.712865000	5.288685000	14.873233000
H	3.485293000	9.739495000	1.854569000
H	2.784407000	11.312809000	1.466501000
H	4.377774000	11.213047000	2.245492000

3a (Ga):

Fe	1.224199000	11.849015000	12.704421000
N	2.077083000	12.737995000	13.904459000
N	0.076954000	10.356882000	13.050284000
N	1.420939000	12.504136000	10.957242000
Si	2.953895000	12.371393000	10.147140000
C	3.919194000	13.989081000	10.084351000
C	3.984680000	11.066049000	11.035725000
C	2.711347000	11.831338000	8.356164000
Si	0.001699000	13.320959000	10.363126000
C	-0.996607000	12.236895000	9.196314000
C	0.452881000	14.921414000	9.476626000
C	-1.102975000	13.755193000	11.828419000
Si	0.340339000	8.848387000	12.208902000
C	0.622932000	9.091829000	10.365299000
C	-1.113977000	7.649242000	12.319193000
C	1.856372000	7.997170000	12.941185000
Si	-0.924361000	10.423422000	14.481810000

C	-0.453628000	9.094051000	15.736025000
C	-0.758259000	12.060826000	15.400037000
C	-2.748008000	10.247315000	14.032596000
C	2.866327000	13.821311000	14.377942000
C	2.391146000	15.136157000	13.728462000
C	2.656550000	13.903364000	15.909492000
C	4.360333000	13.580799000	14.086909000
H	-0.381436000	11.835029000	8.384271000
H	-1.820605000	12.804933000	8.748097000
H	-1.427400000	11.389993000	9.741069000
H	3.406778000	14.727859000	9.458938000
H	4.909324000	13.816206000	9.644885000
H	4.068481000	14.439273000	11.069966000
H	4.064770000	11.254484000	12.113766000
H	5.005488000	11.050982000	10.635364000
H	3.564212000	10.063472000	10.896922000
H	2.464687000	15.070791000	12.638661000
H	3.004117000	15.975987000	14.075470000
H	1.347391000	15.331085000	13.993173000
H	1.609965000	14.115667000	16.143664000
H	3.280696000	14.707124000	16.315551000
H	2.943088000	12.961256000	16.386278000
H	1.020568000	15.594118000	10.129067000
H	-0.460179000	15.443692000	9.166560000
H	1.049071000	14.743822000	8.574957000
H	2.188136000	10.872656000	8.281473000
H	3.685778000	11.722762000	7.864572000
H	2.138680000	12.571233000	7.785396000
H	-0.555595000	8.075817000	15.348354000
H	-1.089651000	9.174225000	16.625907000
H	0.586104000	9.226672000	16.057165000
H	-0.323141000	9.275169000	9.845207000
H	1.067689000	8.184320000	9.939038000
H	1.281879000	9.933602000	10.144536000
H	0.233522000	12.159694000	15.850149000
H	-1.502802000	12.076986000	16.205950000
H	-0.931157000	12.941961000	14.773271000
H	-1.491042000	12.859226000	12.327948000
H	-1.972152000	14.324127000	11.475796000
H	-0.584130000	14.373241000	12.570338000
H	4.692559000	12.650438000	14.557800000
H	4.965441000	14.407057000	14.477074000
H	4.534927000	13.503325000	13.010501000
H	-1.388439000	7.359659000	13.337574000
H	-0.837864000	6.732579000	11.782689000
H	-2.003511000	8.058929000	11.828608000
H	2.745687000	8.634610000	12.867947000
H	2.075041000	7.056452000	12.421937000
H	1.704122000	7.771383000	14.002350000
H	-3.037352000	10.981823000	13.272135000
H	-3.369804000	10.423837000	14.918634000
H	-2.992993000	9.254050000	13.646548000

4a (In):

In	0.000743000	0.000974000	-0.004596000
N	1.672481000	1.480513000	0.007939000
N	1.672535000	-1.478513000	0.007357000
C	-0.937175000	0.000581000	1.952276000
C	-0.902423000	0.001298000	-1.977816000
C	1.484130000	2.809198000	0.006820000
C	3.046889000	1.256080000	0.016104000
C	1.484255000	-2.807226000	0.005707000
C	3.046922000	-1.254017000	0.015736000
H	-0.179515000	0.000436000	2.740764000
H	-1.563113000	-0.889770000	2.061678000
H	-1.563015000	0.890975000	2.061922000
H	-1.526220000	-0.889092000	-2.099156000
H	-1.526547000	0.891489000	-2.098863000
H	-0.130851000	0.001571000	-2.752772000
C	2.727316000	3.491297000	0.014166000
C	0.117458000	3.374956000	-0.002233000
C	3.708155000	2.518357000	0.019967000
C	3.669862000	0.001060000	0.019001000
C	2.727449000	-3.489260000	0.012985000
C	0.117686000	-3.373188000	-0.003983000
C	3.708242000	-2.516252000	0.019145000
H	2.855094000	4.565755000	0.015069000
C	-0.541722000	3.627082000	1.212788000
C	-0.519357000	3.639580000	-1.226906000
H	4.781047000	2.658622000	0.026630000
C	5.165061000	0.000592000	0.025629000
H	2.855272000	-4.563713000	0.013547000
C	-0.541911000	-3.625905000	1.210683000
C	-0.518512000	-3.637668000	-1.229011000
H	4.781106000	-2.656456000	0.025850000
C	-1.847067000	4.117809000	1.182208000
C	0.155340000	3.399284000	2.526874000
C	-1.824562000	4.130336000	-1.215729000
C	0.201791000	3.420393000	-2.529388000
C	5.854301000	0.002666000	1.247302000
C	5.864545000	0.003115000	-1.190673000
C	-1.847085000	-4.117044000	1.179387000
C	0.154600000	-3.398534000	2.525134000
C	-1.823546000	-4.128887000	-1.218552000
C	0.203159000	-3.417703000	-2.531072000
H	-2.361715000	4.307650000	2.122428000
C	-2.506226000	4.367257000	-0.021564000
H	0.680851000	2.439722000	2.542159000
H	-0.558020000	3.417637000	3.355028000
H	0.905518000	4.179322000	2.706680000
H	-2.321715000	4.329887000	-2.163341000
H	0.978440000	4.181212000	-2.675028000
H	-0.491066000	3.475474000	-3.373090000
H	0.700349000	2.446486000	-2.552326000
C	7.249867000	0.005331000	1.231639000
C	5.108904000	0.006250000	2.554510000

C	7.259491000	0.005854000	-1.163708000
C	5.129399000	0.007156000	-2.503692000
H	-2.362059000	-4.307391000	2.119330000
C	-2.505635000	-4.366384000	-0.024741000
H	0.680461000	-2.439178000	2.540818000
H	-0.559174000	-3.416747000	3.352934000
H	0.904384000	-4.178892000	2.705207000
H	-2.320211000	-4.328382000	-2.166429000
H	0.981820000	-4.176685000	-2.675477000
H	-0.488845000	-3.475019000	-3.375317000
H	0.699402000	-2.442606000	-2.554250000
C	-3.930109000	4.852965000	-0.032981000
H	7.786887000	0.010385000	2.178374000
C	7.969125000	0.003612000	0.037064000
H	4.460528000	-0.873248000	2.641427000
H	4.462597000	0.887577000	2.638353000
H	5.803729000	0.006837000	3.397920000
H	7.804199000	0.011305000	-2.106126000
H	5.830691000	0.007868000	-3.341737000
H	4.481576000	-0.872228000	-2.595771000
H	4.483837000	0.888567000	-2.592222000
C	-3.929312000	-4.852682000	-0.036857000
H	-4.626845000	4.006010000	-0.064752000
H	-4.130837000	5.474727000	-0.910444000
H	-4.159571000	5.433035000	0.865580000
C	9.473677000	-0.029564000	0.041864000
H	-4.626435000	-4.005972000	-0.066551000
H	-4.129994000	-5.472629000	-0.915605000
H	-4.158279000	-5.434804000	0.860509000
H	9.838401000	-1.063199000	-0.005212000
H	9.885603000	0.501726000	-0.821352000
H	9.878386000	0.420468000	0.953000000