Supporting Information

Rh(III)-catalyzed switchable C–H functionalization of 2-(1H-pyrazol-1-yl)pyridine with internal alkynes

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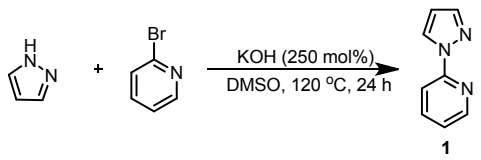
General Information

The ^{1}H NMR, ^{13}C NMR and ^{19}F NMR were recorded with Bruker 400 MHz nuclear spectrometer instruments in $CDCl_3$, CD_3OD and $(CD_3)_2CO$. The chemical shifts (δ) of ^{1}H NMR and ^{13}C NMR were measured in ppm, referenced to residual ^{1}H and ^{13}C signals of nondeuterated $CDCl_3$ (δ = 7.26 and 77.00) ,CD_3OD (δ = 3.31 and 48.80) and $(CD_3)_2CO$ (δ = 2.05 and 206.00, 29.84), as internal standards. All solvents were obtained from commercial sources and were purified according to standard procedures. Purification of products was accomplished by flash chromatography using silica gel (200~300 mesh). Thin layer chromatography (TLC) was performed on Merck silica gel GF254 plates and visualized by UV-light (254 nm). Melting points were obtained on a Yanaco-241 apparatus and are uncorrected. HRMS were recorded on VG ZAB-HS mass spectrometer with ESI resource.

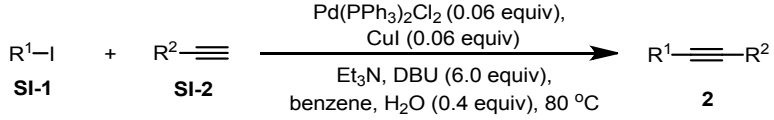
Preparation of Starting Materials:

Synthesis of 1:

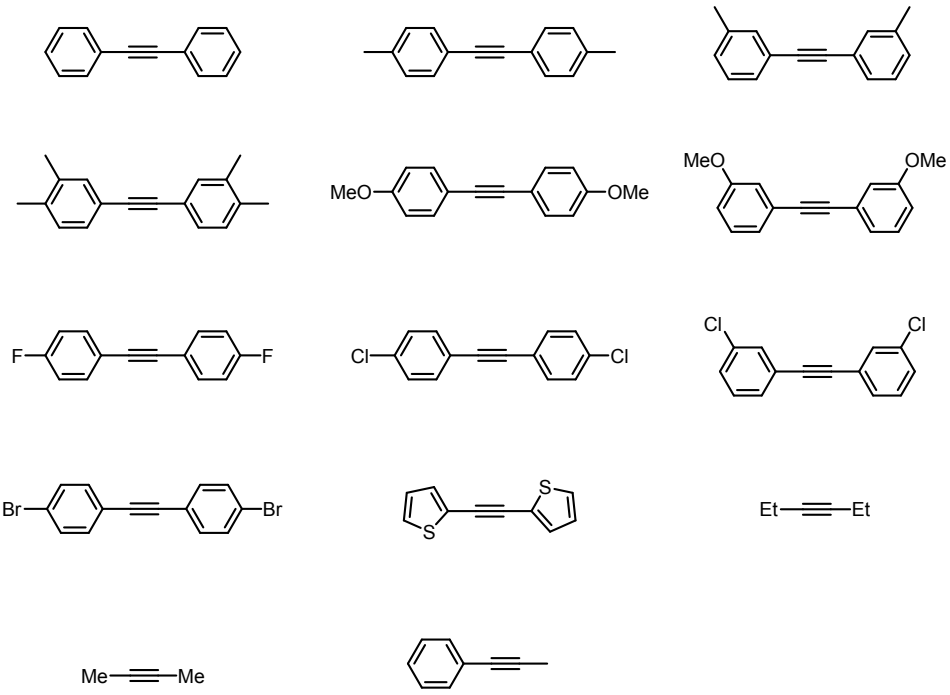


A sealed tube was charged with Pyrazole (70.0 mmol, 4.8 g), 2-bromopyridine (70.0 mmol, 11.0 g), KOH (175.0 mmol, 9.8 g) and dry DMSO (20.0 mL) under argon atmosphere. The resulting mixture was stirred in an oil bath at 120 °C until the end of the reaction. The mixture was quenched with a saturated solution of NH_4Cl and extracted with ethyl acetate (2 × 20.0 mL). The organic phase was dried over $MgSO_4$, followed by evaporation under reduced pressure to remove the solvent. The product was purified by column chromatography on silica gel (hexane/ethyl acetate = 5: 1).

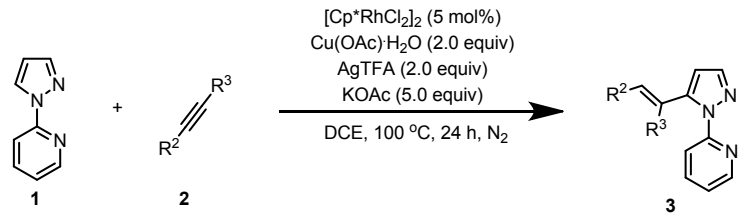
Synthesis of 2:



The preparation of the symmetrical and unsymmetrical alkyne by the coupling of iodide derivatives with alkyne derivatives. In a 50 mL vessel with $Pd(PPh_3)_2Cl_2$ (0.6 mmol), DBU (60.0 mmol), CuI (0.6 mmol) and H_2O (4.0 mmol) in benzene (25.0 mL), **SI-1** (10.0 mmol), **SI-2** (10.0 mmol) were added, respectively. The resulting product was extracted with diethyl ether (2 × 30 mL). The solution was concentrated in vacuo and the residue was purified by column chromatography on silica gel (petroleum ether) to afford the desired pure products **2**.

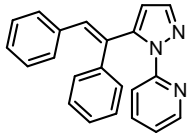


Synthesis of 3:

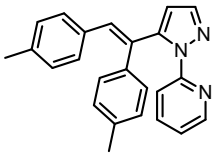


A sealed tube contained **1** (0.2 mmol, 29.0 mg), **2** (0.5 mmol), $[Cp^*RhCl_2]_2$ (5 mol%, 6.18 mg), $Cu(OAc)_2 \cdot H_2O$ (0.4 mmol, 79.8 mg), AgTFA (0.4 mmol, 88.4 mg) and KOAc (1.0 mmol, 98.2 mg) was filled and purged with nitrogen gas three times. Then DCE (2.0 mL) was added to the system via syringe under a nitrogen atmosphere and the reaction was allowed to stir at 100 °C for 24 h. The reaction solution was

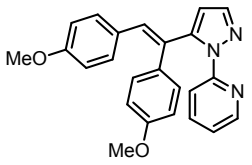
concentrated in vacuo and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate, 10:1) to afford the desired pure product **3**.



2-(5-(1,2-diphenylvinyl)-1H-pyrazol-1-yl)pyridine **3a**: Yellow oil (57 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 – 8.23 (m, 1H), 7.72 (d, *J* = 1.6 Hz, 1H), 7.59 – 7.55 (m, 1H), 7.46 – 7.44 (m, 1H), 7.15 – 6.98 (m, 11H), 6.91 (s, 1H), 6.53 (d, *J* = 1.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 148.0, 145.9, 140.6, 138.0, 137.7, 136.4, 132.4, 130.9, 130.0, 129.5, 127.9, 127.7, 127.3, 127.2, 121.8, 118.0, 110.1. ESI-MS: Calcd for $C_{22}H_{17}N_3$: [M+H$^+$] 324.1495, found 324.1495.

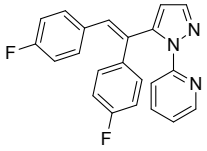


2-(5-(1,2-di-p-tolylvinyl)-1H-pyrazol-1-yl)pyridine **3b**: Yellow oil (60 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 8.25 (m, 1H), 7.69 (d, *J* = 2.0 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.45 – 7.43 (m, 1H), 7.03 – 6.94 (m, 7H), 6.86 – 6.84 (m, 2H), 6.79 (s, 1H), 6.48 (d, *J* = 2.0 Hz, 1H), 2.27 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 148.1, 146.3, 140.6, 137.6, 137.0, 136.9, 135.3, 133.7, 131.5, 130.6, 129.9, 129.4, 128. 7, 128.5, 121.8, 118.1, 109.9, 21.2, 21.1. ESI-MS: Calcd for $C_{24}H_{22}N_3$: [M+H$^+$] 352.1808, found 352.1808.

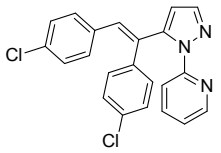


2-(5-(1,2-bis(4-methoxyphenyl)vinyl)-1H-pyrazol-1-yl)pyridine **3c**: Yellow oil (69 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 4.0 Hz, 1H), 7.69 (d, *J* = 1.6 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.45 – 7.42 (m, 1H), 7.06 – 6.98 (m, 5H), 6.77 (s, 1H), 6.70 – 6.67 (m, 2H), 6.60 – 6.56 (m, 2H), 6.49 (d, *J* = 1.6 Hz, 1H), 3.75 (s, 3H), 3.70 (s,

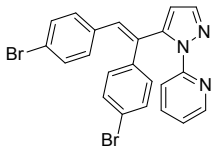
3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 158.7, 152.4, 148.0, 146.5, 140.6, 137.7, 131.3, 130.8, 130.7, 130.0, 129.9, 129.3, 121.8, 118.2, 113.5, 113.3, 109.9, 55.2, 55.1. ESI-MS: Calcd for $C_{24}H_{21}N_3O_2$: [M+H$^+$] 384.1707, found 384.1707.



2-(5-(1,2-bis(4-fluorophenyl)vinyl)-1H-pyrazol-1-yl)pyridine **3d**: Yellow oil (37 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.71 (s, 1H), 7.63 – 7.59 (m, 1H), 7.49 – 7.47 (m, 1H), 7.07 – 7.00 (m, 5H), 6.87 – 6.83 (m, 3H), 6.75 – 6.70 (m, 2H), 6.54 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9 (d, *J* = 246.2 Hz), 152.3, 147.8, 145.4, 140.7, 138.0, 133.9 (d, *J* = 3.4 Hz), 132.4 (d, *J* = 3.3 Hz), 131.8 (d, *J* = 8.0 Hz), 131.5, 131.2 (d, *J* = 7.8 Hz), 129.7 (d, *J* = 1.7 Hz), 122.0, 117.8, 115.0 (d, *J* = 44.1 Hz), 115.0, 110.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.7, -114.0. ESI-MS: Calcd for $C_{22}H_{15}F_2N_3$: [M+H$^+$] 360.1307, found 360.1307.

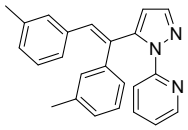


2-(5-(1,2-bis(4-chlorophenyl)vinyl)-1H-pyrazol-1-yl)pyridine ***3e***: Yellow oil (34 mg, 43%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.72 (s, 1H), 7.65 – 7.61 (m, 1H), 7.52 – 7.50 (m, 1H), 7.15 – 7.13 (m, 2H), 7.06 – 6.98 (m, 7H), 6.86 (s, 1H), 6.54 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.8, 145.0, 140.8, 138.1, 136.4, 134.6, 133.3, 133.3, 132.2, 131.4, 130.8, 129.9, 129.9, 128.4, 128.1, 122.0, 117.6, 110.5. ESI-MS: Calcd for $C_{22}H_{15}Cl_2N_3$: [M+H$^+$] 392.0716, found 392.0716.

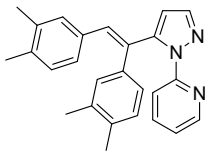


2-(5-(1,2-bis(4-bromophenyl)vinyl)-1H-pyrazol-1-yl)pyridine **3f**: Yellow oil (41 mg, 43%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.72 (s, 1H), 7.65 – 7.61 (m, 1H),

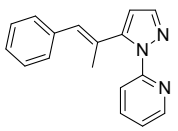
7.52 – 7.48 (m, 1H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.06 – 7.03 (m, 1H), 6.97 – 6.92 (m, 4H), 6.84 (s, 1H), 6.54 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.8, 144.9, 140.8, 138.0, 136.8, 135.1, 132.4, 131.7, 131.4, 131.1, 131.1, 129.9, 129.8, 122.0, 121.6, 121.5, 117.5, 110.5. ESI-MS: Calcd for $C_{22}H_{15}Br_2N_3$: [M+H$^+$] 479.9705, found 479.9705.



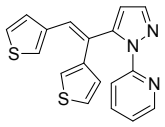
2-(5-(1,2-di-m-tolylvinyl)-1H-pyrazol-1-yl)pyridine **3g**: Yellow oil (42 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.71 (s, 1H), 7.60 – 7.56 (m, 1H), 7.44 – 7.42 (m, 1H), 7.04 – 6.83 (m, 10H), 6.50 (s, 1H), 2.19 (s, 3H), 2.13 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 148.0, 146.2, 140.6, 138.0, 137.7, 137.4, 137.2, 136.4, 132.2, 131.0, 130.5, 130.4, 128.0, 128.0, 127.8, 127.6, 127.3, 126.5, 121.9, 118.3, 109.9, 21.3, 21.1. ESI-MS: Calcd for $C_{24}H_{21}N_3$: [M+H$^+$] 352.1808, found 352.1808.



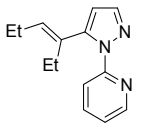
2-(5-(1,2-bis(3,4-dimethylphenyl)vinyl)-1H-pyrazol-1-yl)pyridine **3i**: Yellow oil (52 mg, 69%).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.69 (s, 1H), 7.59 – 7.55 (m, 1H), 7.43 – 7.41 (m, 1H), 7.04 – 7.01 (m, 1H), 6.90 (s, 1H), 6.87 – 6.79 (m, 5H), 6.71 (s, 1H), 6.45 (s, 1H), 2.18 (s, 3H), 2.13 (s, 3H), 2.11 (s, 3H), 2.05 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 148.1, 146.6, 140.5, 137.5, 136.0, 135.8, 135.8, 135.7, 135.5, 134.2, 131.2, 131.0, 130.9, 130.8, 129.2, 129.0, 127.6, 126.7, 121.8, 118.4, 109.7, 19.6, 19.5, 19.4, 19.4. ESI-MS: Calcd for $C_{26}H_{25}N_3$: [M+H$^+$] 380.2127, found 380.2127.



2-(5-(1-phenylprop-1-en-2-yl)-1H-pyrazol-1-yl)pyridine **3j**: Yellow oil (38 mg, 73%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 7.84 – 7.80 (m, 1H), 7.76 – 7.74 (m, 1H), 7.68 (s, 1H), 7.39 – 7.33 (m, 4H), 7.27 – 7.22 (m, 2H), 6.64 (s, 1H), 6.42 (s, 1H), 2.08 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 148.3, 147.3, 140.8, 138.2, 137.3, 130.9, 129.0, 128.8, 128.2, 126.9, 122.0, 117.4, 108.0, 19.0. ESI-MS: Calcd for $C_{17}H_{15}N_3$: [M+H$^+$] 262.1339, found 262.1340.

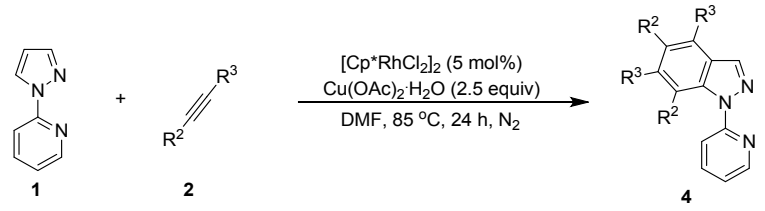


2-(5-(1,2-di(thiophen-3-yl)vinyl)-1H-pyrazol-1-yl)pyridine **3k**: Yellow oil (46 mg, 69%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (s, 1H), 7.73 – 7.68 (m, 2H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.26 – 7.25 (m, 1H), 7.17 – 7.14 (m, 2H), 7.03 (s, 1H), 6.99 (d, *J* = 3.2 Hz, 1H), 6.94 (d, *J* = 2.8 Hz, 1H) 6.92 – 6.89 (m, 1H), 6.86 – 6.84 (m, 1H), 6.49 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.2, 145.0, 140.6, 139.3, 138.6, 138.0, 130.2, 129.2, 127.2, 127.1, 127.0, 126.7, 126.4, 122.9, 122.0, 119.8, 118.1, 109.5. ESI-MS: Calcd for $C_{18}H_{13}N_3S_2$: [M+H$^+$] 336.0624, found 336.0624.

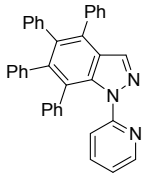


2-(5-(hex-3-en-3-yl)-1H-pyrazol-1-yl)pyridine **3l**: Yellow oil (31 mg, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 7.79 – 7.76 (m, 1H), 7.64 – 7.63 (m, 1H), 7.23 – 7.20 (m, 1H), 6.26 (s, 1H), 5.49 (t, *J* = 7.2 Hz, 1H), 2.25 – 2.10 (m, 4H), 0.96 (t, *J* = 7.6 Hz, 3H), 0.87 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 148.3, 145.7, 140.6, 138.0, 133.8, 132.3, 121.9, 117.7, 108.5, 23.8, 21.2, 13.8, 13.1. ESI-MS: Calcd for $C_{14}H_{17}N_3$: [M+H$^+$] 228.1495, found 228.1495.

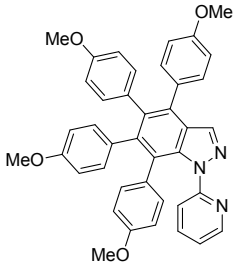
Synthesis of 4:



A sealed tube contained **1** (0.2 mmol, 29 mg), **2** (0.5 mmol), $[Cp^*RhCl_2]_2$ (5 mol%, 6.18 mg) and $Cu(OAc)_2 \cdot H_2O$ (0.5 mmol, 99.8 mg) was filled and purged with nitrogen gas three times. Then DMF (2.0 mL) was added to the system via syringe under a nitrogen atmosphere and the reaction was allowed to stir at 85 °C for 24 h. The reaction solution was concentrated in vacuum and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate, 10:1) to afford the desired pure product **4**.

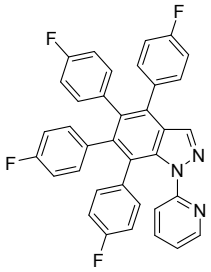


4,5,6,7-tetraphenyl-1-(pyridin-2-yl)-1H-indazole **4a**: Wight solid (85 mg, 87%). M.p.: 95 − 97 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.94 (d, J = 3.6 Hz, 1H), 7.44 – 7.40 (m, 1H), 7.30 – 7.22 (m, 5H), 7.17 (d, J = 8.0 Hz, 1H), 6.94 – 6.76 (m, 16H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 147.9, 141.4, 139.9, 138.7, 137.6, 137.5, 136.9, 136.6, 135.2, 133.5, 131.9, 131.6, 130.6, 130.5, 127.8, 126.9, 126.8, 126.8, 126.6, 125.8, 125.8, 125.5, 125.5, 124.3, 121.5, 119.9. ESI-MS: Calcd for $C_{36}H_{25}N_3$: [M+H$^+$] 500.2121, found 500.2121.

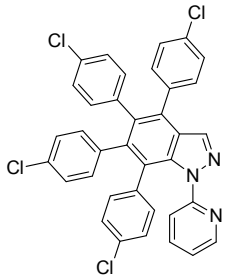


4,5,6,7-tetrakis(4-methoxyphenyl)-1-(pyridin-2-yl)-1H-indazole **4b**: Yellow solid (85 mg, 87%). M.p.: 98 − 100 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 8.03 (d, J =

4.0 Hz, 1H), 7.44 – 7.40 (m, 1H), 7.20 – 7.18 (m, 2H), 7.11 – 7.09 (m, 1H), 6.97 – 6.94 (m, 1H), 6.82 – 6.80 (m, 2H), 6.72 – 6.66 (m, 6H), 6.49 – 6.43 (m, 4H), 6.34 – 6.32 (m, 2H), 3.80 (s, 3H), 3.66 (s, 3H), 3.63 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 157.6, 157.2, 157.1, 152.5, 147.9, 141.4, 137.9, 136.8, 136.6, 135.0, 133.1, 132.9, 132.6, 132.6, 132.5, 131.6, 131.6, 131.3, 130.1, 125.8, 123.8, 121.3, 120.1, 113.3, 112.5, 112.4, 112.2, 55.1, 55.1, 54.9, 54.9. ESI-MS: Calcd for $C_{40}H_{33}N_3O_4$: [M+H$^+$] 620.2544, found 620.2544.

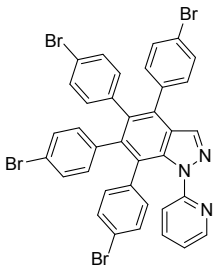


4,5,6,7-tetrakis(4-fluorophenyl)-1-(pyridin-2-yl)-1H-indazole **4c**: Yellow solid (61 mg, 53%). M.p.: 85 − 87 ºC.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.95 (d, *J* = 4.0 Hz, 1H), 7.57 – 7.53 (m, 1H), 7.28 (s, 1H), 7.23 – 7.20 (m, 2H), 7.04 – 6.97 (m, 4H), 6.78 – 6.60 (m, 9H), 6.54 – 6.50 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9 (d, *J* = 245.0 Hz), 161.2 (d, *J* = 245.0 Hz), 161.0 (d, *J* = 244.0 Hz), 152.2, 147.9, 140.5, 137.6, 137.3, 136.4, 135.4 (d, *J* = 4.0 Hz), 134.2, 134.2, 133.3 (d, *J* = 3.0 Hz), 133.2 (d, J = 8.0 Hz), 133.0, 132.9 (d, *J* = 8.0 Hz), 132.0 (d, *J* = 7.0 Hz), 132.0 (d, *J* = 8.0 Hz), 125.9, 123.8, 121.8, 120.0, 115.2, 115.0, 114.3, 114.1, 114.1, 113.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.7, -115.8, -116.1, -116.2. ESI-MS: Calcd for $C_{36}H_{21}F_4N_3$: [M+H$^+$] 572.1744, found 572.1744.

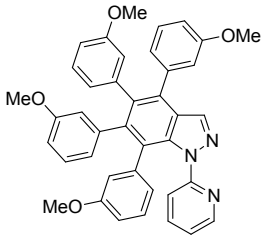


4,5,6,7-tetrakis(4-chlorophenyl)-1-(pyridin-2-yl)-1H-indazole **4d**: Yellow solid (60 mg, 47%). M.p.: 88 − 90 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.92 (d, *J* = 4.0 Hz, 1H), 7.59 – 7.54 (m, 1H), 7.29 – 7.26 (m, 3H), 7.18 – 7.16 (m, 2H), 7.06 –

7.03 (m, 1H), 6.96 – 6.91 (m, 4H), 6.81 – 6.79 (m, 2H), 6.73 – 6.67 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 147.9, 139.8, 137.6, 137.5, 137.4, 136.5, 136.3, 135.6, 133.7, 133.3, 132.9, 132.6, 132.3, 132.2, 132.1, 131.6, 131.6, 128.4, 127.6, 127.4, 127.3, 125.8, 123.7, 121.8, 119.9. ESI-MS: Calcd for $C_{36}H_{21}Cl_4N_3$: [M+H$^+$] 636.0562, found 636.0566.

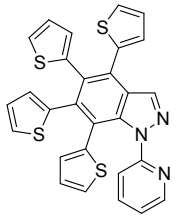


4,5,6,7-tetrakis(4-bromophenyl)-1-(pyridin-2-yl)-1H-indazole **4e**: Yellow solid (82 mg, 50%). M.p.: 83 − 85 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.92 (d, *J* = 4.0 Hz, 1H), 7.59 – 7.55 (m, 1H), 7.44 – 7.42 (m, 2H), 7.29 – 7.26 (m, 1H), 7.12 – 7.04 (m, 7H), 6.96 – 6.94 (m, 2H), 6.67 – 6.61 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 147.9, 139.7, 138.1, 137.5, 136.9, 136.2, 136.0, 133.5, 133.2, 132.9, 132.8, 132.0, 131.9, 131.7, 131.4, 131.1, 130.5, 130.4, 130.3, 125.8, 123.6, 121.8, 121.6, 120.6, 120.5, 120.5, 119.9. ESI-MS: Calcd for $C_{36}H_{21}Br_4N_3$: [M+H$^+$] 811.8542, found 811.8551.

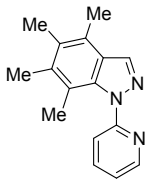


4,5,6,7-tetrakis(3-methoxyphenyl)-1-(pyridin-2-yl)-1H-indazole **4f**: Yellow solid (87 mg, 70%). M.p.: 87 − 89 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (s, 1H), 8.01 (d, *J* = 3.6 Hz, 1H), 7.48 – 7.44 (m, 1H), 7.24 – 7.18 (m, 2H), 6.98 – 6.95 (m, 2H), 6.87 – 6.79 (m, 4H), 6.74 – 6.70 (m, 1H), 6.51 – 6.41 (m, 9H), 3.64 (s, 3H), 3.48 – 3.43 (m, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 158.5, 158.3, 152.5, 147.9, 141.2, 141.1, 140.9, 139.9, 138.7, 137.4, 136.9, 136.7, 134.7, 133.4, 128.8, 127.9, 127.8, 127.6, 125.7, 124.6, 124.3, 124.0, 123.3, 123.0, 121.6, 119.8, 117.1, 116.9, 115.7, 115.3,

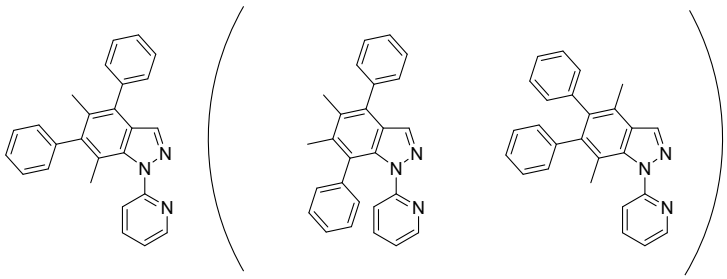
113.3, 112.9, 112.4, 112.3, 112.2, 55.1, 55.1, 55.0. ESI-MS: Calcd for $C_{40}H_{33}N_3O_4$: [M+H$^+$] 620.2544, found 620.2554.



1-(pyridin-2-yl)-4,5,6,7-tetra(thiophen-2-yl)-1H-indazole **4g**: Yellow solid (65mg, 62%). M.p.: 90 − 92 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.12 (d, *J* = 3.6 Hz, 1H), 7.57 – 7.53 (m, 1H), 7.36 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 7.17 – 7.14 (m, 2H), 7.10 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.07 – 7.04 (m, 2H), 6.99 (dd, *J* = 4.0, 2.0 Hz, 1H), 6.78 – 6.76 (m, 1H), 6.72 – 6.70 (m, 1H), 6.67 – 6.66 (m, 1H), 6.62 – 6.61 (m, 1H), 6.46 – 6.44 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 148.1, 140.4, 140.1, 139.1, 138.4, 137.9, 137.2, 136.9, 136.5, 130.0, 129.8, 129.2, 129.2, 129.1, 128.7, 127.2, 126.7, 126.6, 126.4, 126.3, 126.0, 125.7, 125.6, 121.8, 119.6, 119.4. ESI-MS: Calcd for $C_{28}H_{17}N_3S_4$: [M+H$^+$] 524.0378, found 524.0378.



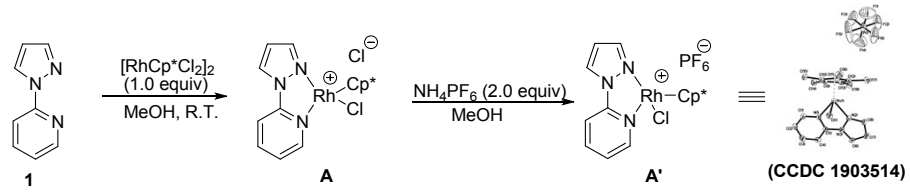
4,5,6,7-tetraethyl-1-(pyridin-2-yl)-1H-indazole **4h**: Yellow solid (37 mg, 73%). M.p.: 59 − 61 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 – 8.54 (m, 1H), 8.17 (s, 1H), 7.89 – 7.85 (m, 1H), 7.69 – 7.67 (m, 1H), 7.29 – 7.27 (m, 1H), 2.55 (s, 3H), 2.33 (s, 3H), 2.31 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.3, 148.1, 138.5, 138.1, 136.1, 135.9, 129.2, 125.2, 121.9, 119.9, 117.1, 17.4, 16.7, 16.1, 15.9. ESI-MS: Calcd for $C_{16}H_{17}N_3$: [M+H$^+$] 252.1495, found 252.1495.



5,7-dimethyl-4,6-diphenyl-1-(pyridin-2-yl)-1H-indazole 5,6-dimethyl-4,7-diphenyl-1-(pyridin-2-yl)-1H-indazole 4,7-dimethyl-5,6-diphenyl-1-(pyridin-2-yl)-1H-indazole

4i: White solid (50 mg, 67%, 2.3:1:1). M.p.: 77 − 79 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.0 Hz, 1.00H), 8.54 (d, *J* = 5.6 Hz, 0.44H), 8.33 (s, 0.47H), 8.31 (s, 0.82H), 8.05 (d, *J* = 6.0 Hz, 0.47H), 7.92 – 7.89 (m, 1.00H), 7.78 – 7.76 (m, 1.00H), 7.37 – 7.31 (m, 1.54H), 7.20 – 6.96 (m, 19.00H), 6.90 – 6.82 (m, 2.00H), 2.48 (s, 1.31H), 2.39 (s, 3.00H), 2.38 (s, 1.33H), 1.96 (s, 3.00H), 1.89 (s, 1.32H), 1.87 (s, 1.30H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.0, 152.0, 148.1, 144.2, 143.5, 142.2, 141.7, 141.0, 141.0, 140.8, 140.7, 140.3, 140.0, 139.0, 138.9, 138.2, 136.1, 135.8, 135.4, 131.2, 130.9, 130.7, 130.7, 130.5, 130.4, 130.3, 130.0, 129.9, 129. 8, 129.0, 128.9, 128.2, 127.6, 127.5, 127.4, 127.3, 127.3, 127.1, 126.3, 126.2, 126.0, 125.9, 125.9, 125.8, 125.6, 125.3, 125.1, 122.5, 120.5, 119.3, 117.4, 116.7, 18.9, 18.4, 17.3, 17.0, 16.8, 16.8. ESI-MS: Calcd for $C_{26}H_{21}N_3$: [M+H$^+$] 376.1808, found 376.1808.

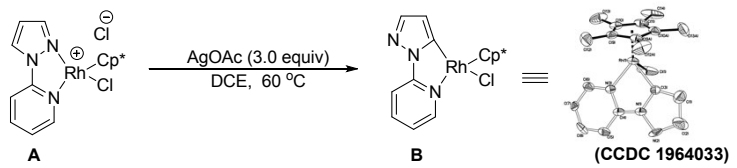
Mechanistic studies:



A sealed tube contained $[Cp^*RhCl_2]_2$ (0.1 mmol, 61.8 mg) and **1** (0.24 mmol, 35.0 mg) was filled and purged with nitrogen gas three times. Then MeOH (10.0 mL) was added to the system via syringe under a nitrogen atmosphere and the reaction was allowed to stir at room temperature for 1 h. The reaction solution was concentrated in vacuum and the residue was washed with ether to remove excess ligand. Cyclometalated compound **A** was isolated as an orange solid (91 mg, 99%).After **A** was formed, NH_4PF_6 (0.4 mmol, 65.2 mg) were added to the reaction solution and strred for another 1 h. The precipitate **A'** was formed. The mixture was filtered through Celite and evaporated to dryness. **A'** was recrystallized from MeOH at −10 °C.

A: ^{1}H NMR (400 MHz, CD_3OD) δ 8.95 (d, *J* = 3.2 Hz, 1H), 8.80 (d, *J* = 5.2 Hz, 1H), 8.43 (d, *J* = 2.0 Hz, 1H), 8.32 – 8.28 (m, 1H), 8.18 – 8.16 (m, 1H), 7.73 – 7.70 (m, 1H), 7.01 – 7.00 (m, 1H), 1.80 (s, 15H). ^{13}C NMR (100 MHz, CD_3OD) δ 151.7, 149.5, 145.4, 143.7, 132.3, 126.3, 113.7, 113.4, 99.0, 9.1.

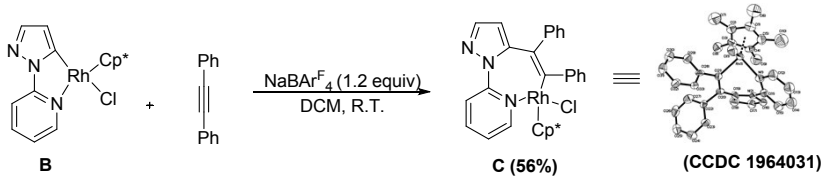
A': ^{1}H NMR (400 MHz, Acetone) δ 9.00 (d, *J* = 3.2 Hz, 1H), 8.93 (d, *J* = 5.6 Hz, 1H), 8.49 (d, *J* = 2.0 Hz, 1H), 8.39 – 8.35 (m, 1H), 8.26 – 8.24 (m, 1H), 7.78 – 7.75 (m, 1H), 7.06 – 7.05 (m, 1H), 1.86 (s, 15H). ^{13}C NMR (100 MHz, Acetone) δ 151.5, 149.0, 144.8, 143.2, 131.8, 125.9, 113.3, 113.0, 98.2, 9.1.



A sealed tube contained **A** (0.2 mmol, 91.0 mg) and AgOAc (0.6 mmol, 100.1 mg) was filled and purged with nitrogen gas three times. Then DCE (10.0 mL) was added to the system via syringe under a nitrogen atmosphere and the reaction was allowed to

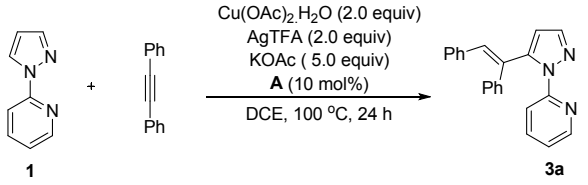
stir at 84 °C for 3 h. The reaction solution was concentrated in vacuum and the residue was purified by column chromatography on aluminium oxide gel (ethyl acetate) to afford the desired pure product **B**. Cyclometalated compound **B** was isolated as an orange solid (57.0 mg, 72%). **B** were recrystallized from n-hexane/CH_2Cl_2 (2:1) at −10 °C.

B: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 5.6 Hz, 1H), 7.82 – 7.80 (m, 2H), 7.74 (d, *J* = 1.6 Hz, 1H), 7.11 – 7.07 (m, 1H), 6.48 (d, *J* = 1.6 Hz, 1H), 1.72 (s, 15H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 148.3, 143.7, 138.6, 118.9, 110.7, 110.4, 95.4, 95.3, 8.4.

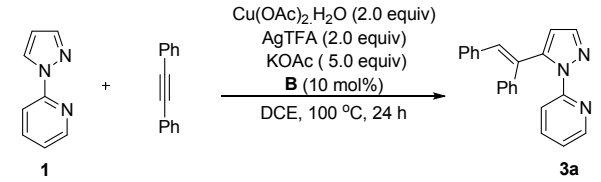


A sealed tube contained **B** (0.2 mmol, 80.0 mg), diphenylacetylene (0.24mmol, 43.0 mg) and $NaBAr^F_4$ (0.24 mmol, 213.0 mg) was filled and purged with nitrogen gas three times. Then DCE (10.0 mL) was added to the system via syringe under a nitrogen atmosphere and the reaction was allowed to stir at room temperature for 0.5 h. The reaction solution was concentrated in vacuum and the residue was purified by column chromatography on aluminium oxide gel (petroleum ether/ethyl acetate, 1:1) to afford the desired pure product **C**. Cyclometalated compound **C** was isolated as an orange solid (63.0 mg, 56%). **C** were recrystallized from n-hexane/CH2Cl2 (2:1) at −10 °C.

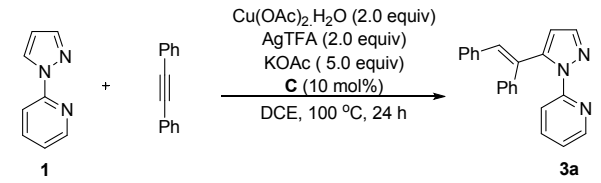
C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.74 (dd, *J* = 5.6, 1.6 Hz, 1H), 7.95 – 7.91 (m, 1H), 7.80 – 7.78(m, 1H), 7.59 (d, *J* = 1.6 Hz, 1H), 7.35 – 7.31 (m, 1H), 7.08 – 6.75 (m, 10H), 5.95 (d, *J* = 2.0 Hz, 1H), 1.40 (s, 15H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 174.7, 155.3, 153.3, 151.0, 148.9, 144.5, 141.1, 138.2, 130.4, 129.6, 126.2, 124.1, 122.5, 122.4, 122.0, 109.8, 95.5, 7.9.



A sealed tube contained **1** (0.2 mmol, 29.0 mg), diphenylacetylene (0.5 mmol, 89.0 mg), **A** (10 mol%, 11.0 mg), $Cu(OAc)_2 \cdot H_2O$ (0.4 mmol, 80.0 mg), AgTFA (0.4 mmol, 88.0 mg) and KOAc (1.0 mmol, 98.0 mg) was filled and purged with nitrogen gas three times. Then DCE (2.0 mL) was added to the system via syringe under a nitrogen atmosphere and the reaction was allowed to stir at 100 °C for 24 h. The product **3a** was obtained in 80% isolated yield.

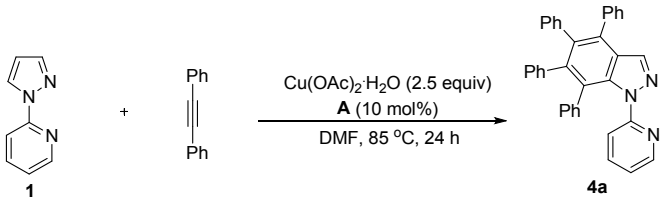


A sealed tube contained **1** (0.2 mmol, 29.0 mg), diphenylacetylene (0.5 mmol, 89.0 mg), **B** (10 mol%, 8.0 mg), $Cu(OAc)_2 \cdot H_2O$ (0.4 mmol, 80.0 mg), AgTFA (0.4 mmol, 88.0 mg) and KOAc (1.0 mmol, 98.0 mg) was filled and purged with nitrogen gas three times. Then DCE (2.0 mL) and acetic acid (5.0 ul, 0.08 mmol) were added to the system via syringe under a nitrogen atmosphere and the reaction was allowed to stir at 100 °C for 24 h. The product **3a** was obtained in 77% isolated yield.

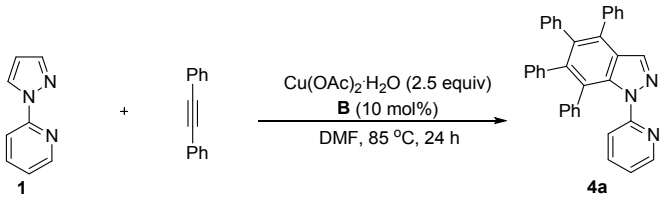


A sealed tube contained **1** (0.2 mmol, 29.0 mg), diphenylacetylene (0.5 mmol, 89.0 mg), **C** (10 mol%, 12.0 mg), $Cu(OAc)_2 \cdot H_2O$ (0.4 mmol, 80.0 mg), AgTFA (0.4 mmol, 88.0 mg) and KOAc (1.0 mmol, 98.0 mg) was filled and purged with nitrogen gas three times. Then DCE (2.0 mL) and acetic acid (5.0 ul, 0.08 mmol) were added to the

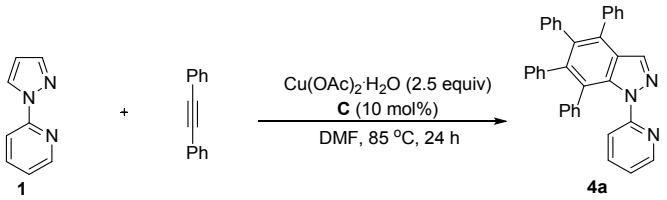
system via syringe under a nitrogen atmosphere and the reaction was allowed to stir at 100 °C for 24 h. The product **3a** was obtained in 82% isolated yield.



A sealed tube contained **1** (0.2 mmol, 29.0 mg), diphenylacetylene (0.5 mmol, 89.0 mg), **A** (10 mol%, 11.0 mg), $Cu(OAc)_2 \cdot H_2O$ (0.5 mmol, 100.0 mg) was filled and purged with nitrogen gas three times. Then DMF (2.0 mL) was added to the system via syringe under a nitrogen atmosphere and the reaction was allowed to stir at 85 °C for 24 h. The product **4a** was obtained in 90% isolated yield.

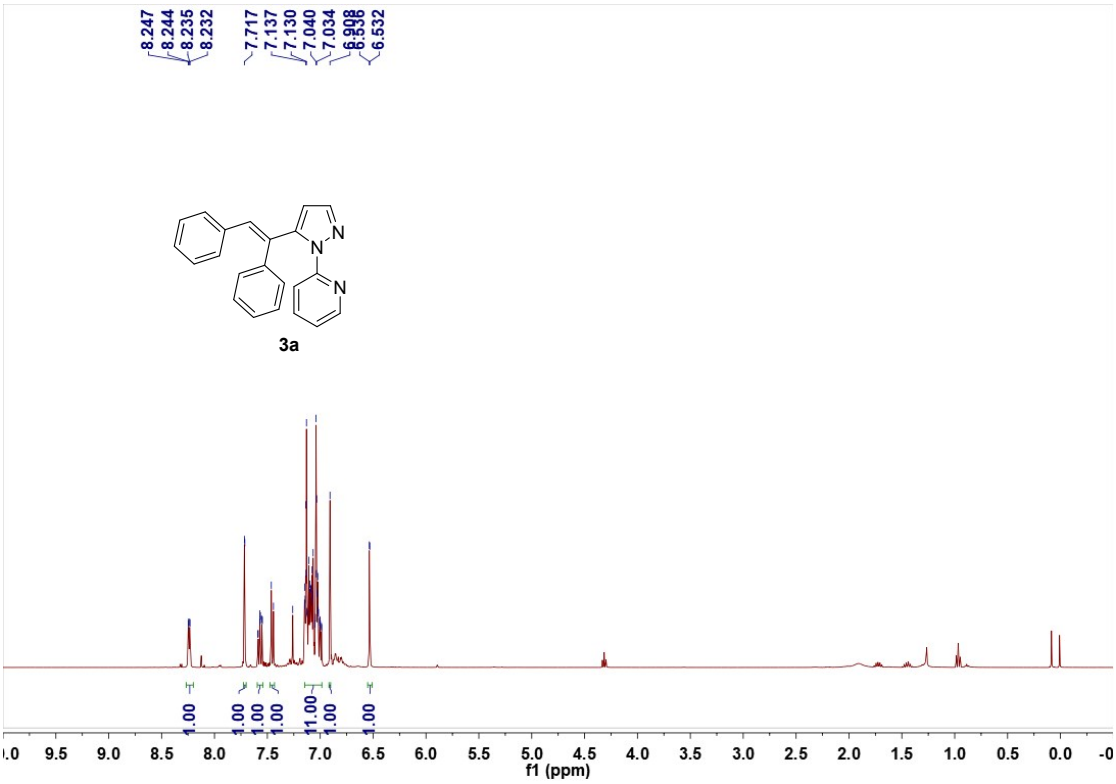


A sealed tube contained **1** (0.2 mmol, 29.0 mg), diphenylacetylene (0.5 mmol, 89.0 mg), **B** (10 mol%, 8.0 mg), $Cu(OAc)_2 \cdot H_2O$ (0.5 mmol, 100.0 mg) was filled and purged with nitrogen gas three times. Then DMF (2.0 mL) was added to the system via syringe under a nitrogen atmosphere and the reaction was allowed to stir at 85 °C for 24 h. The product **4a** was obtained in 91% isolated yield.



A sealed tube contained **1** (0.2 mmol, 29.0 mg), diphenylacetylene (0.5 mmol, 89.0 mg), **C** (10 mol%, 12.0 mg), $Cu(OAc)_2 \cdot H_2O$ (0.5 mmol, 100.0 mg) was filled and purged with nitrogen gas three times. Then DMF (2.0 mL) was added to the system via syringe under a nitrogen atmosphere and the reaction was allowed to stir at 85 °C for 24 h. The product **4a** was obtained in 90% isolated yield.

NMR Spectra:


8.247
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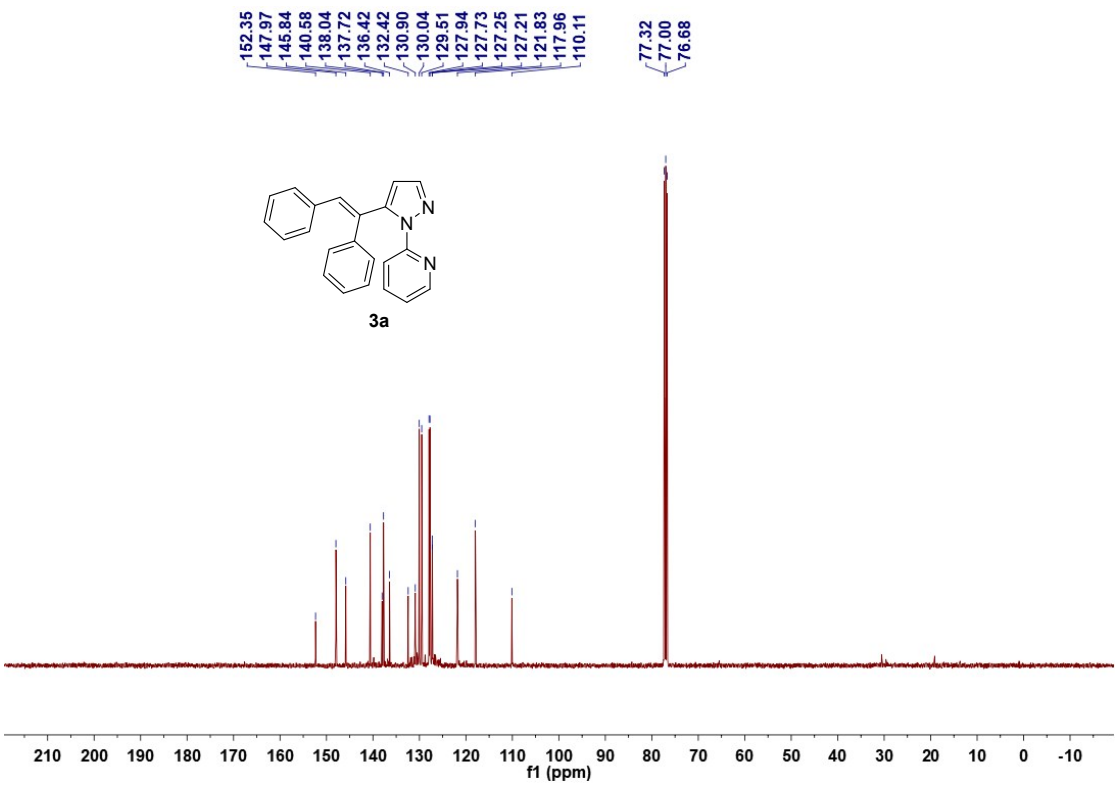
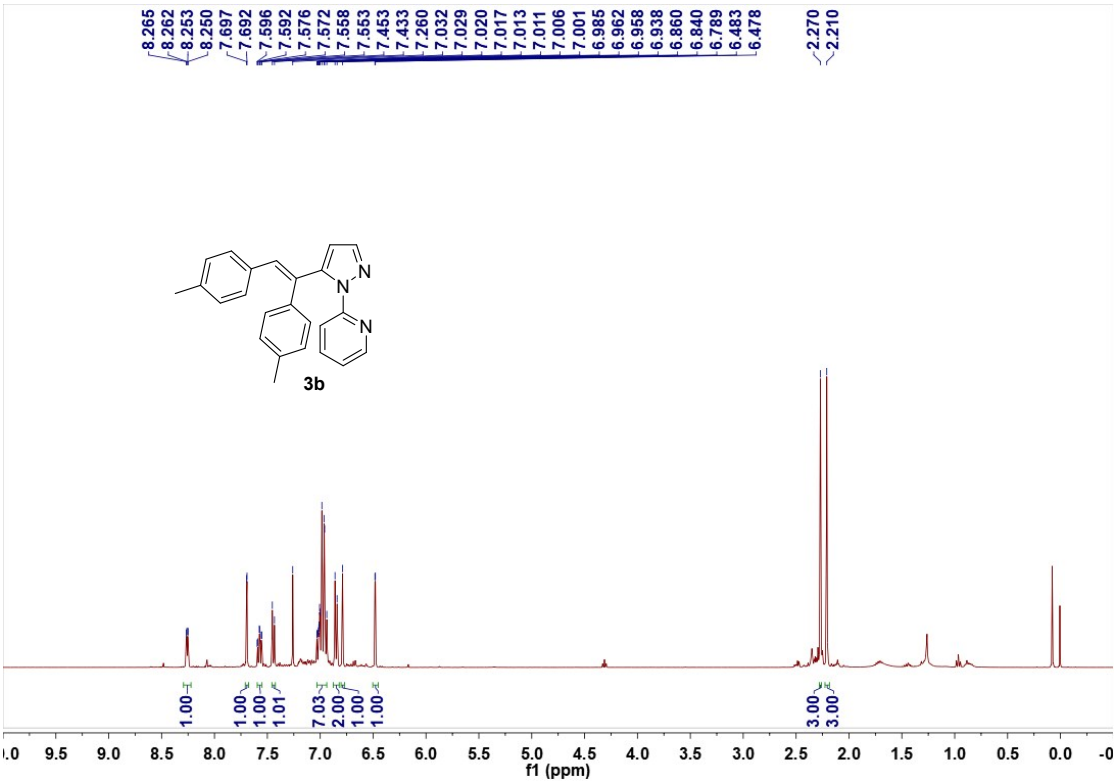
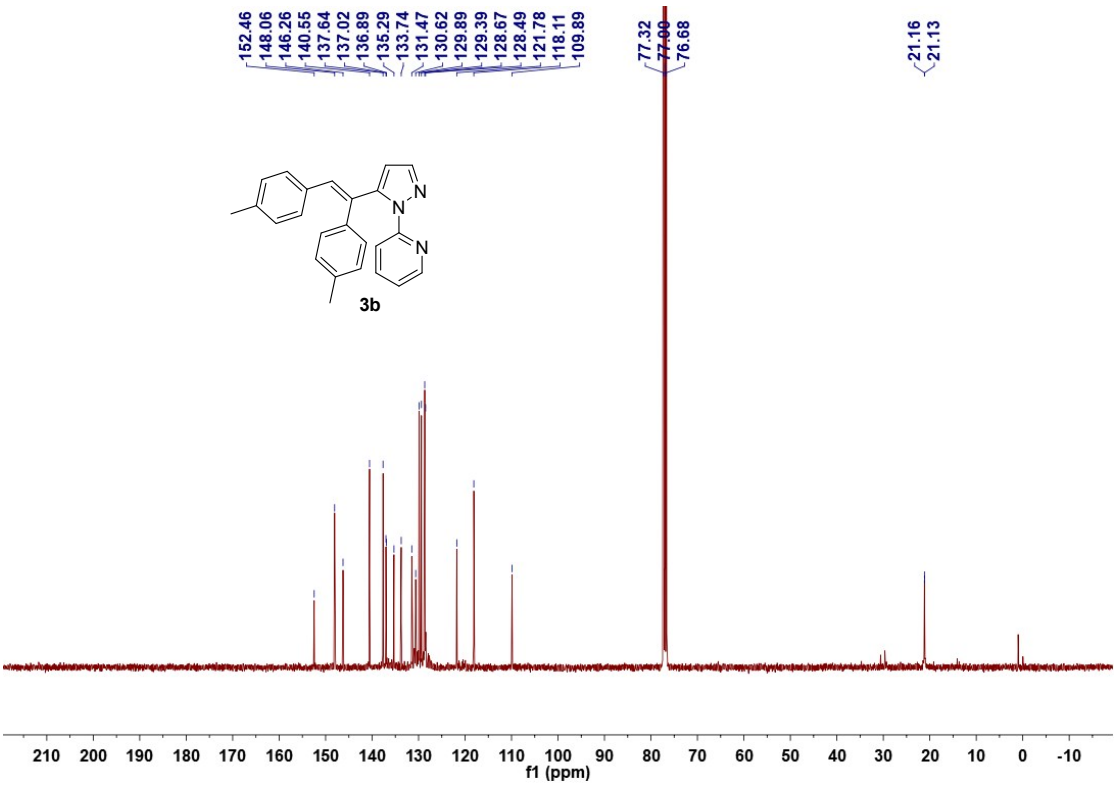
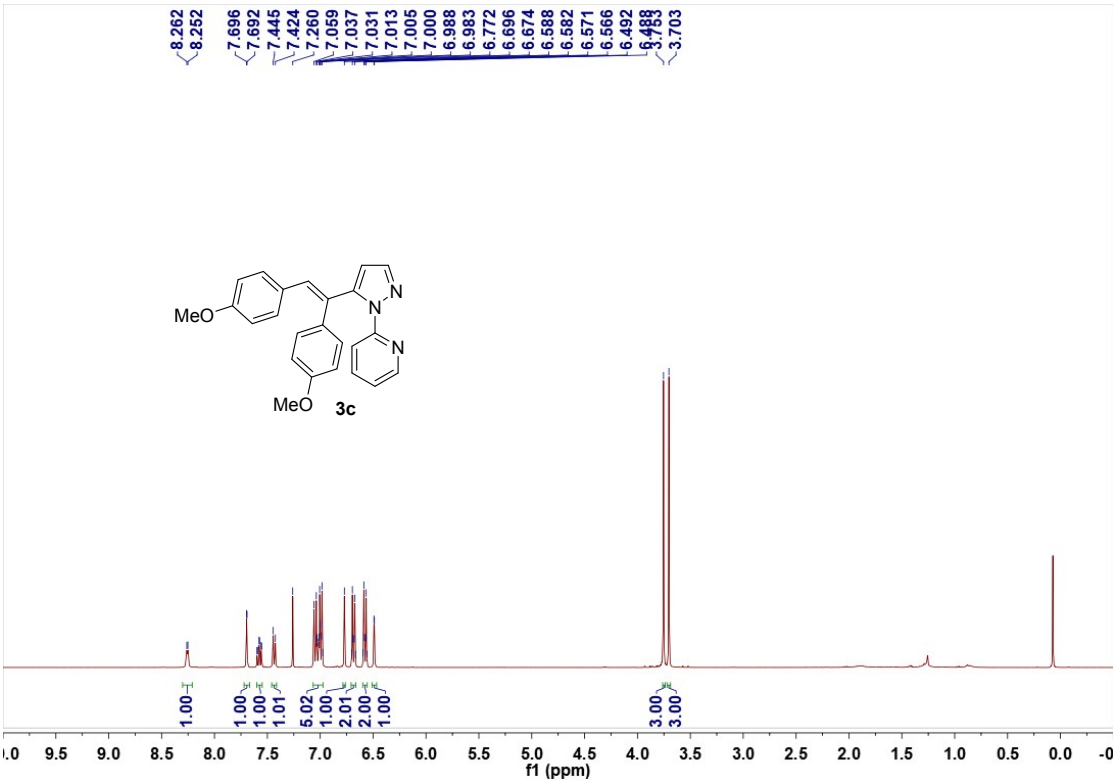
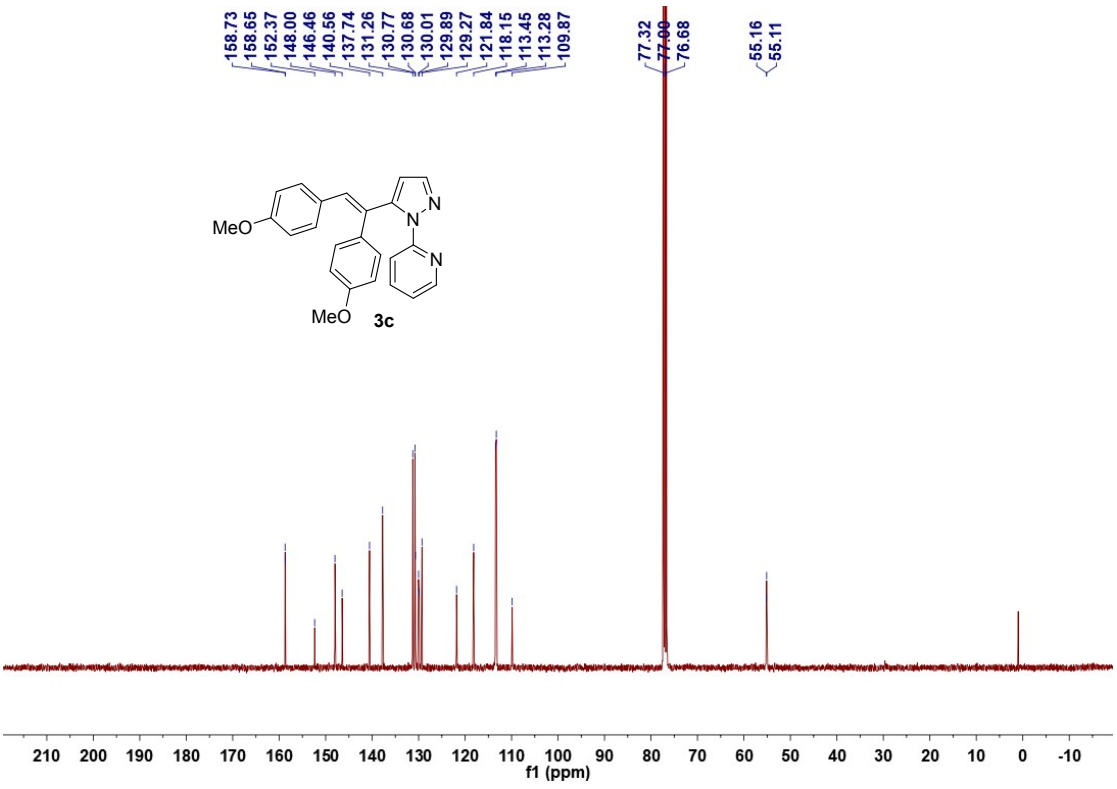
8.235
8.232
7.717
7.137
7.130
7.040
7.034
6.532
3a
1.00
1.00
1.00
1.00
11.00
1.00
1.00
f1 (ppm)


152.35
147.97
145.84
140.58
138.04
137.72
136.42
132.42
130.90
130.04
129.51
127.94
127.73
127.25
127.21
121.83
117.96
110.11
77.32
77.00
76.68
3a
f1 (ppm)


8.265
8.262
8.253
8.250
7.697
7.692
7.596
7.592
7.576
7.572
7.558
7.553
7.453
7.433
7.260
7.032
7.029
7.020
7.017
7.013
7.011
7.006
7.001
6.985
6.962
6.958
6.938
6.860
6.840
6.789
6.483
6.478
2.270
2.210
N
N
N
3b
1.00
1.00
1.00
1.01
7.03
2.00
1.00
1.00
3.00
3.00
f1 (ppm)


152.46
148.06
146.26
140.55
137.64
137.02
136.89
135.29
133.74
131.47
130.62
129.89
129.39
128.67
128.49
121.78
118.11
109.89
77.32
77.00
76.68
21.16
21.13
N
N
N
3b
f1 (ppm)


8.262
8.252
7.696
7.692
7.445
7.424
7.260
7.059
7.037
7.031
7.013
7.005
7.000
6.988
6.983
6.772
6.696
6.674
6.588
6.582
6.571
6.566
6.492
6.488
3.783
3.703
MeO
MeO
3c
1.00
1.00
1.00
1.01
5.02
1.00
2.01
2.00
1.00
3.00
3.00
f1 (ppm)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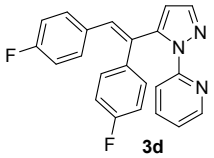
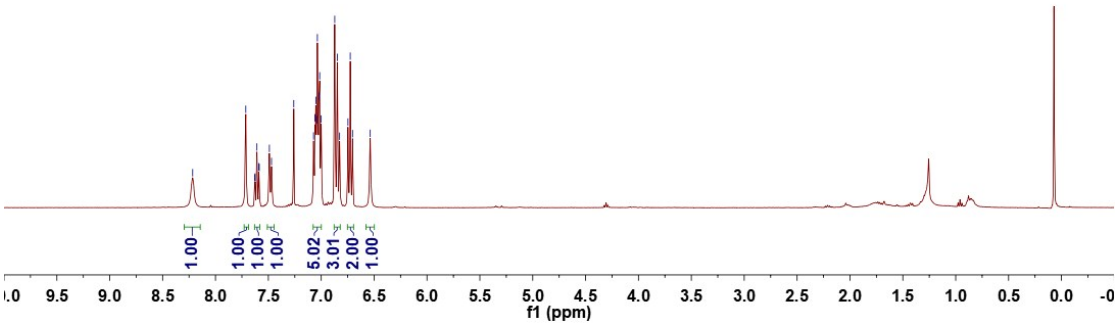
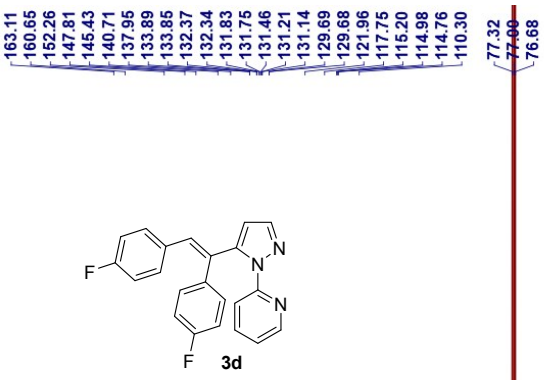
152.37
148.00
146.46
140.56
137.74
131.26
130.77
130.68
130.01
129.89
129.27
121.84
118.15
113.45
113.28
109.87
77.32
77.00
76.68
55.16
55.11
MeO
MeO
3c
f1 (ppm)


8.216
7.713
7.629
7.625
7.608
7.590
7.586
7.490
7.470
7.260
7.073
7.059
7.051
7.043
7.036
7.022
7.015
7.001
6.872
6.848
6.826
6.747
6.726
6.704
6.537

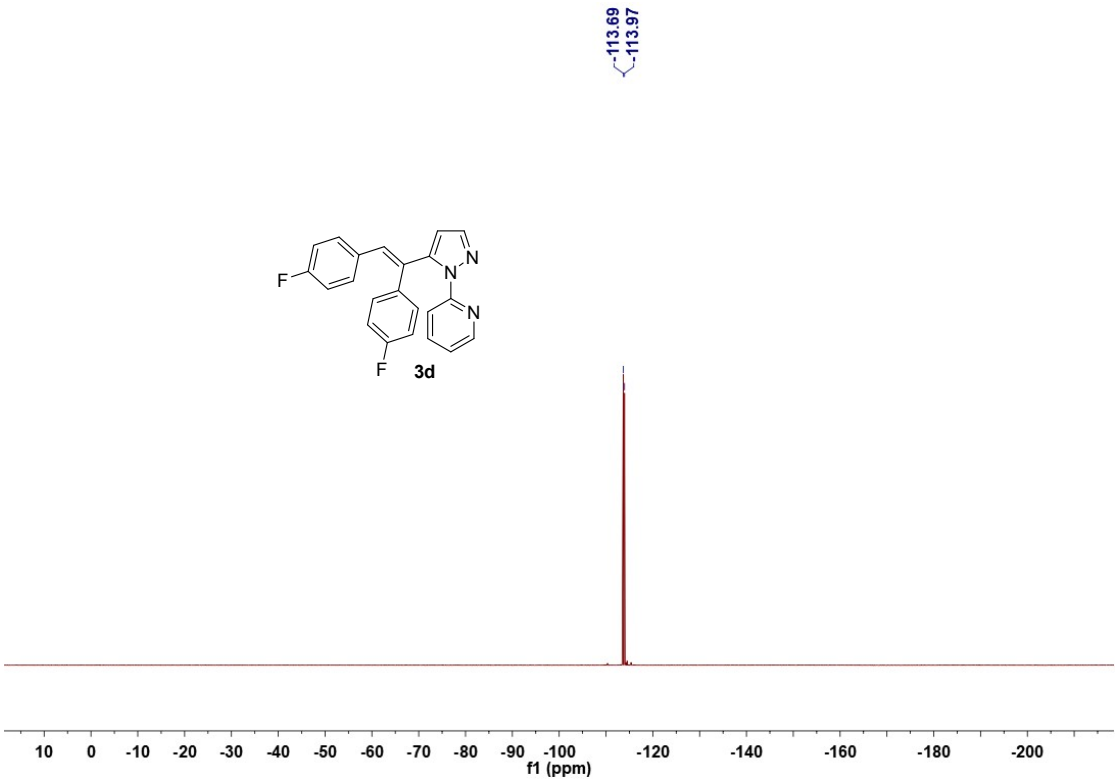

F
N
N
N
F
3d

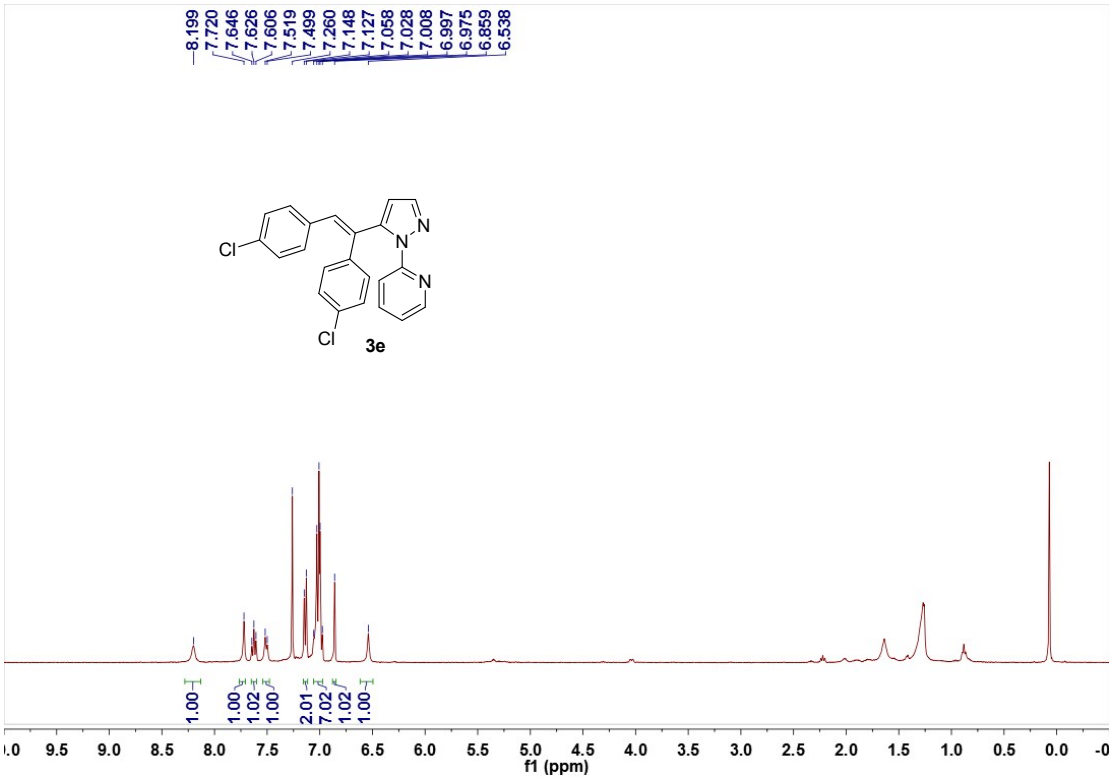

1.00
1.00
1.00
1.00
5.02
3.01
2.00
1.00
f1 (ppm)

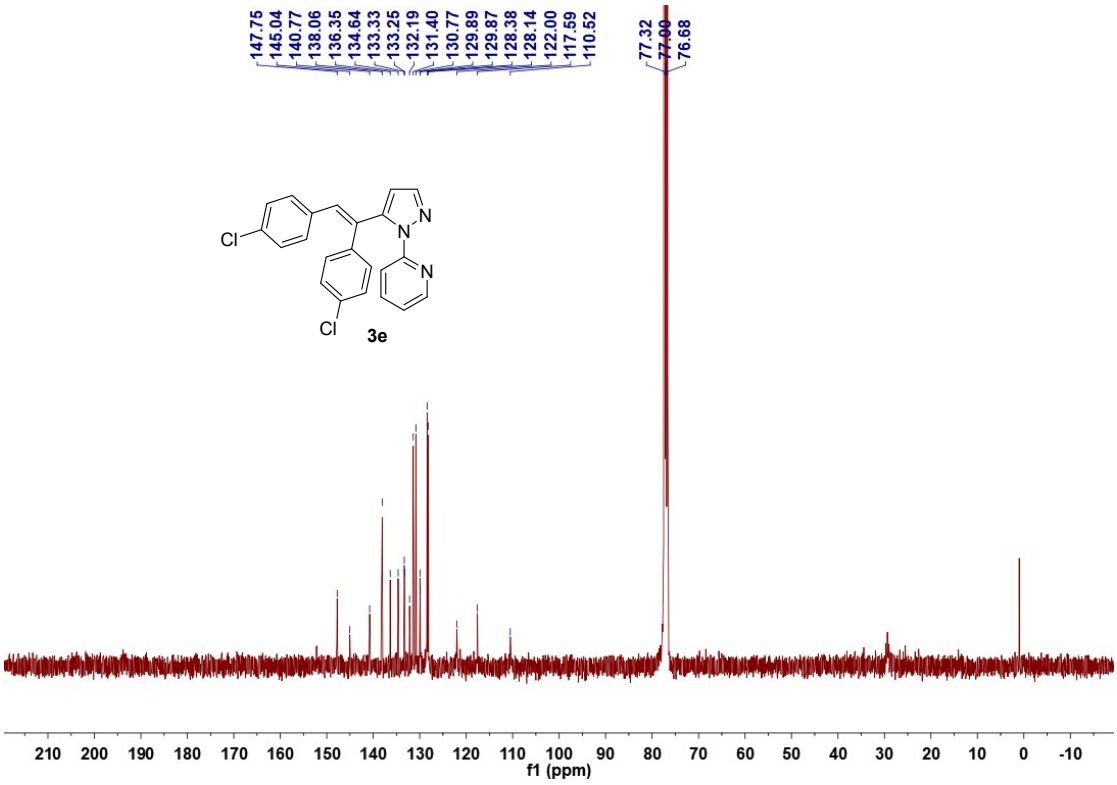

F
N
N
N
F
3d

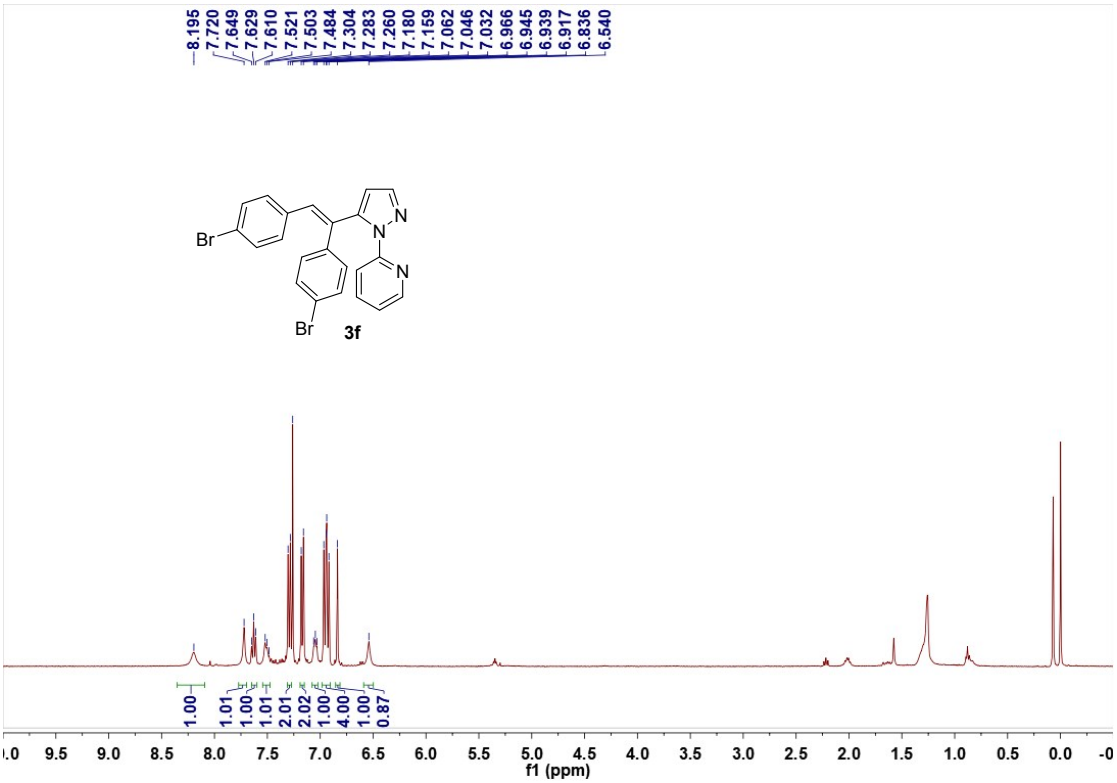
163.11
160.65
152.26
147.81
145.43
140.71
137.95
133.89
133.85
132.37
132.34
131.83
131.75
131.46
131.21
131.14
129.69
129.68
121.96
117.75
115.20
114.98
114.76
110.30
77.32
77.00
76.68
f1 (ppm)

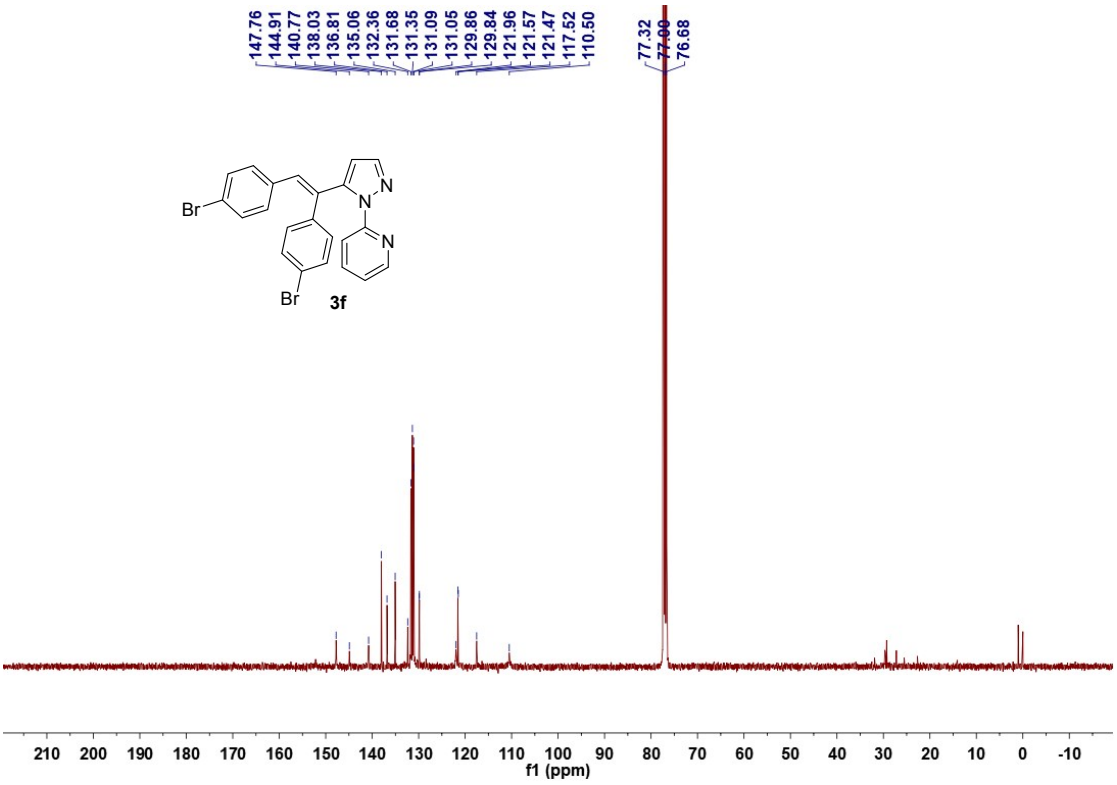
-

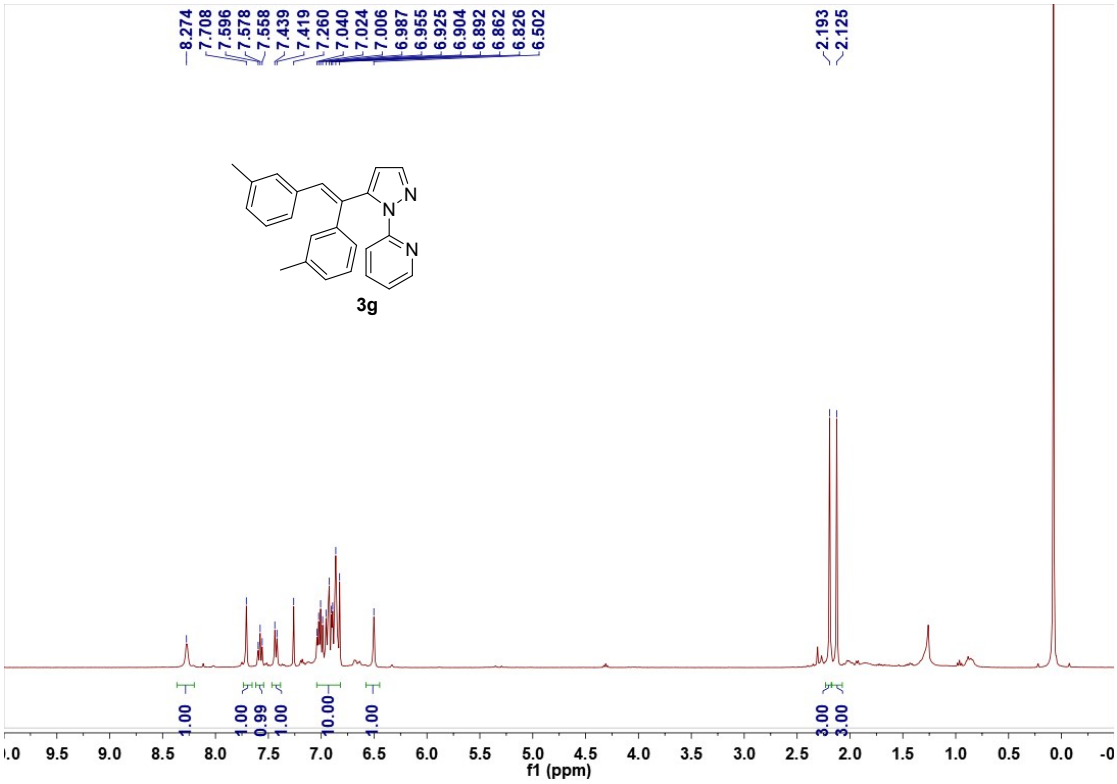

-113.69
-113.97
F
N
N
F
3d
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

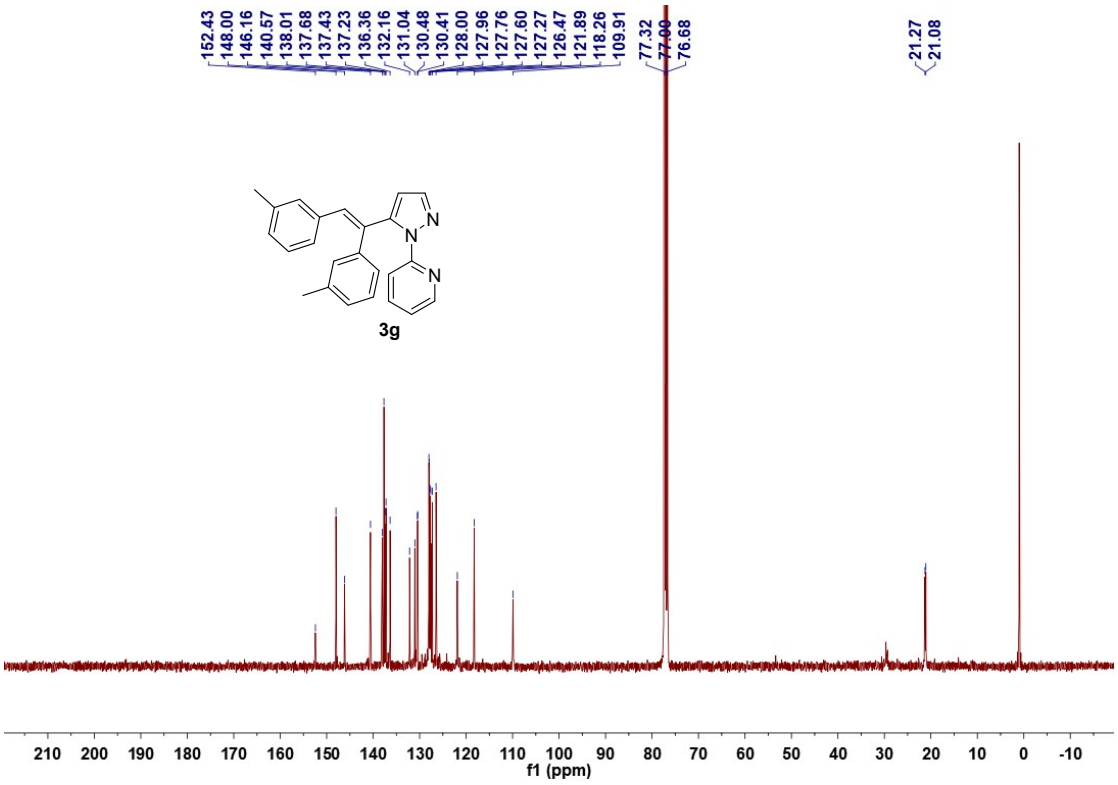

8.199
7.720
7.646
7.626
7.606
7.519
7.499
7.260
7.148
7.127
7.058
7.028
7.008
6.997
6.975
6.859
6.538
Cl
N
N
N
Cl
3e
1.00
1.00
1.02
1.00
2.01
7.02
1.02
1.00
f1 (ppm)

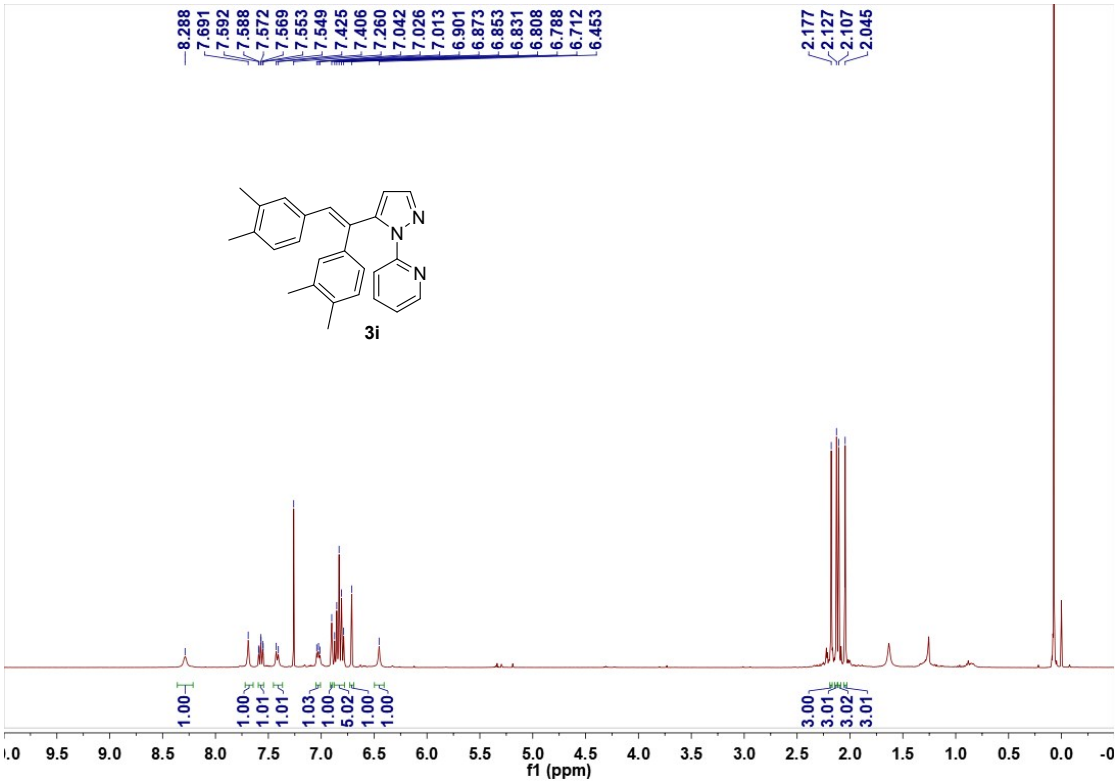

147.75
145.04
140.77
138.06
136.35
134.64
133.33
133.25
132.19
131.40
130.77
129.89
129.87
128.38
128.14
122.00
117.59
110.52
77.32
77.00
76.68
Cl
N
N
N
Cl
3e
f1 (ppm)

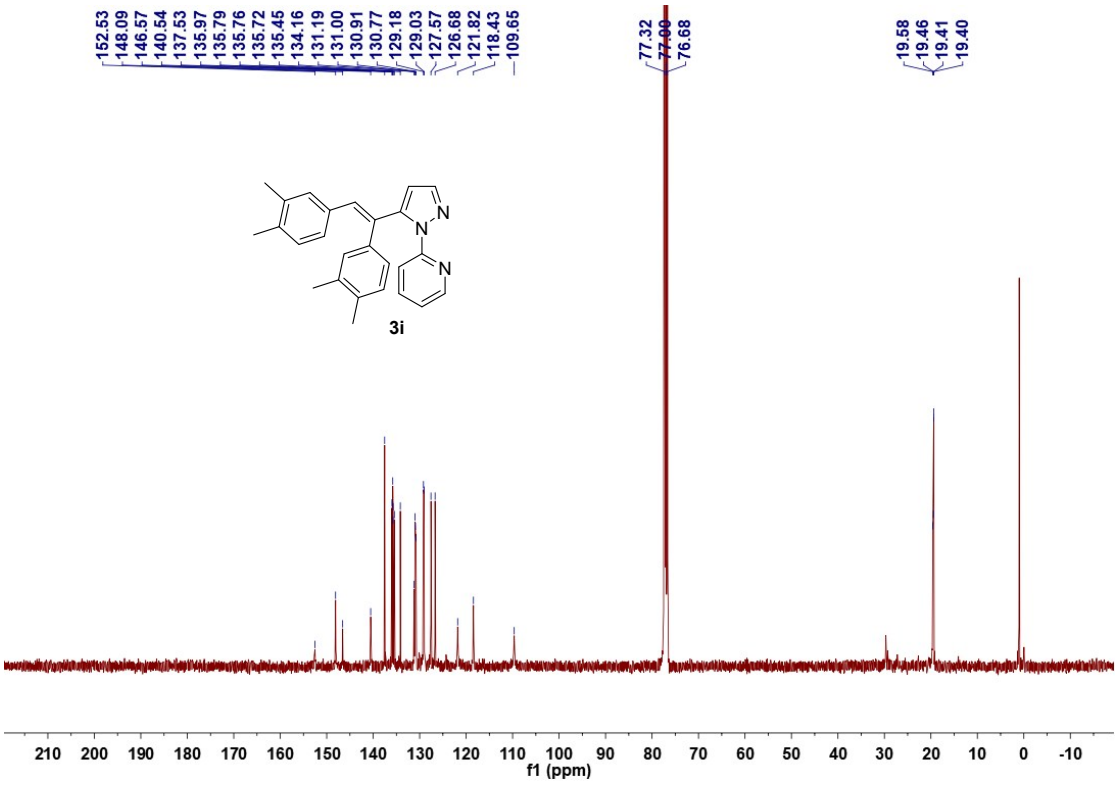

8.195
7.720
7.649
7.629
7.610
7.521
7.503
7.484
7.304
7.283
7.260
7.180
7.159
7.062
7.046
7.032
6.966
6.945
6.939
6.917
6.836
6.540
Br
N
N
N
Br
3f
1.00
1.01
1.00
1.01
2.01
2.02
1.00
4.00
1.00
0.87
f1 (ppm)

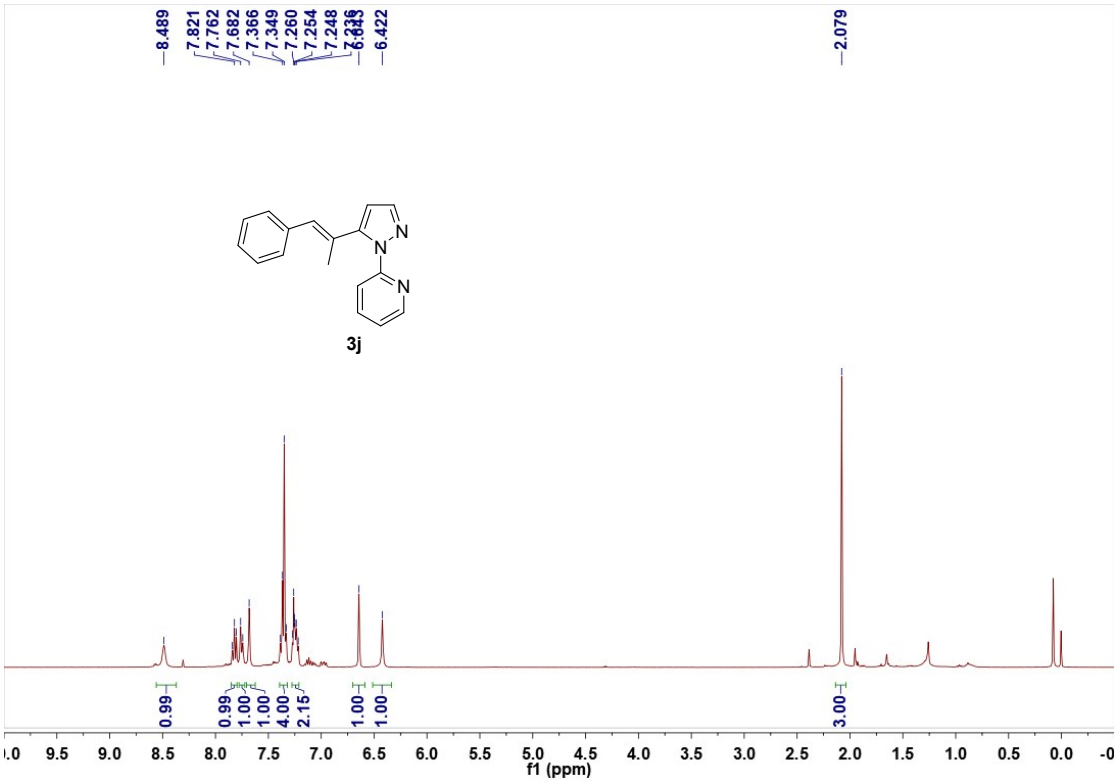

147.76
144.91
140.77
138.03
136.81
135.06
132.36
131.68
131.35
131.09
131.05
129.86
129.84
121.96
121.57
121.47
117.52
110.50
77.32
77.00
76.68
Br
N
N
N
Br
3f
f1 (ppm)

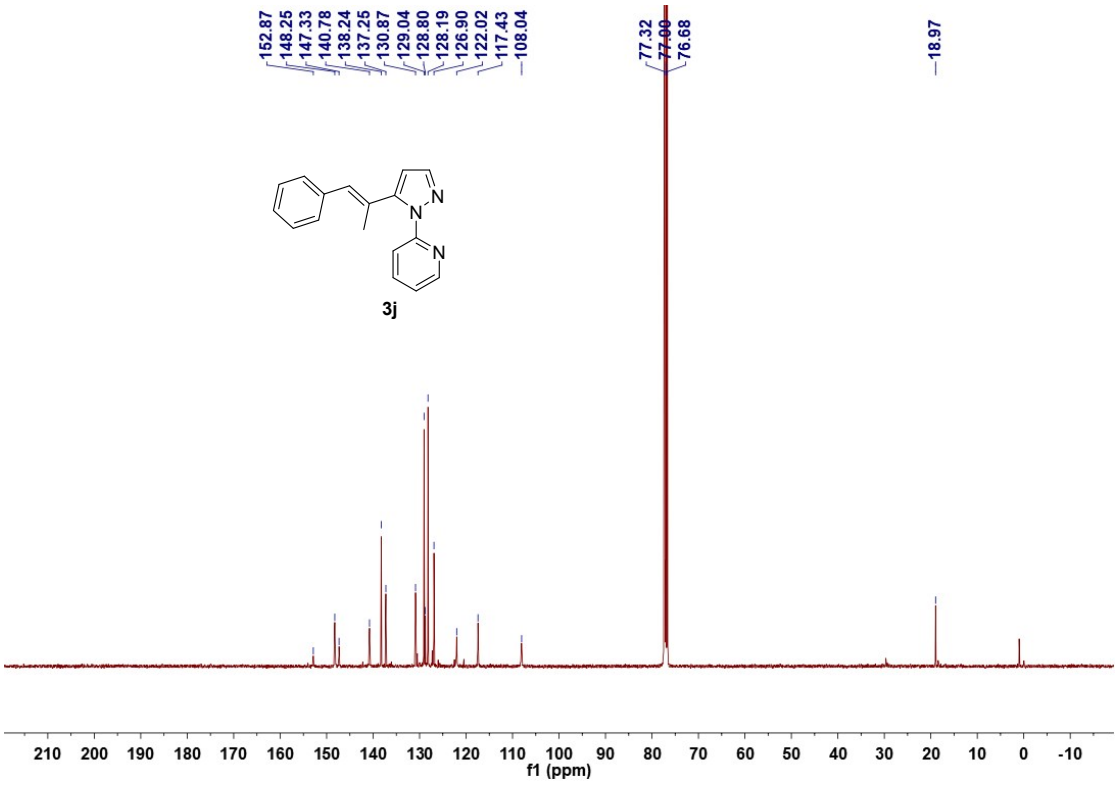

8.274
7.708
7.596
7.578
7.558
7.439
7.419
7.260
7.040
7.024
7.006
6.987
6.955
6.925
6.904
6.892
6.862
6.826
6.502
2.193
2.125
3g
1.00
1.00
0.99
1.00
10.00
1.00
3.00
3.00
f1 (ppm)

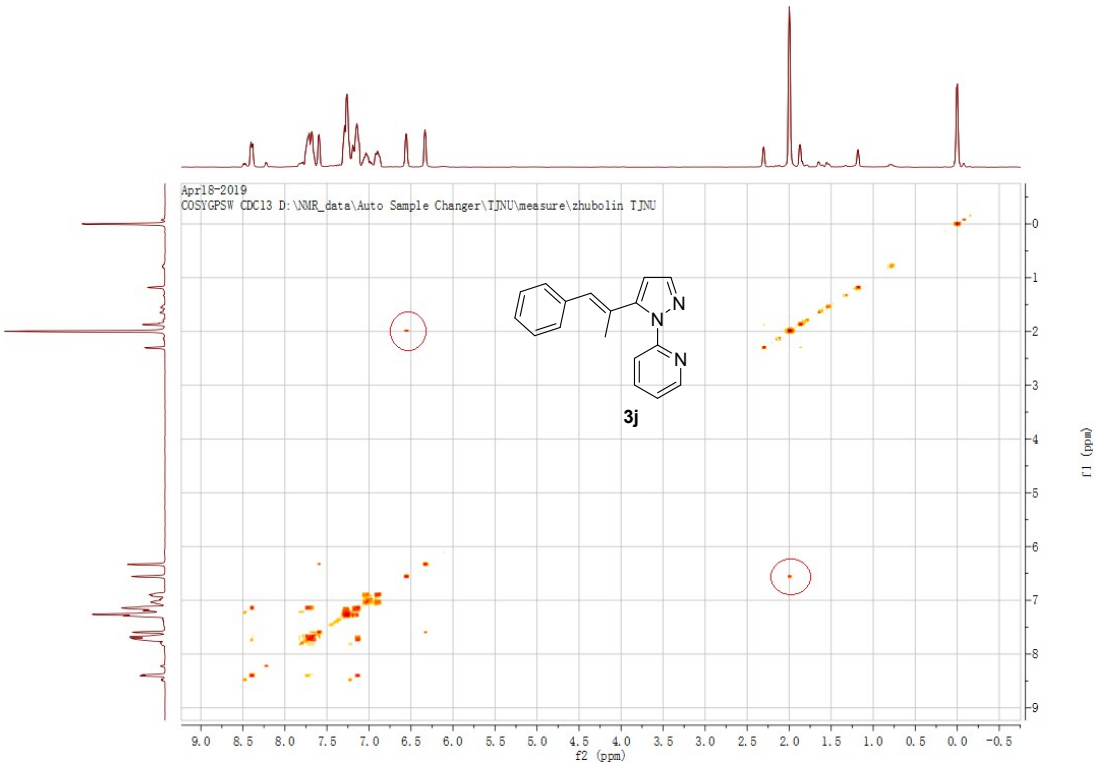

152.43
148.00
146.16
140.57
138.01
137.68
137.43
137.23
136.36
132.16
131.04
130.48
130.41
128.00
127.96
127.76
127.60
127.27
126.47
121.89
118.26
109.91
77.32
77.00
76.68
21.27
21.08
3g
f1 (ppm)

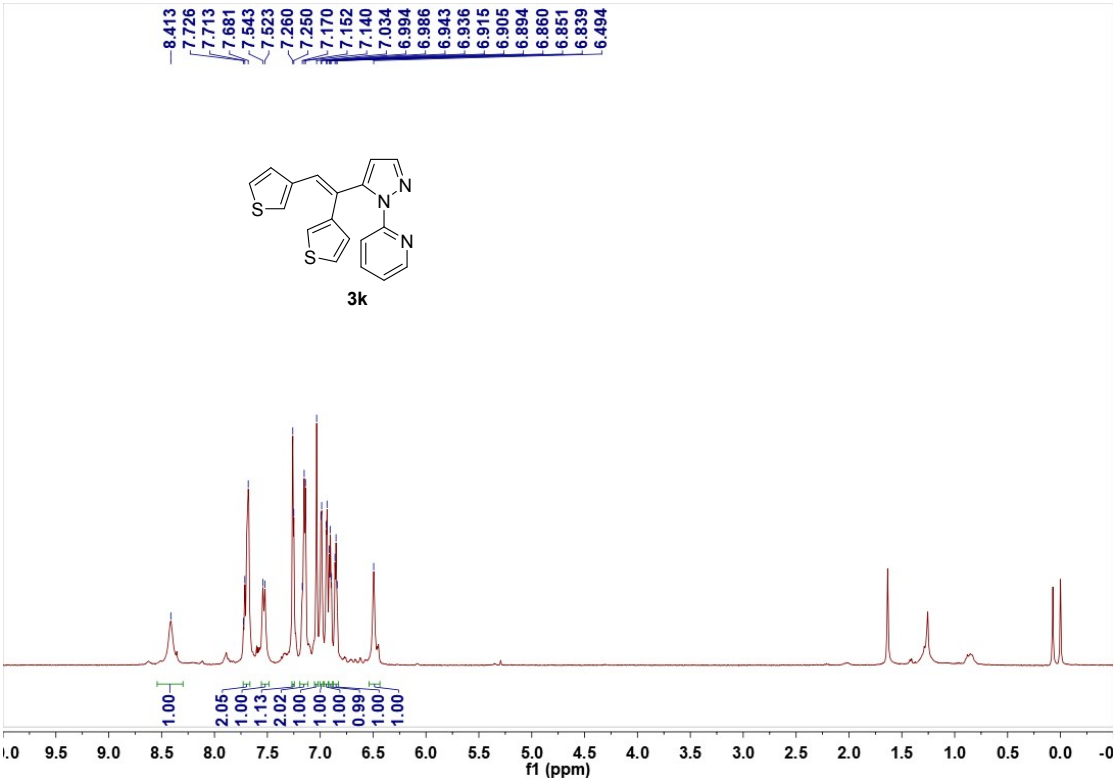

8.288
7.691
7.592
7.588
7.572
7.569
7.553
7.549
7.425
7.406
7.260
7.042
7.026
7.013
6.901
6.873
6.853
6.831
6.808
6.788
6.712
6.453
2.177
2.127
2.107
2.045
3i
1.00
1.00
1.01
1.01
1.03
1.00
5.02
1.00
1.00
3.00
3.01
3.02
3.01
f1 (ppm)

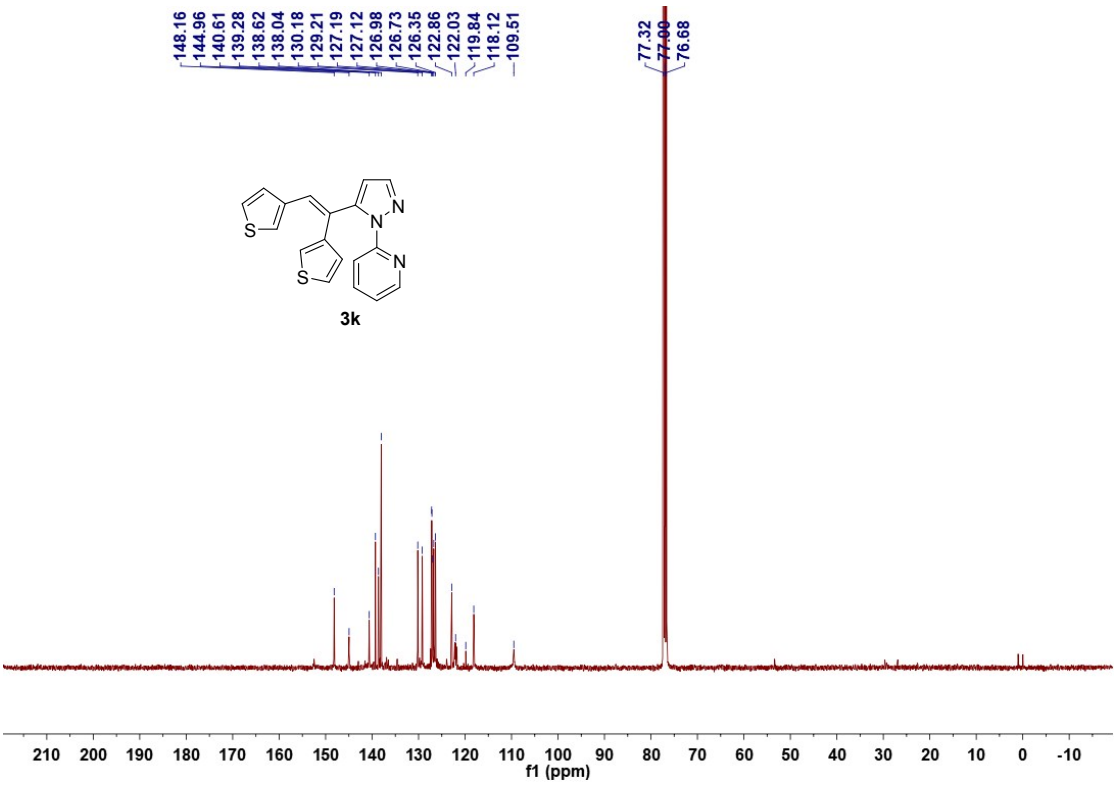

152.53
148.09
146.57
140.54
137.53
135.97
135.79
135.76
135.72
135.45
134.16
131.19
131.00
130.91
130.77
129.18
129.03
127.57
126.68
121.82
118.43
109.65
77.32
77.00
76.68
19.58
19.46
19.41
19.40
3i
f1 (ppm)


8.489
7.821
7.762
7.682
7.366
7.349
7.260
7.254
7.248
6.422
2.079
3j
0.99
0.99
1.00
1.00
4.00
2.15
1.00
1.00
3.00
f1 (ppm)


152.87
148.25
147.33
140.78
138.24
137.25
130.87
129.04
128.80
128.19
126.90
122.02
117.43
108.04
77.32
77.00
76.68
18.97
3j
f1 (ppm)


Apr18-2019
COSYGPSW CDC13 D:\\NMR_data\Auto Sample Changer\TJNU\measure\zhubolin TJNU
N
N
N
3j
f2 (ppm)
f1 (ppm)


8.413
7.726
7.713
7.681
7.543
7.523
7.260
7.250
7.170
7.152
7.140
7.034
6.994
6.986
6.943
6.936
6.915
6.905
6.894
6.860
6.851
6.839
6.494
S
N
N
S
N
3k
1.00
2.05
1.00
1.13
2.02
1.00
1.00
1.00
0.99
1.00
1.00
f1 (ppm)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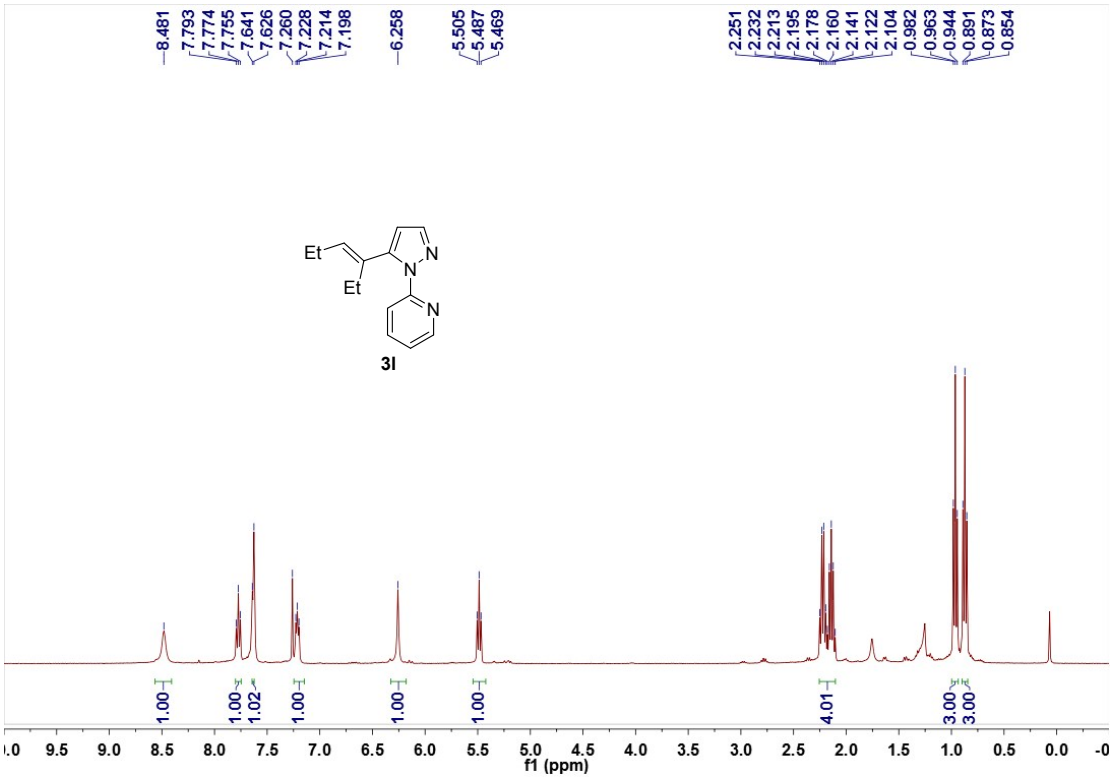
144.96
140.61
139.28
138.62
138.04
130.18
129.21
127.19
127.12
126.98
126.73
126.35
122.86
122.03
119.84
118.12
109.51
77.32
77.00
76.68
S
N
N
S
N
3k
f1 (ppm)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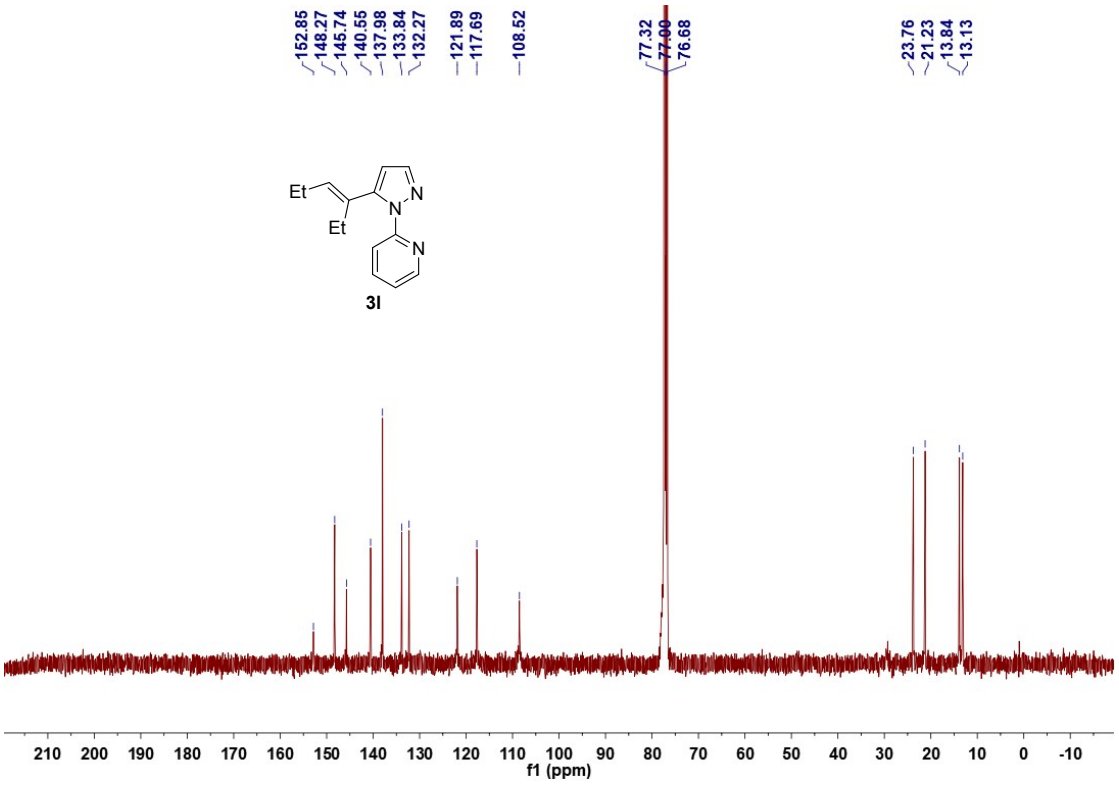
7.774
7.755
7.641
7.626
7.260
7.228
7.214
7.198
6.258
5.505
5.487
5.469
2.251
2.232
2.213
2.195
2.178
2.160
2.141
2.122
2.104
0.982
0.963
0.944
0.891
0.873
0.854
Et
Et
N
N
N
3l
1.00
1.00
1.02
1.00
1.00
1.00
4.01
3.00
3.00
f1 (ppm)


152.85
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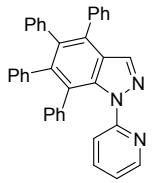
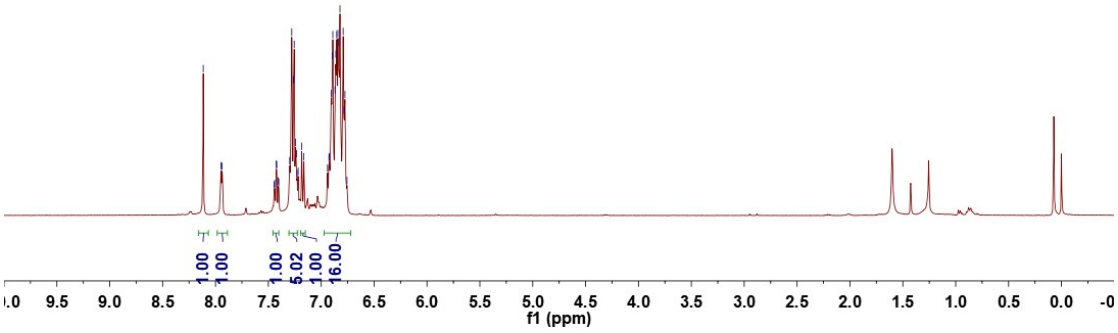
145.74
140.55
137.98
133.84
132.27
121.89
117.69
108.52
77.32
77.00
76.68
23.76
21.23
13.84
13.13
Et
Et
N
N
N
3l
f1 (ppm)


8.116
7.947
7.938
7.444
7.440
7.425
7.421
7.406
7.402
7.298
7.279
7.261
7.255
7.242
7.235
7.228
7.218
7.184
7.164
6.940
6.927
6.923
6.906
6.897
6.890
6.870
6.862
6.854
6.843
6.834
6.823
6.793
6.784
6.776
6.756


Ph
Ph
Ph
Ph
N
N
N

4a


1.00
1.00
1.00
5.02
1.00
16.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


152.39
147.92
141.43
139.88
138.70
137.55
137.53
136.91
136.62
135.15
133.54
131.92
131.62
130.62
130.52
127.76
126.87
126.80
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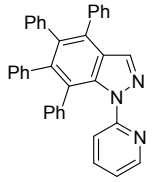
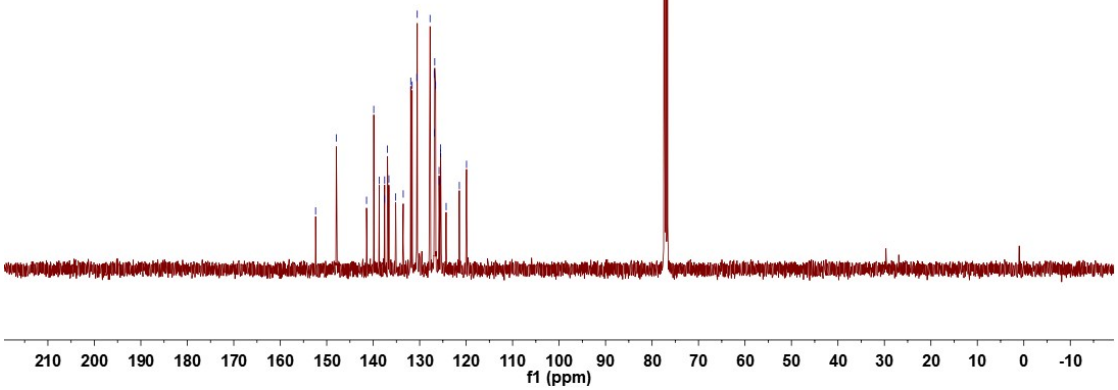
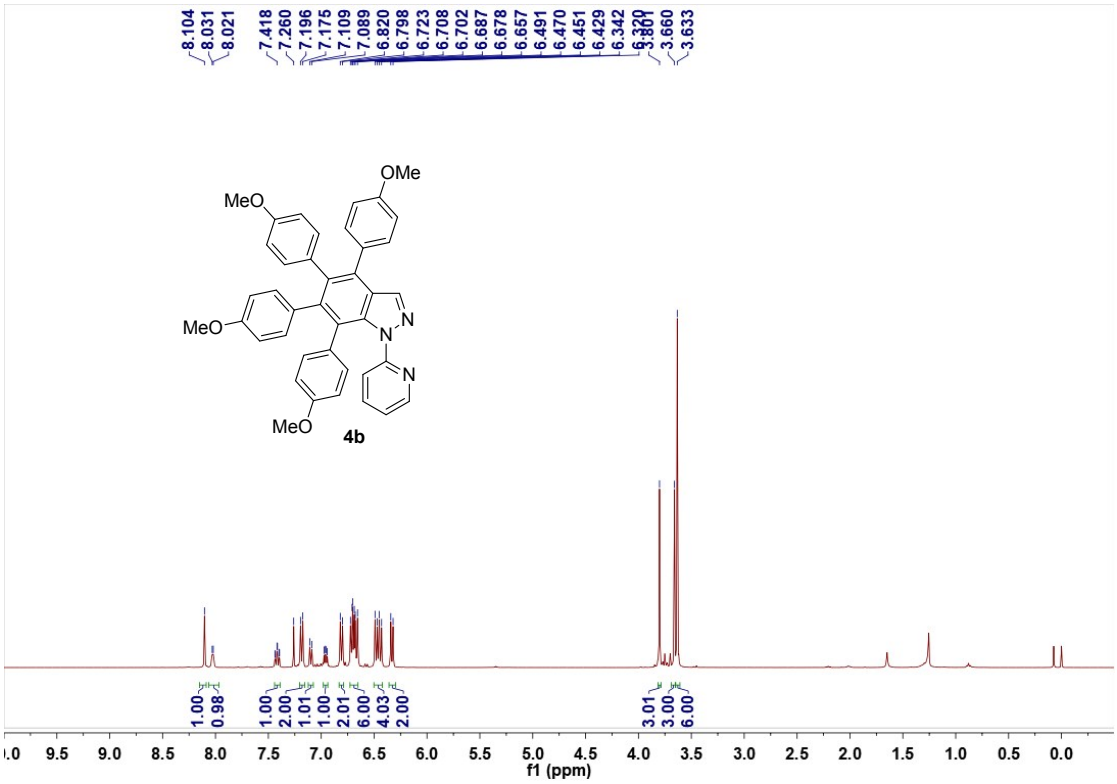
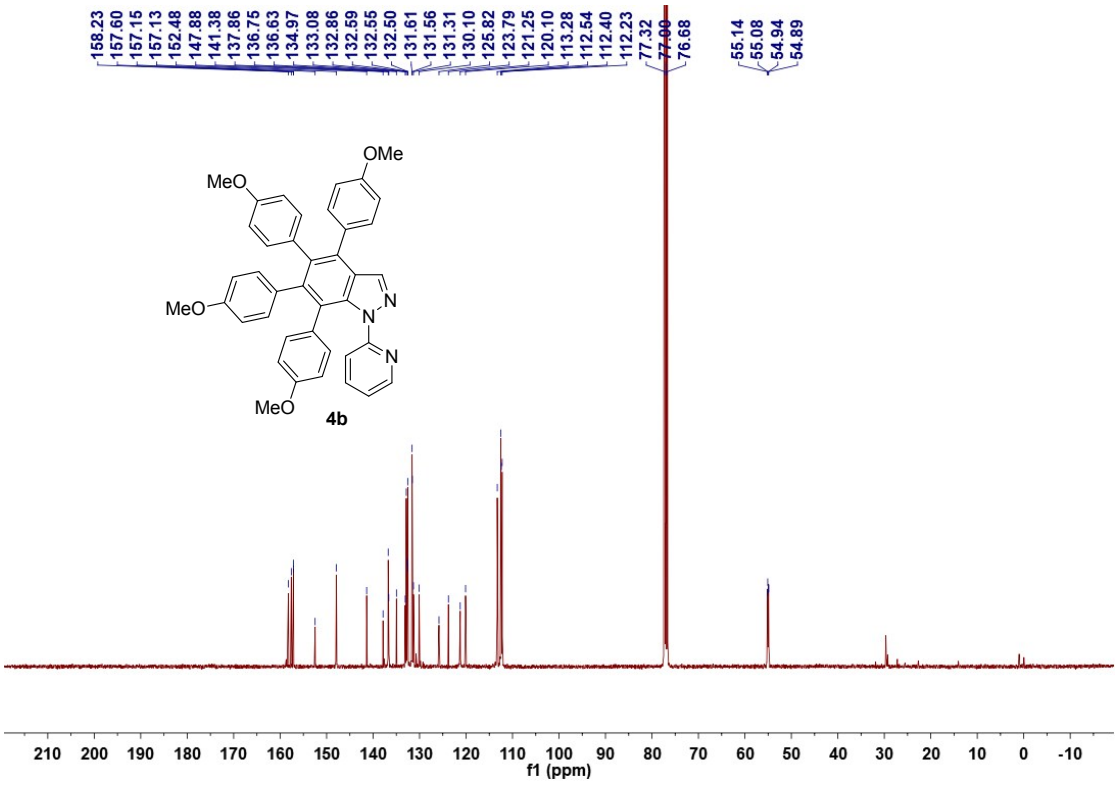
124.30
121.46
119.91
77.32
77.00
76.68

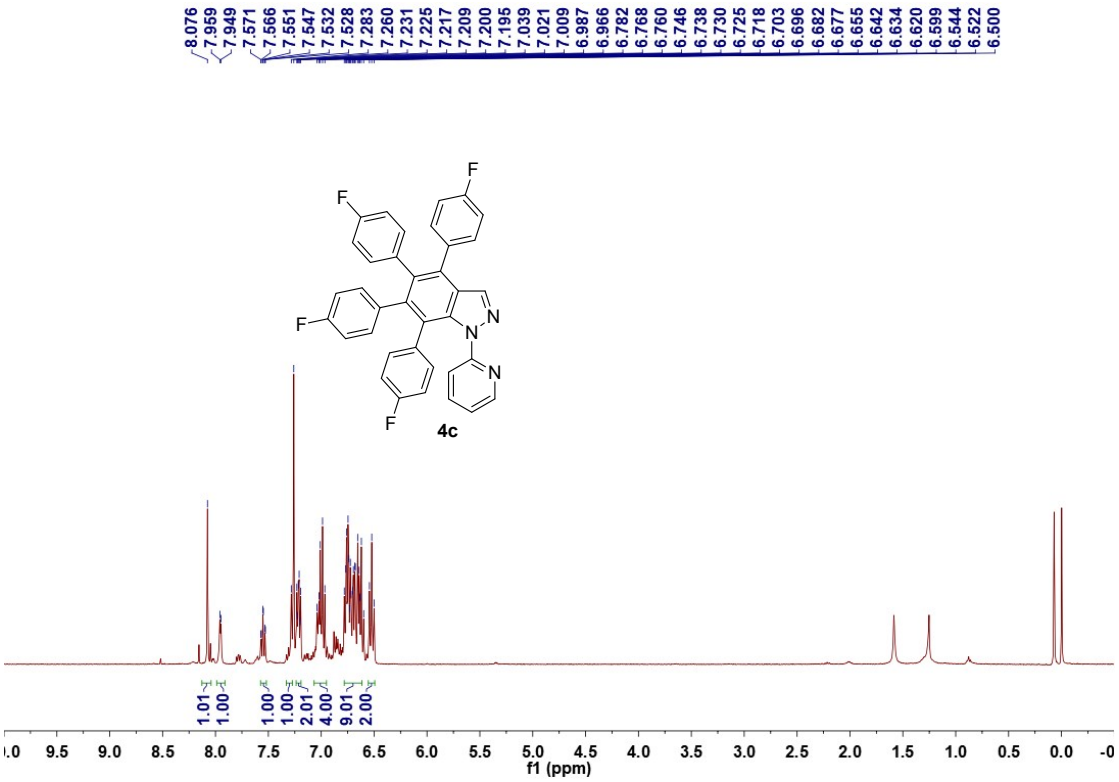

Ph
Ph
Ph
Ph
N
N
N

4a


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.104
8.031
8.021
7.418
7.260
7.196
7.175
7.109
7.089
6.820
6.798
6.723
6.708
6.702
6.687
6.678
6.657
6.491
6.470
6.451
6.429
6.342
3.801
3.660
3.633
OMe
MeO
MeO
MeO
N
N
N
4b
1.00
0.98
1.00
2.00
1.01
1.00
2.01
6.00
4.03
2.00
3.01
3.00
6.00
f1 (ppm)


158.23
157.60
157.15
157.13
152.48
147.88
141.38
137.86
136.75
136.63
134.97
133.08
132.86
132.59
132.55
132.50
131.61
131.56
131.31
130.10
125.82
123.79
121.25
120.10
113.28
112.54
112.40
112.23
77.32
77.00
76.68
55.14
55.08
54.94
54.89
OMe
MeO
MeO
MeO
N
N
N
4b
f1 (ppm)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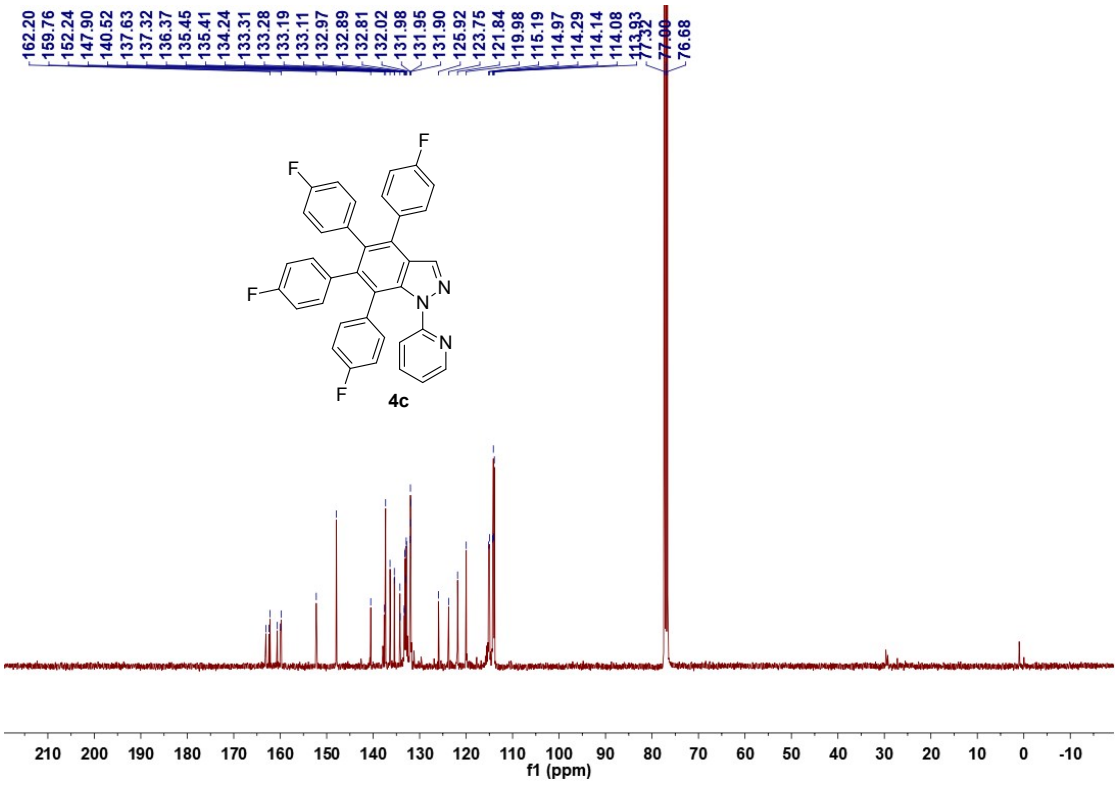
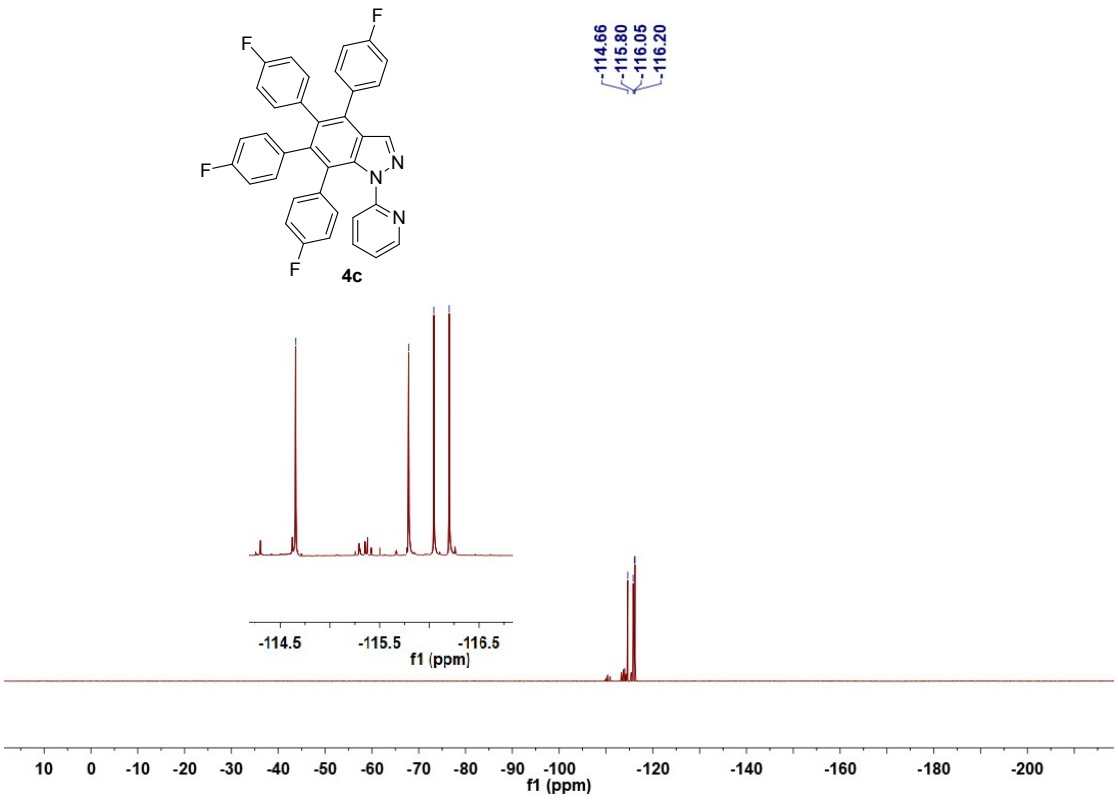
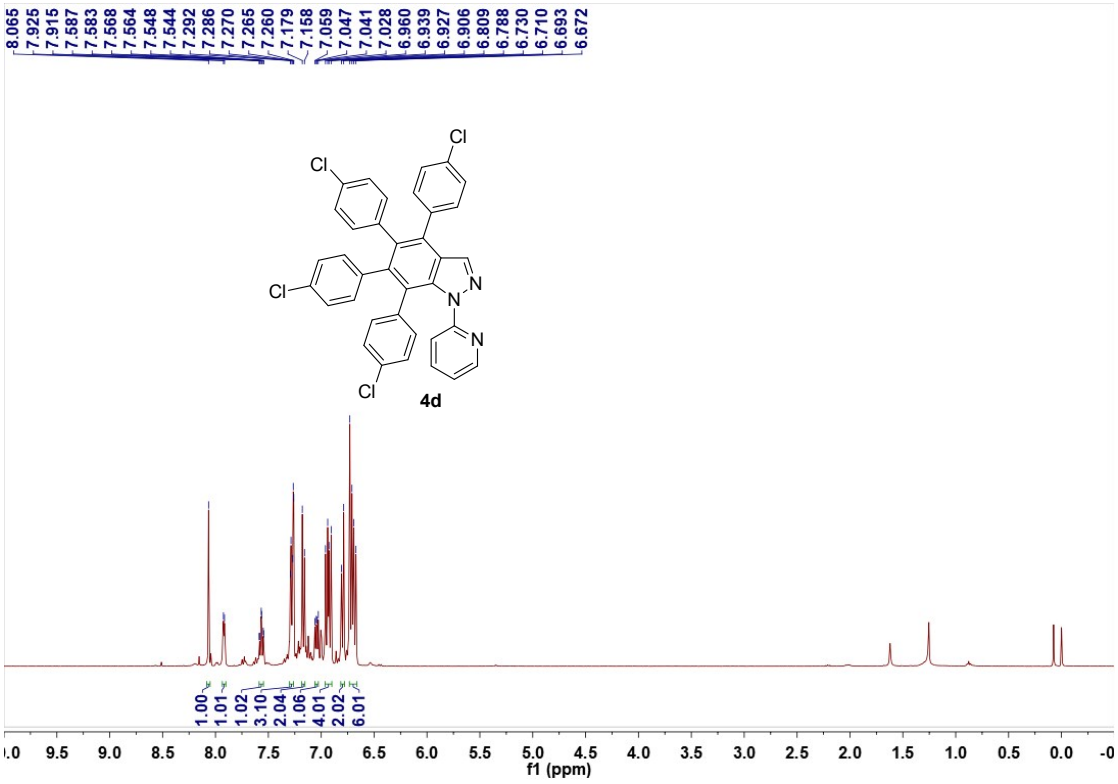
7.959
7.949
7.571
7.566
7.551
7.547
7.532
7.528
7.283
7.260
7.231
7.225
7.217
7.209
7.200
7.195
7.039
7.021
7.009
6.987
6.966
6.782
6.768
6.760
6.746
6.738
6.730
6.725
6.718
6.703
6.696
6.682
6.677
6.655
6.642
6.634
6.620
6.599
6.544
6.522
6.500
F
F
F
F
N
N
N
4c
1.01
1.00
1.00
1.00
2.01
4.00
9.01
2.00
f1 (ppm)


162.20
159.76
152.24
147.90
140.52
137.63
137.32
136.37
136.45
135.41
134.24
133.31
133.28
133.19
133.11
132.97
132.89
132.81
132.02
131.98
131.95
131.90
125.92
123.75
121.84
119.98
115.19
114.97
114.29
114.14
114.08
77.00
76.68
F
F
F
F
N
N
N
4c
f1 (ppm)


F
F
F
F
N
N
N
F
4c
-114.66
-115.80
-116.05
-116.20
-114.5
-115.5
-116.5
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)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7.915
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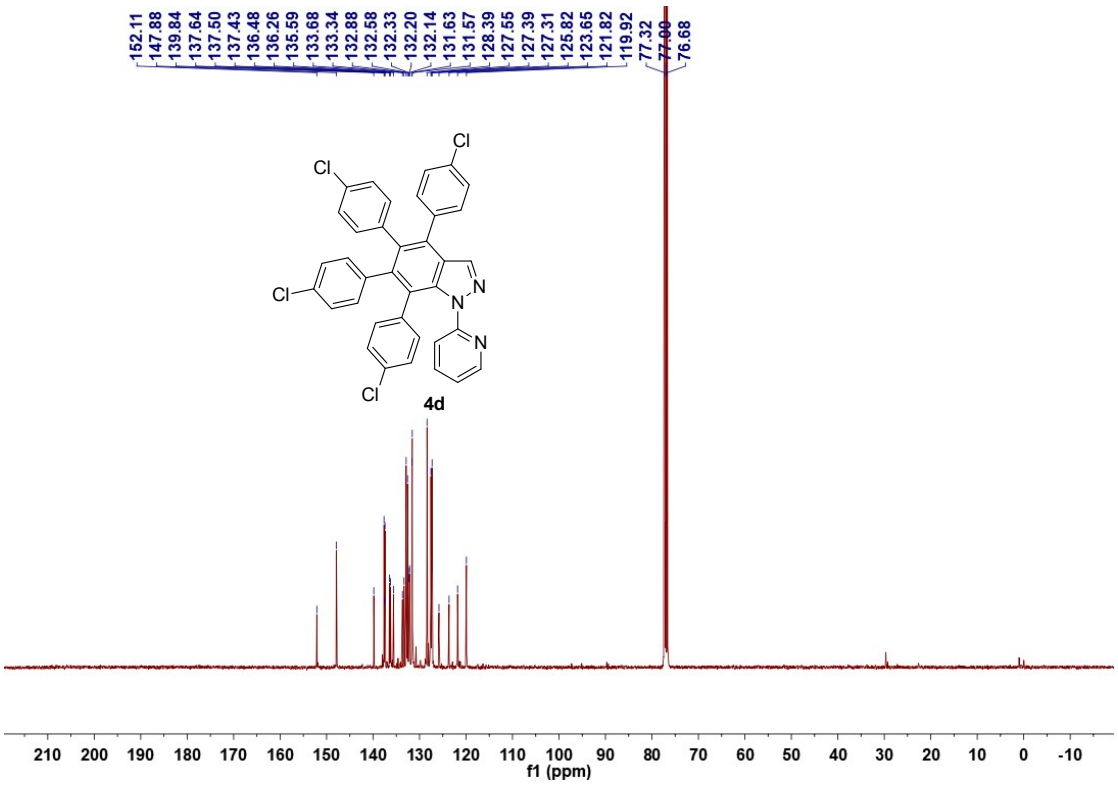
7.568
7.564
7.548
7.544
7.292
7.286
7.270
7.265
7.260
7.179
7.158
7.059
7.047
7.041
7.028
6.960
6.939
6.927
6.906
6.809
6.788
6.730
6.710
6.693
6.672
Cl
Cl
Cl
Cl
N
N
N
Cl
4d
1.00
1.01
1.02
3.10
2.04
1.06
4.01
2.02
6.01
f1 (ppm)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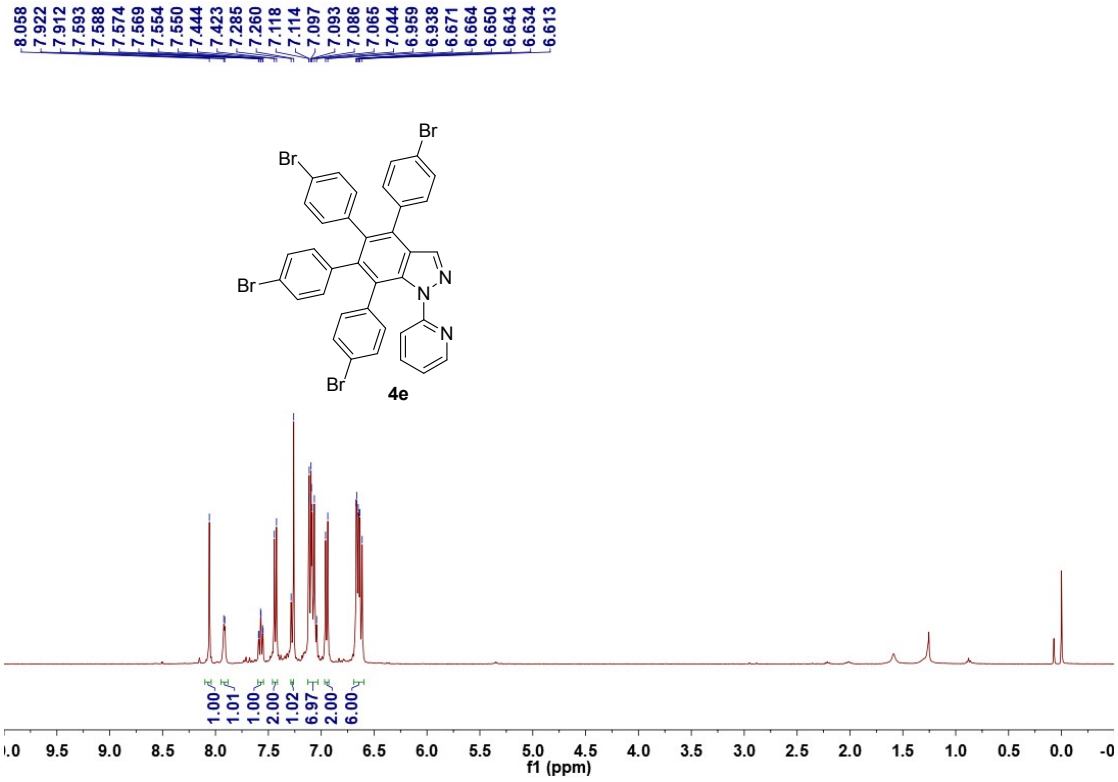
139.84
137.64
137.50
137.43
136.48
136.26
135.59
133.68
133.34
132.88
132.58
132.33
132.20
132.14
131.63
131.57
128.39
127.55
127.39
127.31
125.82
123.65
121.82
119.92
77.32
77.00
76.68
Cl
Cl
Cl
Cl
N
N
N
Cl
4d
f1 (ppm)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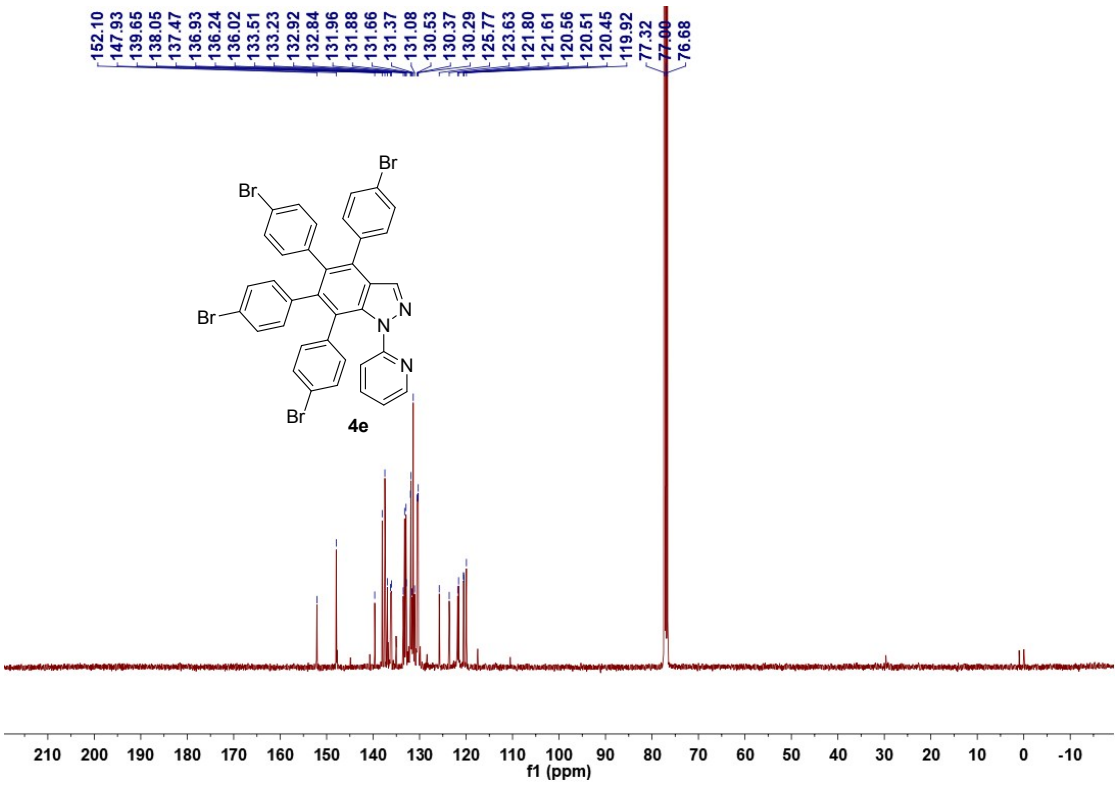
7.922
7.912
7.593
7.588
7.574
7.569
7.554
7.550
7.444
7.423
7.285
7.260
7.118
7.114
7.097
7.093
7.086
7.065
7.044
6.959
6.938
6.671
6.664
6.650
6.643
6.634
6.613
Br
Br
Br
Br
N
N
N
4e
1.00
1.01
1.00
2.00
1.02
6.97
2.00
6.00
f1 (ppm)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137.47
136.93
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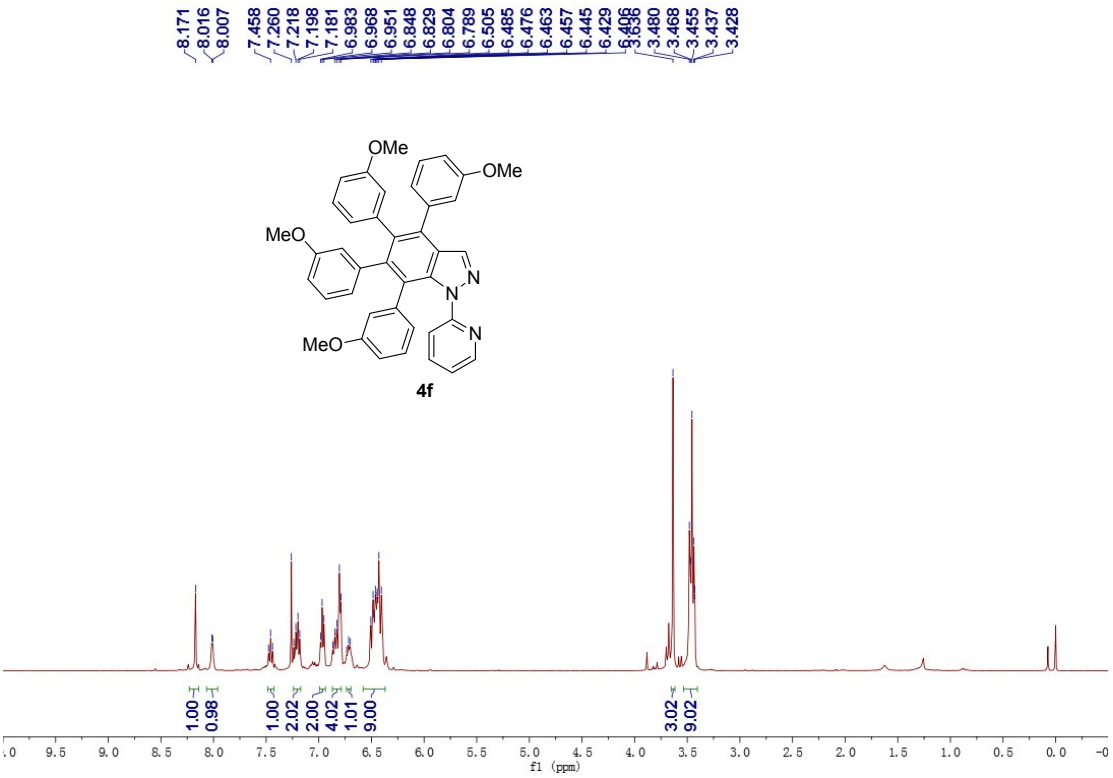
136.02
133.51
133.23
132.92
132.84
131.96
131.88
131.66
131.37
131.08
130.53
130.37
130.29
125.77
123.63
121.80
121.61
120.56
120.51
120.45
119.92
77.32
77.00
76.68
Br
Br
Br
Br
N
N
N
4e
f1 (ppm)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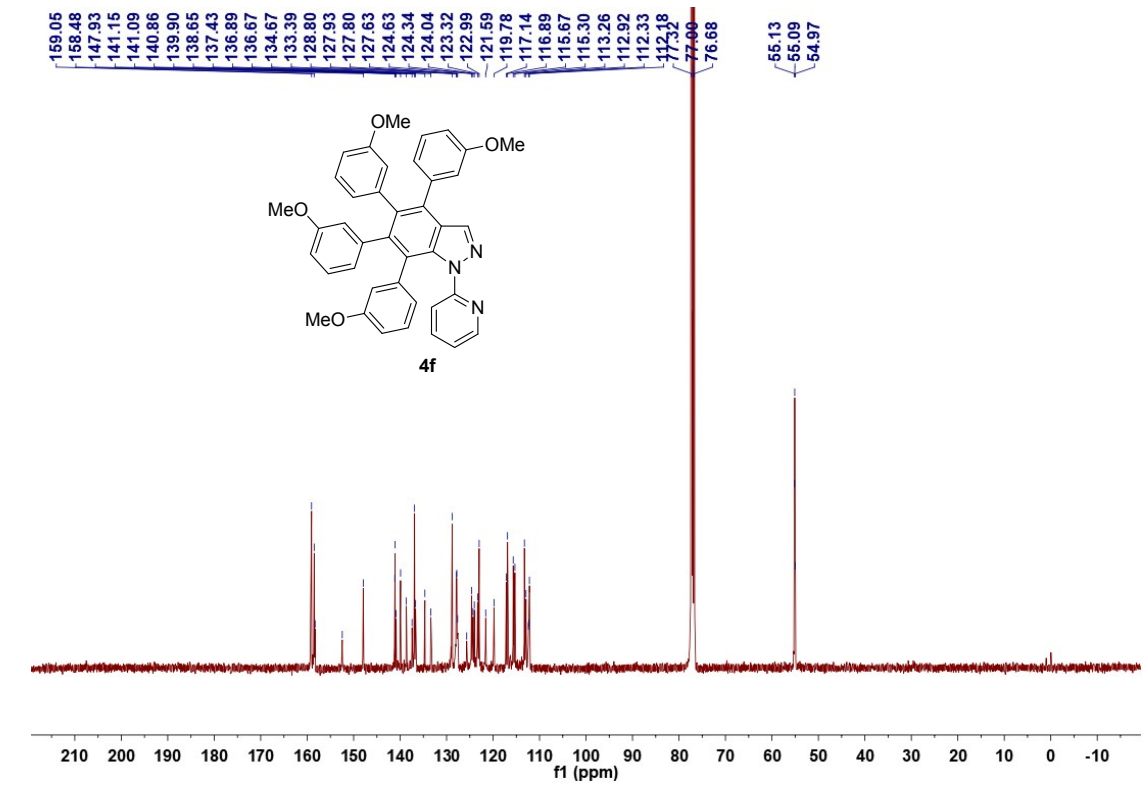
8.016
8.007
7.458
7.260
7.218
7.198
7.181
6.983
6.968
6.951
6.848
6.829
6.804
6.789
6.505
6.485
6.476
6.463
6.457
6.445
6.429
3.480
3.468
3.455
3.437
3.428
OMe
OMe
MeO
MeO
N
N
N
4f
1.00
0.98
1.00
2.02
2.00
4.02
1.01
9.00
3.02
9.02
f1 (ppm)


159.05
158.48
147.93
141.15
141.09
140.86
139.90
138.65
137.43
136.89
136.67
134.67
133.39
128.80
127.93
127.80
127.63
124.63
124.34
124.04
123.32
122.99
121.59
119.78
117.14
116.89
115.67
115.30
113.26
112.92
112.33
112.18
77.32
77.00
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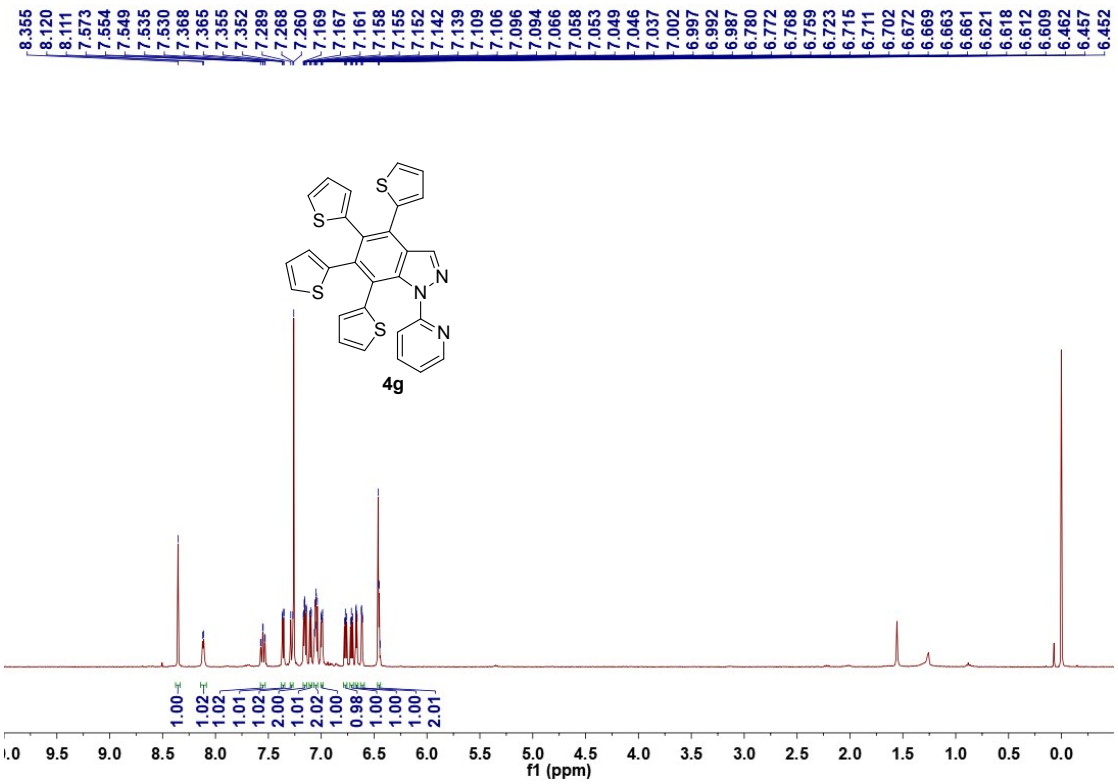
55.09
54.97
OMe
OMe
MeO
MeO
N
N
N
4f
f1 (ppm)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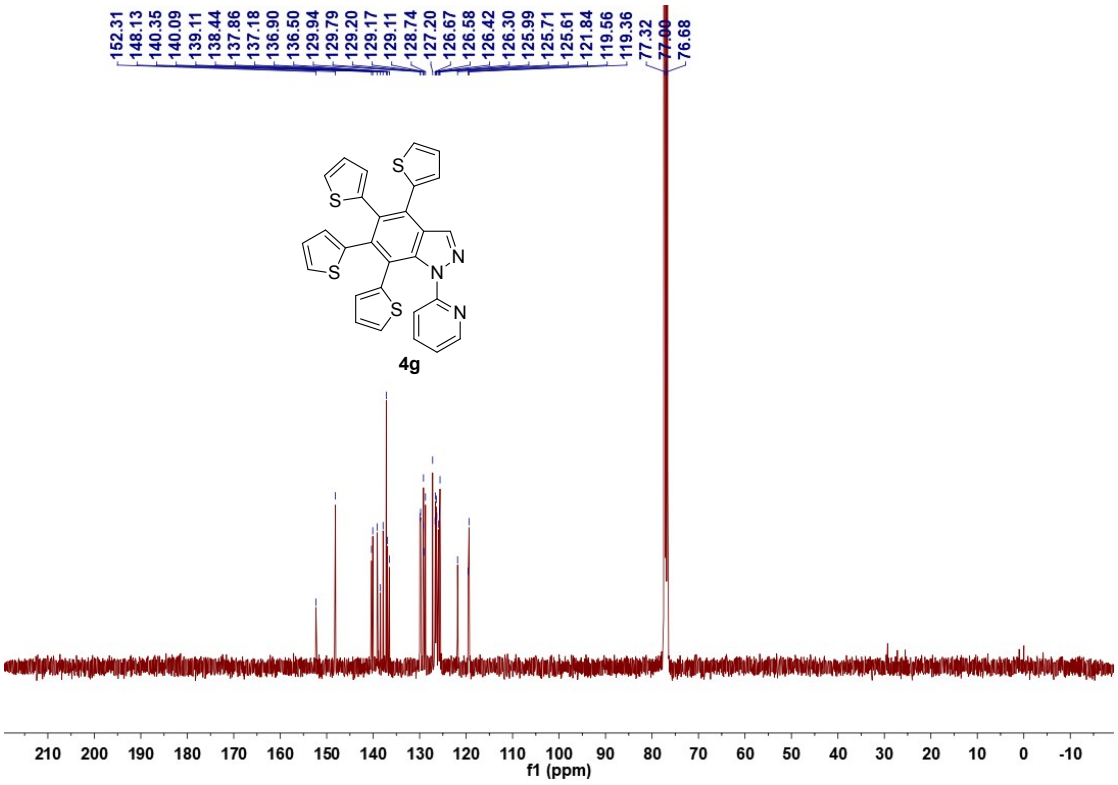
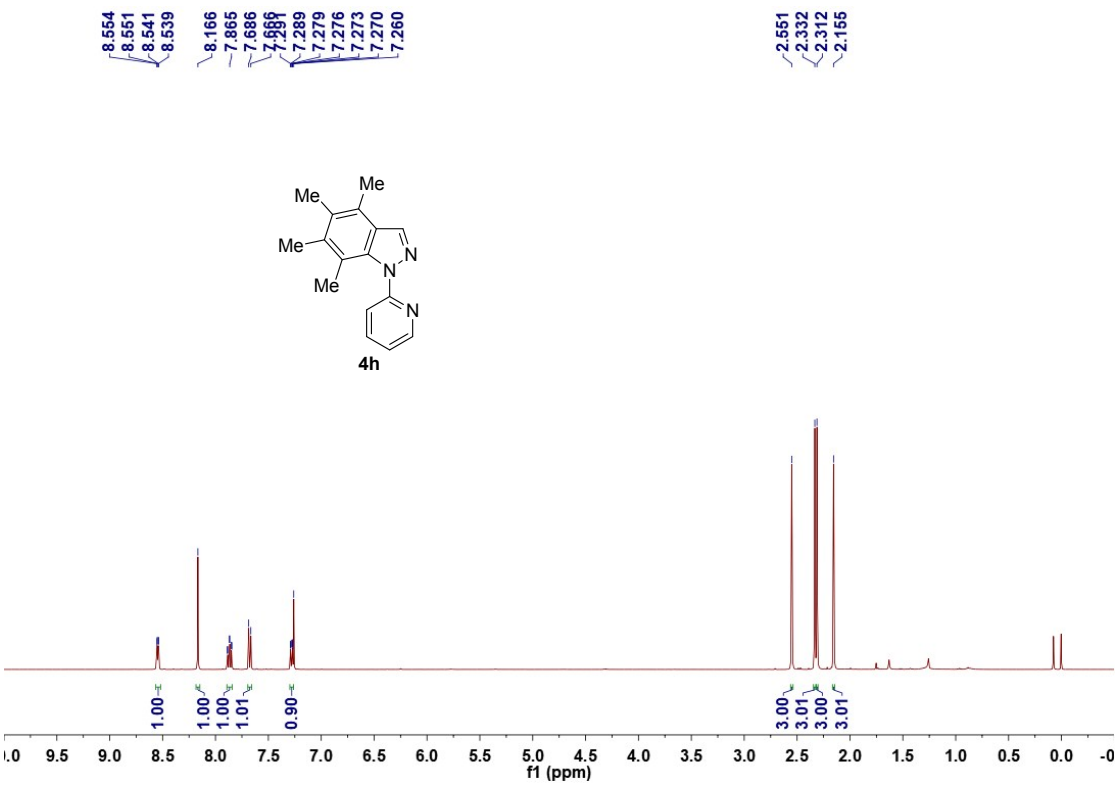
8.111
7.573
7.554
7.549
7.535
7.530
7.368
7.365
7.355
7.352
7.289
7.268
7.260
7.169
7.167
7.161
7.158
7.155
7.152
7.142
7.139
7.109
7.106
7.096
7.094
7.066
7.058
7.053
7.049
7.046
7.037
7.002
6.997
6.992
6.987
6.780
6.772
6.768
6.759
6.723
6.715
6.711
6.702
6.672
6.669
6.663
6.661
6.621
6.618
6.612
6.609
6.462
6.457
6.452
4g
1.00
1.02
1.02
1.01
1.02
2.00
1.01
2.02
1.00
0.98
1.00
1.00
1.00
2.01
f1 (ppm)


152.31
148.13
140.35
140.09
139.11
138.44
137.86
137.18
136.90
136.50
129.94
129.79
129.20
129.17
129.11
128.74
127.20
126.67
126.58
126.42
126.30
125.99
125.71
125.61
121.84
119.56
119.36
77.32
77.00
76.68
4g
f1 (ppm)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8.551
8.541
8.539
8.166
7.865
7.686
7.289
7.279
7.276
7.273
7.270
7.260
2.551
2.332
2.312
2.155
Me
Me
Me
Me
N
N
4h
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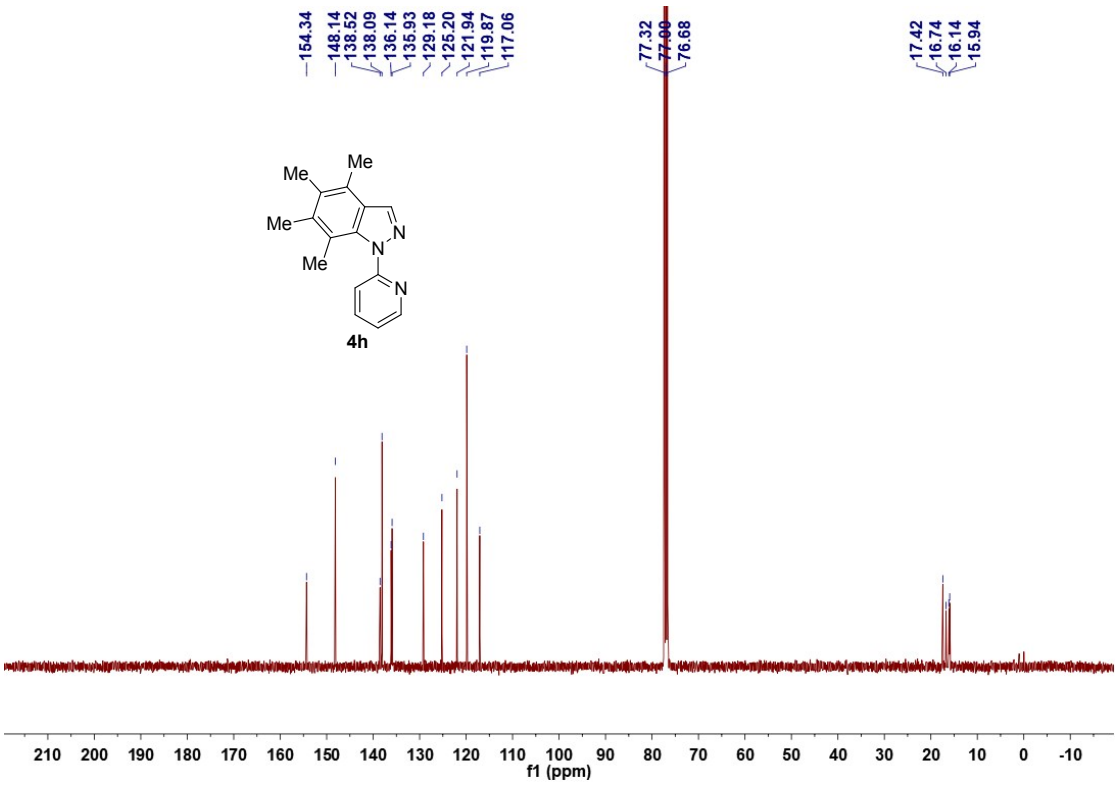
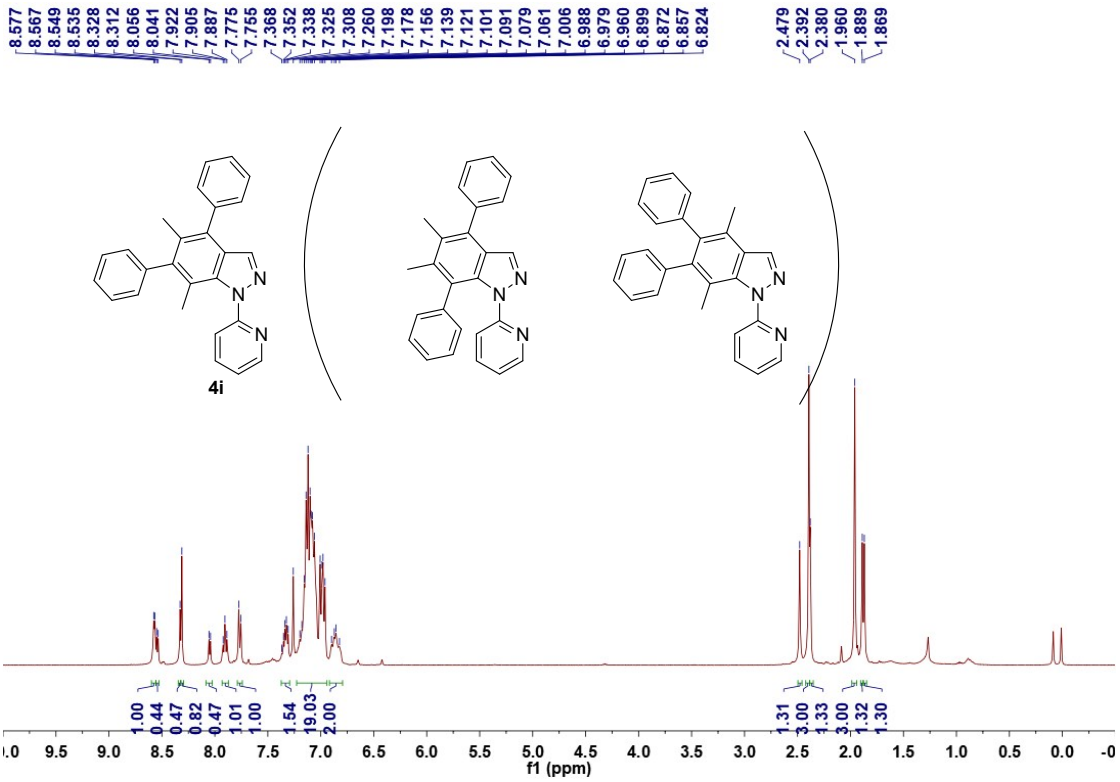
1.00
1.00
1.01
0.90
3.00
3.01
3.00
3.01
f1 (ppm)


154.34
148.14
138.52
138.09
136.14
135.93
129.18
125.20
121.94
119.87
117.06
77.32
77.00
76.68
17.42
16.74
16.14
15.94
Me
Me
Me
Me
N
N
4h
f1 (ppm)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8.549
8.535
8.328
8.312
8.056
8.041
7.922
7.905
7.887
7.775
7.755
7.368
7.352
7.338
7.325
7.308
7.260
7.198
7.178
7.156
7.139
7.121
7.101
7.091
7.079
7.061
7.006
6.988
6.979
6.960
6.899
6.872
6.857
6.824
2.479
2.392
2.380
1.960
1.889
1.869
4i
1.00
0.44
0.47
0.82
0.47
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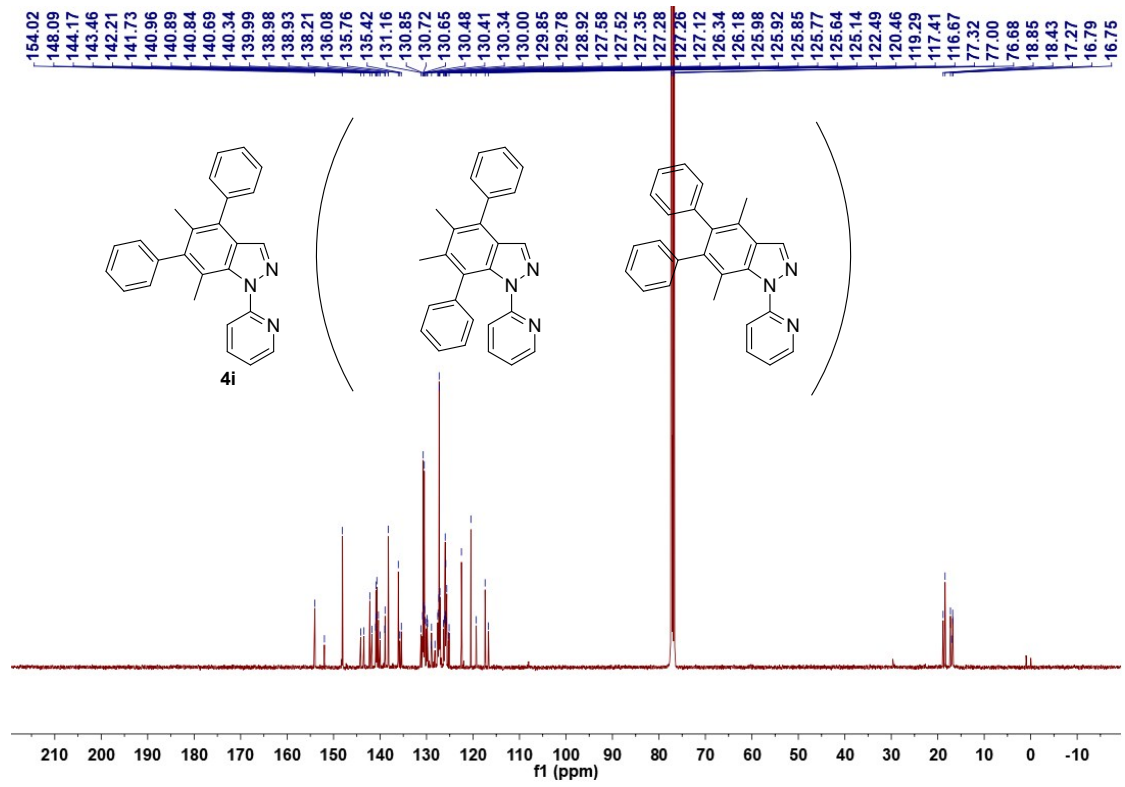
1.00
1.54
19.03
2.00
1.31
3.00
1.33
3.00
1.32
1.30
f1 (ppm)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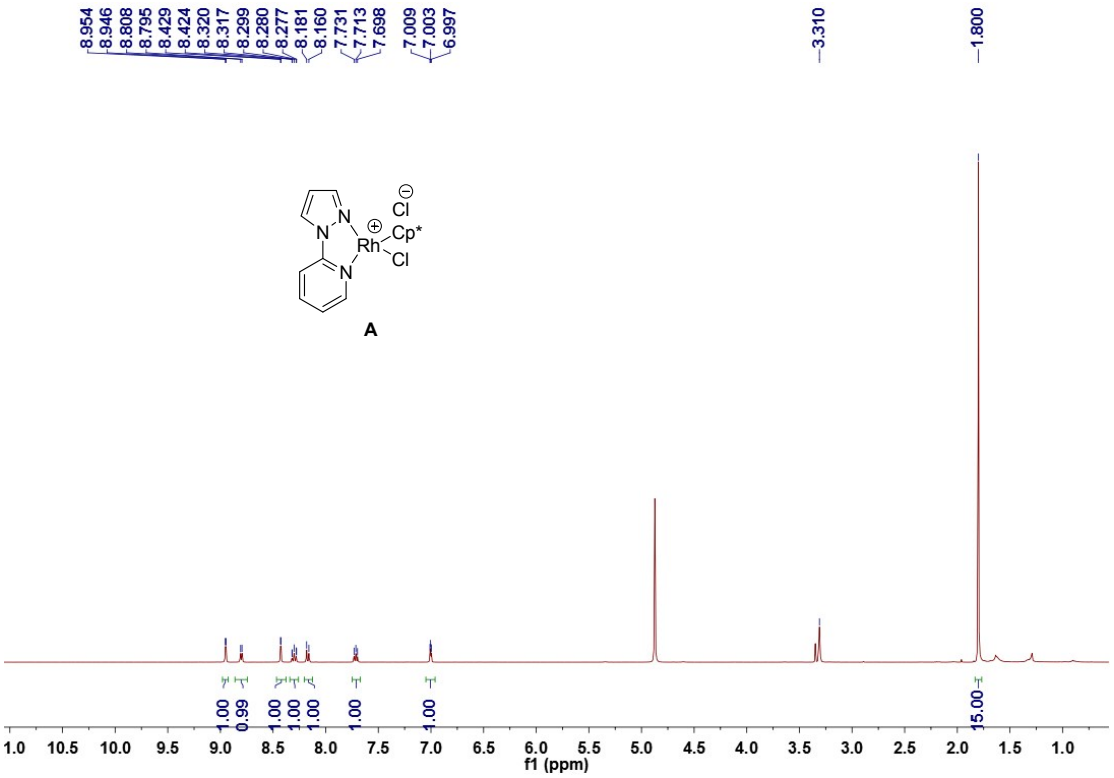
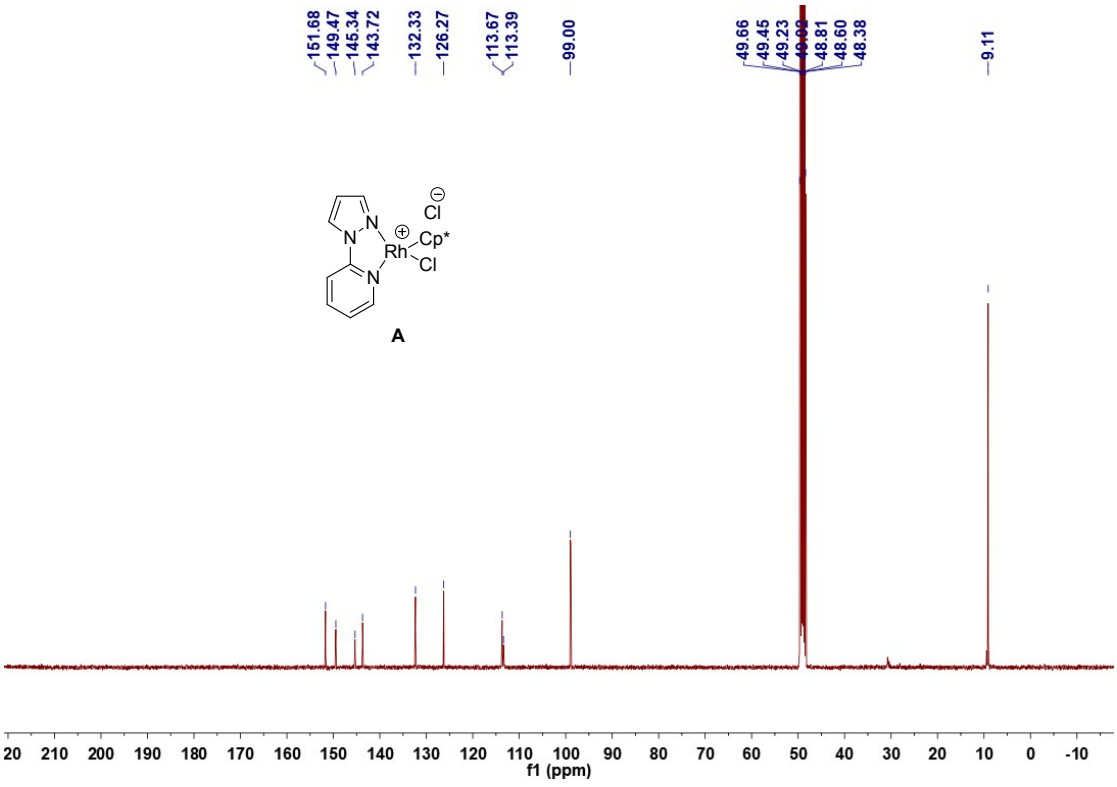
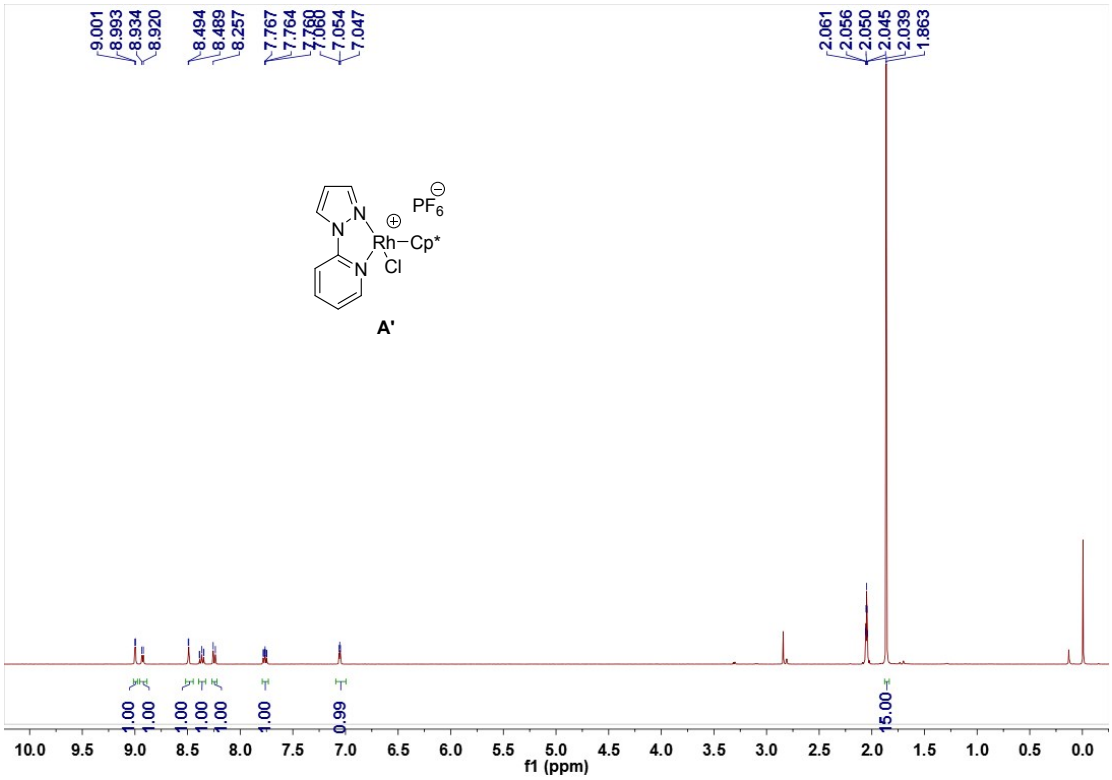
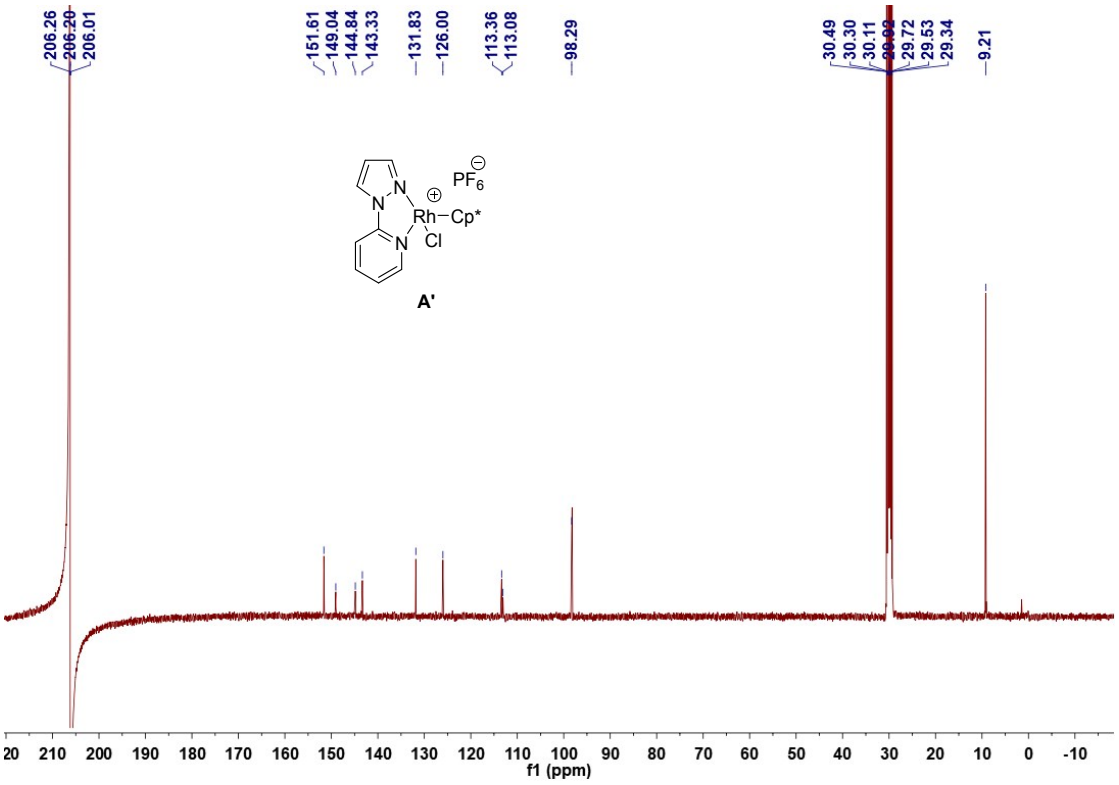
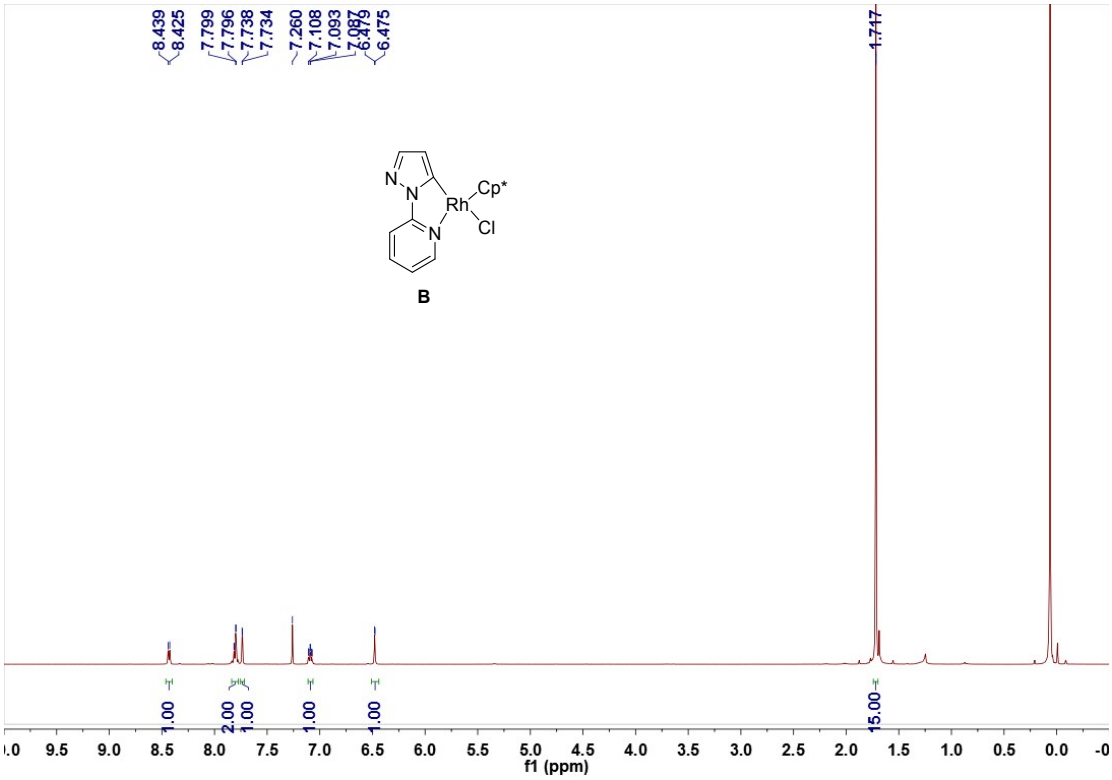
144.17
143.46
142.21
141.73
140.96
140.89
140.84
140.69
140.34
139.99
138.98
138.93
138.21
136.08
135.76
135.42
131.16
130.85
130.72
130.65
130.48
130.41
130.34
130.00
129.85
129.78
128.92
127.58
127.52
127.35
127.28
127.26
127.12
126.34
126.18
125.98
125.92
125.85
125.77
125.64
125.14
122.49
120.46
119.29
117.41
116.67
77.32
77.00
76.68
18.85
18.43
17.27
16.79
16.75
4i
f1 (ppm)

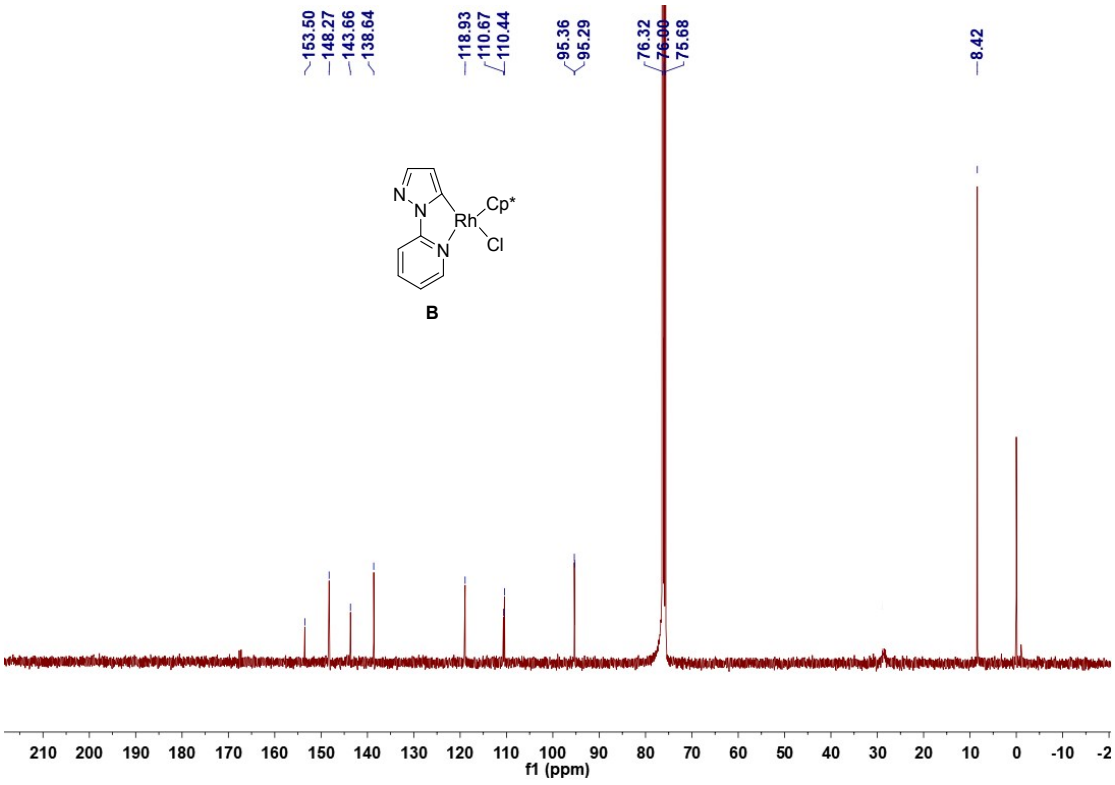

8.954
8.946
8.808
8.795
8.429
8.424
8.320
8.317
8.299
8.280
8.277
8.181
8.160
7.731
7.713
7.698
7.009
7.003
6.997
3.310
1.800
Cl
Cp*
Rh
Cl
N
N
N
A
1.00
0.99
1.00
1.00
1.00
1.00
1.00
15.00
f1 (ppm)

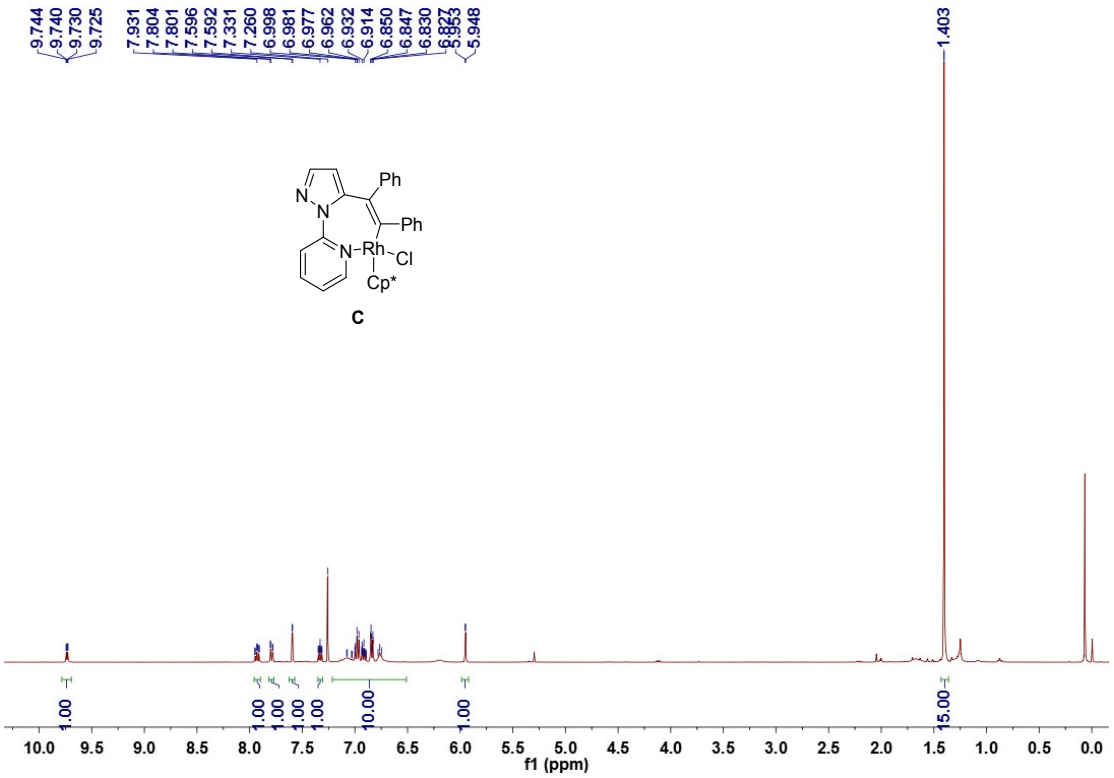

151.68
149.47
145.34
143.72
132.33
126.27
113.67
113.39
99.00
49.66
49.45
49.23
48.81
48.60
48.38
9.11
Cl
Cp*
Rh
Cl
N
N
N
A
f1 (ppm)

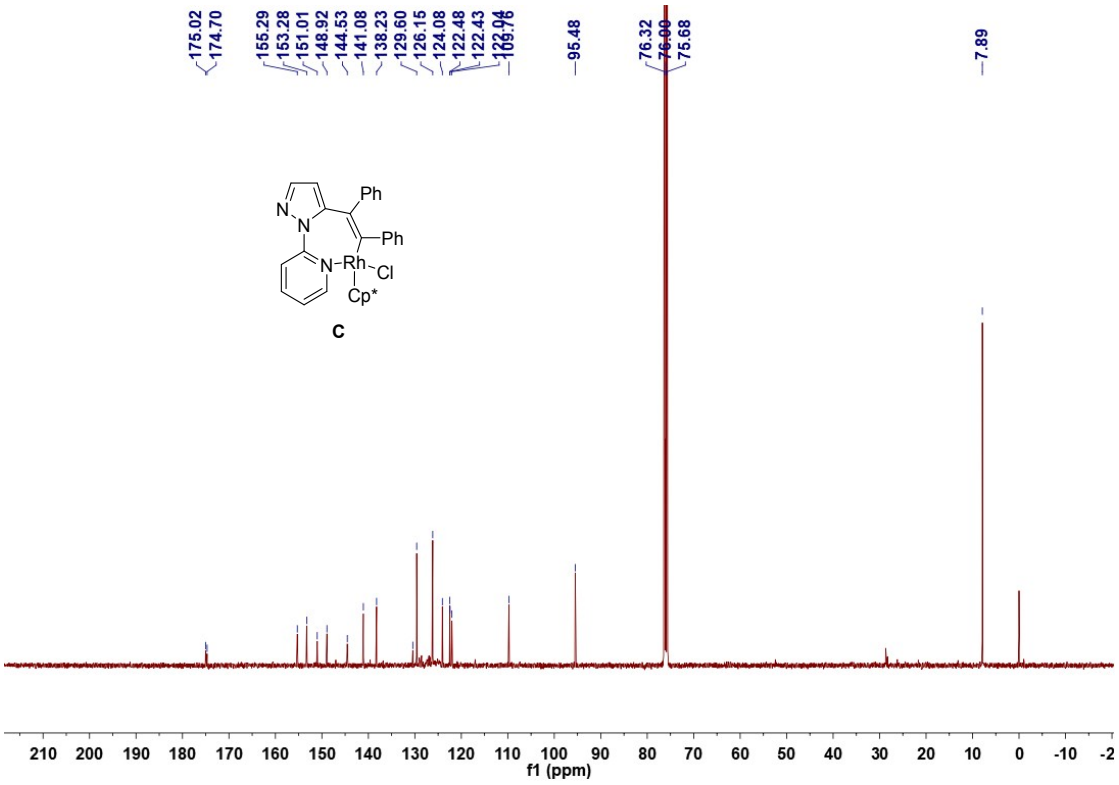

9.001
8.993
8.934
8.920
8.494
8.489
8.257
7.767
7.764
7.760
7.088
7.054
7.047
2.061
2.056
2.050
2.045
2.039
1.863
PF6
Rh−Cp*
Cl
A'
1.00
1.00
1.00
1.00
1.00
1.00
0.99
15.00
f1 (ppm)


206.26
206.20
206.01
151.61
149.04
144.84
143.33
131.83
126.00
113.36
113.08
98.29
30.49
30.30
30.11
29.72
29.53
29.34
9.21
PF6
Rh−Cp*
Cl
A'
f1 (ppm)


8.439
8.425
7.799
7.796
7.738
7.734
7.260
7.108
7.093
6.475
1.717
Cp*
Rh
Cl
N
N
N
B
1.00
2.00
1.00
1.00
1.00
15.00
f1 (ppm)


153.50
148.27
143.66
138.64
118.93
110.67
110.44
95.36
95.29
76.32
76.00
75.68
8.42
Cp*
Rh
Cl
N
N
N
B
f1 (ppm)


9.744
9.740
9.730
9.725
7.931
7.804
7.801
7.596
7.592
7.331
7.260
6.998
6.981
6.977
6.962
6.932
6.914
6.850
6.847
6.830
6.827
5.953
5.948
1.403
Ph
Ph
N-Rh-Cl
Cp*
C
1.00
1.00
1.00
1.00
10.00
1.00
15.00
f1 (ppm)


175.02
174.70
155.29
153.28
151.01
148.92
144.53
141.08
138.23
129.60
126.15
124.08
122.48
122.43
95.48
76.32
76.00
75.68
7.89
Ph
Ph
N-Rh-Cl
Cp*
C
f1 (ppm)

X-Ray Crystallographic Data of 3a, 4e, A', B and C:

X-Ray Crystallographic Data of 3a

Table 1. Crystal Data and Summary of X-ray Data Collection for **3a.**

	3a
formula	$C_{22}H_{17}N_3$
fw	323.38
T (K)	293(2)
crystsyst	monoclinic
space group	C2/c
a (Å)	12.9558(3)
b (Å)	15.3650(4)
c (Å)	17.5580(4)
α (deg)	90
β (deg)	104.709(3)
γ (deg)	90
V (Å^3)	3380.66(14)
Z	8
D_{calc} (g·cm^{-3})	1.271
μ (mm^{-1})	0.593
F(000)	1360.0
cryst size (mm)	0.25 × 0.24 × 0.2
max. 2θ (deg)	134.16
no. of reflns collected	9641
no. of indepreflns/R_{int}	3017/0.0634
no. of params	227
goodness-of-fit on F^2	1.040
R_1, wR_2 [I> 2σ(I)]	0.0628, 0.1689
R_1, wR_2 (all data)	0.0673, 0.1772
largest diff peak and hole (e Å^{-3})	0.45, −0.38

Table 2. Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement Parameters (Å2×103) for **3a**. Ueq is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
N1	7499.5(10)	4655.8(9)	7880.9(8)	20.2(3)
N2	6731.8(11)	5909.1(8)	7249.8(7)	18.6(3)
N3	6627.0(12)	6788.6(9)	7343.1(8)	25.1(4)
C1	7641.5(13)	5482.2(11)	7714.4(9)	20.4(4)
C2	8347.8(13)	4226.2(12)	8303.6(10)	25.9(4)
C3	9341.2(15)	4595.6(14)	8582.0(12)	37.3(5)
C4	9459.8(17)	5465.9(15)	8412.0(14)	48.1(6)
C5	8602.6(16)	5922.8(13)	7973.7(12)	37.4(5)
C6	5670.3(15)	6970.7(10)	6893.7(10)	24.7(4)
C7	5145.4(14)	6234.9(11)	6508.3(9)	22.8(4)
C8	5846.6(12)	5558.7(10)	6742.1(9)	17.4(4)
C9	5741.7(12)	4649.6(10)	6455.2(8)	16.7(4)
C10	6579.3(12)	4322.8(10)	6077.7(9)	16.4(4)
C11	7111.4(12)	3539.1(10)	6314.2(9)	20.6(4)
C12	7822.6(13)	3208.9(11)	5916.2(10)	25.3(4)
C13	8023.2(13)	3658.3(12)	5279.9(11)	26.8(4)
C14	7519.7(13)	4446.3(11)	5052.9(10)	25.1(4)
C15	6810.9(13)	4784.6(10)	5457(1)	20.6(4)
C16	4857.0(12)	4206.6(10)	6478.2(9)	17.4(4)
C17	4468.9(11)	3366.5(10)	6113.9(9)	16.6(4)
C18	4672.0(12)	3072.2(10)	5409.4(9)	18.8(4)
C19	4223.9(13)	2306.8(11)	5059.7(9)	21.7(4)
C20	3555.5(13)	1817.5(11)	5396.4(10)	23.8(4)
C21	3342.0(13)	2098.8(11)	6091.4(10)	24.7(4)
C22	3794.7(12)	2862.1(11)	6445.7(9)	21.1(4)

Table 3. Anisotropic Displacement Parameters ($Å^2×10^3$) for **3a**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	23.4(7)	21.3(7)	15.3(7)	-0.4(5)	3.9(5)	-2.5(5)

N2	29.1(7)	14.9(7)	12.8(7)	-1.6(5)	7.0(6)	-1.3(5)
N3	44.2(9)	15.1(7)	21.5(8)	-2.6(5)	18.2(7)	-3.9(6)
C1	27.2(9)	23.8(8)	9.8(7)	-2.2(6)	4.0(6)	-5.6(6)
C2	27.8(9)	26.6(9)	19.6(9)	3.0(7)	-0.7(7)	0.3(7)
C3	28.5(10)	45.1(12)	30.8(11)	7.1(9)	-6.4(8)	-4.6(8)
C4	34.2(11)	53.2(14)	44.5(13)	8.6(11)	-12.5(9)	-22(1)
C5	40.7(11)	32.9(10)	30.7(11)	3.1(8)	-5.6(8)	-18.1(8)
C6	40.0(9)	19.7(8)	19.6(8)	3.7(6)	17.3(7)	6.8(7)
C7	30.9(8)	25.5(9)	14.3(8)	3.3(6)	9.7(7)	7.6(7)
C8	24.8(8)	20.9(8)	7.8(7)	0.6(6)	6.6(6)	1.0(6)
C9	24.1(8)	18.5(8)	6.8(7)	1.1(5)	2.6(6)	1.8(6)
C10	19.3(7)	18.2(8)	10.8(7)	-3.6(6)	2.1(6)	-2.5(6)
C11	24.0(8)	20.5(8)	14.8(8)	-1.1(6)	0.5(6)	-0.7(6)
C12	23.9(8)	23.1(8)	26.9(9)	-7.2(7)	2.8(7)	3.2(6)
C13	22.9(8)	31.7(9)	27.5(9)	-15.3(7)	9.6(7)	-4.2(7)
C14	30.8(9)	28.9(9)	18.8(8)	-5.7(7)	12.1(7)	-9.6(7)
C15	26.3(8)	19.6(8)	16.9(8)	-1.2(6)	7.3(6)	-2.7(6)
C16	20.9(8)	24.0(8)	7.1(7)	-0.5(6)	3.3(6)	3.3(6)
C17	17.1(7)	22.2(8)	8.8(7)	2.0(6)	0.2(6)	3.6(6)
C18	21.3(8)	23.9(8)	10.9(7)	-0.2(6)	3.7(6)	-2.8(6)
C19	24.9(8)	25.3(8)	14.2(8)	-2.0(6)	3.7(6)	0.0(6)
C20	26.0(8)	19.7(8)	23.8(9)	-0.1(7)	2.9(7)	-2.2(6)
C21	24.7(8)	26.2(9)	24.9(9)	6.2(7)	9.4(7)	-1.5(7)

C22	22.7(8)	27.3(9)	14.2(8)	3.7(6)	6.2(6)	2.6(6)

Table 4. Bond Lengths for **3a**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.326(2)	C9	C16	1.342(2)
N1	C2	1.334(2)	C10	C11	1.397(2)
N2	N3	1.3721(18)	C10	C15	1.395(2)
N2	C1	1.413(2)	C11	C12	1.386(2)
N2	C8	1.371(2)	C12	C13	1.393(3)
N3	C6	1.319(2)	C13	C14	1.385(3)
C1	C5	1.389(2)	C14	C15	1.396(2)
C2	C3	1.378(3)	C16	C17	1.471(2)
C3	C4	1.387(3)	C17	C18	1.403(2)
C4	C	1.373(3)	C17	C22	1.400(2)
C6	C7	1.402(2)	C18	C19	1.384(2)
C7	C8	1.373(2)	C19	C20	1.387(2)
C8	C9	1.479(2)	C20	C21	1.387(2)
C9	C10	1.495(2)	C21	C22	1.386(2)

Table 5. Bond Angles for **3a**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C2	117.10(14)	C16	C9	C10	124.37(14)
N3	N2	C1	118.79(13)	C11	C10	C9	121.11(14)
C8	N2	N3	111.87(13)	C15	C10	C9	119.98(14)
C8	N2	C1	129.07(13)	C15	C10	C11	118.86(14)
C6	N3	N2	104.12(14)	C12	C11	C10	120.43(15)
N1	C1	N2	115.45(14)	C11	C12	C13	120.41(15)

N1	C1	C5	123.89(16)	C14	C13	C12	119.61(14)
C5	C1	N2	120.66(15)	C13	C14	C15	120.13(15)
N1	C2	C3	123.83(17)	C10	C15	C14	120.49(15)
C2	C3	C4	117.74(18)	C9	C16	C17	129.19(13)
C5	C4	C3	119.71(18)	C18	C17	C16	123.09(13)
C4	C5	C1	117.71(18)	C22	C17	C16	119.01(13)
N3	C6	C7	112.62(14)	C22	C17	C18	117.70(14)
C8	C7	C6	105.25(15)	C19	C18	C17	120.89(14)
N2	C8	C7	106.14(14)	C18	C19	C20	120.55(15)
N2	C8	C9	125.55(14)	C21	C20	C19	119.44(15)
C7	C8	C9	128.05(15)	C22	C21	C20	120.15(14)
C8	C9	C10	116.99(13)	C21	C22	C17	121.27(14)
C16	C9	C8	118.28(13)				

Table 6. Torsion Angles for **3a**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C1	C5	C4	1.7(3)	C8	N2	C1	C5	157.15(17)
N1	C2	C3	C4	0.1(3)	C8	C9	C10	C11	129.20(15)
N2	N3	C6	C7	-0.01(17)	C8	C9	C10	C15	-53.4(2)
N2	C1	C5	C4	-178.95(18)	C8	C9	C16	C17	168.44(14)
N2	C8	C9	C10	-54.09(19)	C9	C10	C11	C12	174.70(14)
N2	C8	C9	C16	132.45(16)	C9	C10	C15	C14	-174.12(14)
N3	N2	C1	N1	150.12(13)	C9	C16	C17	C18	-30.3(2)
N3	N2	C1	C5	-29.3(2)	C9	C16	C17	C22	154.96(16)
N3	N2	C8	C7	-0.65(16)	C10	C9	C16	C17	-4.5(3)
N3	N2	C8	C9	173.82(13)	C10	C11	C12	C13	0.6(3)
N3	C6	C7	C8	-0.38(17)	C11	C10	C15	C14	3.4(2)
C1	N1	C2	C3	1.1(3)	C11	C12	C13	C14	1.0(3)
C1	N2	N3	C6	-174.17(13)	C12	C13	C14	C15	-0.4(3)
C1	N2	C8	C7	173.23(14)	C13	C14	C15	C10	-1.8(3)

C1	N2	C8	C9	-12.3(2)	C15	C10	C11	C12	-2.8(2)
C2	N1	C1	N2	178.51(13)	C16	C9	C10	C11	-57.8(2)
C2	N1	C1	C5	-2.1(2)	C16	C9	C10	C15	119.66(17)
C2	C3	C4	C5	-0.6(3)	C16	C17	C18	C19	-175.19(15)
C3	C4	C5	C1	-0.3(3)	C16	C17	C22	C21	175.01(14)
C6	C7	C8	N2	0.60(15)	C17	C18	C19	C20	0.6(2)
C6	C7	C8	C9	-173.69(14)	C18	C17	C22	C21	0.0(2)
C7	C8	C9	C10	119.16(17)	C18	C19	C20	C21	-0.3(3)
C7	C8	C9	C16	-54.3(2)	C19	C20	C21	C22	-0.1(3)
C8	N2	N3	C6	0.41(16)	C20	C21	C22	C17	0.3(3)
C8	N2	C1	N1	-23.4(2)	C22	C17	C18	C19	-0.4(2)

Table 7. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3a**.

Atom	x	y	z	U(eq)
H2	8264	3643	8417	31
H3	9913	4273	8874	45
H4	10117	5739	8594	58
H5	8663	6507	7855	45
H6	5376	7527	6839	30
H7	4467	6210	6167	27
H11	6988	3237	6741	25
H12	8168	2684	6075	30
H13	8492	3431	5009	32
H14	7654	4751	4630	30
H15	6491	5322	5312	25
H16	4429	4468	6765	21
H18	5114	3396	5174	23
H19	4372	2119	4595	26
H20	3253	1305	5158	29
H21	2894	1775	6320	30
H22	3648	3043	6913	25

X-Ray Crystallographic Data of 4e

Table 1. Crystal Data and Summary of X-ray Data Collection for **4e**

	4e
formula	$C_{36}H_{21}Br_4N_3$
fw	815.20
T (K)	150.00(10)
crystsyst	monoclinic
space group	$P2_1/c$
a (Å)	16.89621(19)
b (Å)	26.8711(3)
c (Å)	25.9578(3)
α (deg)	90
β (deg)	100.2322(10)
γ (deg)	90
V (Å^3)	11597.9(2)
Z	12
D_{calc} (g·cm^{-3})	1.401
μ (mm^{-1})	5.274
F(000)	4776.0
cryst size (mm)	0.25 × 0.22 × 0.2
max. 2θ (deg)	134.15
no. of reflns collected	44595
no. of indepreflns/R_{int}	20695/0.0321
no. of params	1162
goodness-of-fit on F^2	1.022
R_1, wR_2 [I> 2σ(I)]	0.0569, 0.1463
R_1, wR_2 (all data)	0.0704, 0.1564
largest diff peak and hole (e Å^{-3})	2.11, −1.65

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4e**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
Br1	10783.1(6)	8574.8(4)	10265.8(3)	85.3(3)
Br2	6178.6(4)	8361.9(3)	10232.5(2)	52.57(16)
Br3	3355.2(3)	8208.5(2)	7781.7(2)	41.68(13)
Br4	5092.0(5)	8226.1(5)	5053.0(3)	90.4(3)
N1	9401(2)	8385.2(16)	7617.8(17)	36.0(9)
N2	9385(3)	8390.6(18)	7087.4(18)	41.2(10)
N3	10285(3)	7962.9(18)	8301(2)	47.3(11)
C1	8628(3)	8365.2(18)	7731.5(19)	30.0(10)
C2	8107(3)	8347.4(18)	7251.1(19)	31.2(10)
C3	7268(3)	8331.4(18)	7217.4(19)	31.2(10)
C4	6978(3)	8325.3(17)	7689.4(19)	30.1(10)
C5	7514(3)	8346.0(17)	8177.9(18)	27.5(9)
C6	8352(3)	8372.3(17	8214.0(19)	27.8(9)
C7	8624(3)	8370(2)	6868(2)	40.5(12)
C8	8907(3)	8424.0(18)	8723.4(19)	30.3(10)
C9	8959(3)	8063.8(19)	9112(2)	34.4(11)
C10	9509(3)	8111(2)	9574(2)	42.6(12)
C11	10004(3)	8524(2)	9645(2)	45.2(13)
C12	9958(3)	8887(2)	9271(2)	41.6(12)
C13	9403(3)	8835.7(18)	8810(2)	32.4(10)
C14	7175(3)	8343.5(18)	8671.6(18)	28.0(9)
C15	7209(3)	8772.1(19)	8974(2)	37.4(11)
C1	6913(3)	8778(2)	9434(2)	42.7(13)
C17	6569(3)	8355(2)	9590.9(18)	35.1(11)
C18	6513(3)	7925(2)	9296.5(19)	36.4(11)
C1	6810(3)	7921.8(19)	8835.6(19)	33.1(10)
C20	6093(3)	8297.8(18)	7686.3(17)	28.9(10)
C21	5666(3)	7858.8(19)	7575(2)	36.4(11)
C22	4853(3)	7827.8(19)	7605(2)	37.6(11)
C23	4467(3)	8246.8(19)	7734.0(18)	31.8(10)
C24	4862(3)	8695(2)	7822(2)	38.0(11)
C25	5674(3)	8716.2(19)	7808(2)	35.7(11)
C26	6743(3)	8316(2)	6695.0(19)	34.7(11)
C27	6836(3)	7940(2)	6347(2)	44.0(13)

C28	6353(4)	7912(3)	5853(2)	54.6(16)
C29	5774(3)	8269(3)	5718(2)	56.1(18)
C30	5682(4)	8653(3)	6049(2)	63.3(19)
C31	6159(4)	8675(2)	6542(2)	48.7(14)
C32	10166(3)	8351.4(19)	7950(2)	35.9(11)
C34	11032(4)	7944(2)	8617(3)	49.2(14)
C35	11614(4)	8303(3)	8563(3)	68(2)
C36	11443(4)	8671(3)	8184(3)	65.0(19)
C37	10705(3)	8694(2)	7876(2)	43.1(13)
Br5	8000.5(4)	6645.5(2)	6169.8(2)	46.05(15)
Br6	12681.5(3)	6448.4(2)	6194.0(2)	42.73(14)
Br7	15495.1(4)	6525.9(4)	8647.7(3)	73.7(3)
Br8	13816.4(5)	6915.5(4)	11341.8(3)	72.6(2)
N4	9469(2)	6739.6(16)	8829.3(16)	32.3(9)
N5	9510(3)	6768.8(18)	9361.7(17)	39.6(10)
N6	8541(3)	7098.6(17)	8128.8(19)	44.2(11)
C38	10224(3)	6704.2(17)	8701.4(18)	26.6(9)
C39	10765(3)	6725.2(18)	9176.3(18)	29.6(10)
C40	11604(3)	6700.1(18)	9195.1(18)	29.7(10)
C41	11873(3)	6647.3(17)	8720.6(18)	27.1(9)
C42	11317(3)	6631.0(16)	8236.3(17)	24.3(9)
C43	10487(3)	6655.7(16)	8215.9(18)	26.1(9)
C44	10277(3)	6761(2)	9567.5(19)	37.2(11)
C45	9912(3)	6641.0(18)	7707.3(18)	27.4(9)
C46	9384(3)	6243.7(17)	7591.5(19)	28.6(9)
C47	8817(3)	6236.6(18)	7128.2(19)	31.5(10)
C48	8792(3)	6636.8(19)	6790.3(19)	32.3(10)
C49	9320(3)	7030(2)	6890(2)	37.2(11)
C50	9880(3)	7030.7(19)	7351.0(19)	32.5(10)
C51	11643(3)	6592.2(17)	7738.7(18)	26.7(9)
C52	12126(3)	6964.2(19)	7588.6(18)	30.9(10)
C53	12437(3)	6920.5(19)	7129.6(19)	32.4(10)
C54	12254(3)	6508.3(19)	6819.2(18)	32.8(10)
C55	11757(3)	6136.5(19)	6951.3(19)	33.5(10)
C56	11458(3)	6180.4(18)	7412.9(19)	31.4(10)
C57	12757(3)	6612.7(19)	8718.7(17)	28.9(10)
C58	13092(3)	6172(2)	8583(2)	42.1(12)
C59	13914(4)	6141(3)	8567(3)	54.1(16)

C60	14385(3)	6555(3)	8679(2)	45.4(14)
C61	14061(3)	6993(2)	8807(2)	46.4(14)
C62	13255(3)	7019(2)	8829(2)	38.3(12)
C63	12143(3)	6737.1(19)	9712.1(19)	31.8(10)
C64	12669(3)	6363(2)	9914(2)	42.3(12)
C65	13167(4)	6412(2)	10401(2)	49.0(14)
C66	13127(4)	6839(3)	10682(2)	49.3(14)
C67	12592(4)	7216(3)	10499(2)	61.6(18)
C68	12108(4)	7163(3)	10018(2)	53.7(16)
C69	8686(3)	6751.1(18)	8511(2)	31.4(10)
C71	7793(4)	7082(2)	7820(2)	51.8(16)
C72	7230(3)	6733(2)	7912(3)	58.8(19)
C73	7419(3)	6418(2)	8324(3)	53.9(17)
C74	8153(3)	6414.3(19)	8630(2)	36.4(11)
Br9	9273.4(6)	4474.9(4)	9921.5(3)	80.3(3)
Br10	5144.5(4)	4854.0(3)	8504.9(3)	63.5(2)
Br11	4267.1(5)	5023.2(5)	5516.2(4)	90.8(3)
Br12	8220.6(4)	4974.8(2)	4042.8(2)	44.74(14)
N7	10181(2)	4963.4(15)	7410.3(16)	33.4(9)
N8	10547(3)	4996.2(16)	6981.4(17)	37.1(9)
N9	10490(3)	5326.3(16)	8235.5(17)	37.3(9)
C75	9355(3)	4970.6(17)	7266.3(19)	30.6(10)
C76	9198(3)	5014.7(18)	6718.9(19)	31.8(10)
C77	8402(3)	5013.1(18)	6431.4(19)	32.2(10)
C78	7776(3)	4982.5(17)	6712.7(19)	31.9(10)
C79	7950(3)	4935.4(18)	7271.4(19)	31.0(10)
C80	8727(3)	4915.8(17)	7561.2(19)	31.7(10)
C81	9966(3)	5031.0(19)	6573(2)	35.8(11)
C82	8294(3)	5024.3(18)	5852.3(19)	31.9(10)
C83	7897(3)	4641.7(19)	5546(2)	35.5(11)
C84	7855(3)	4632(2)	5011(2)	38.0(11)
C85	8226(3)	5004(2)	4773.6(19)	36.1(11)
C86	8622(3)	5395(2)	5063(2)	39.0(12)
C87	8658(3)	5399(2)	5598(2)	39.0(12)
C88	6923(3)	4988.6(19)	6427.8(19)	32.7(10)
C89	6416(3)	4587(2)	6442(2)	40.7(12)
C90	5628(3)	4588(2)	6173(2)	49.5(14)
C91	5348(4)	5005(3)	5886(2)	53.6(16)

C92	5831(4)	5413(3)	5862(2)	52.4(15)
C93	6626(3)	5400(2)	6132(2)	44.6(13)
C94	7257(3)	4909.6(18)	7561.2(18)	31.4(10)
C95	6742(3)	5314(2)	7565(2)	35.4(11)
C96	6112(3)	5300(2)	7843(2)	40.8(12)
C97	6014(3)	4879(2)	8123(2)	40.7(12)
C98	6498(3)	4469(2)	8125(2)	41.3(12)
C99	7129(3)	4488(2)	7847(2)	37.6(11)
C100	8891(3)	4832.8(18)	8128.9(19)	31.7(10)
C101	8645(3)	5163(2)	8483(2)	35.5(11)
C102	8771(3)	5069(2)	9013(2)	42.4(12)
C103	9156(4)	4629(2)	9198(2)	49.2(14)
C104	9431(4)	4304(2)	8867(3)	53.8(15)
C105	9305(3)	4402(2)	8333(2)	42.1(12)
C106	10679(3)	4984.3(19)	7913(2)	32.8(10)
C108	10955(4)	5350(2)	8712(2)	43.5(13)
C109	11608(4)	5045(3)	8866(2)	52.9(15)
C110	11807(4)	4701(3)	8517(3)	57.8(16)
C111	11329(3)	4666(2)	8021(2)	46.5(13)

Table 3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **4e**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
Br1	76.0(5)	98.4(6)	63.4(5)	22.1(4)	-37.4(4)	-40.0(5)
Br2	48.2(3)	80.5(5)	30.4(3)	-3.8(3)	11.0(2)	10.8(3)
Br3	21.6(2)	52.9(3)	50.1(3)	-1.8(2)	5.1(2)	-2.5(2)
Br4	44.7(4)	185.2(11)	36.2(3)	-19.9(5)	-6.4(3)	20.4(5)
N1	25(2)	43(2)	42(2)	3.1(19)	12.7(18)	1.7(17)
N2	33(2)	52(3)	41(2)	9(2)	13.7(19)	1(2)
N3	33(2)	41(3)	65(3)	3(2)	0(2)	6(2)
C1	24(2)	31(2)	37(3)	3.8(19)	10.6(19)	0.5(18)
C2	29(2)	30(2)	35(3)	3.7(19)	9(2)	5.3(19)
C3	29(2)	31(2)	33(2)	0.6(19)	5.8(19)	7.3(19)
C4	25(2)	30(2)	34(2)	-2.9(19)	3.7(19)	3.9(18)
C5	22(2)	28(2)	33(2)	0.1(18)	5.4(18)	1.9(17)
C6	22(2)	25(2)	36(2)	-1.8(18)	5.4(18)	1.8(17)
C7	36(3)	52(3)	36(3)	9(2)	15(2)	1(2)
C8	21(2)	33(2)	38(3)	-3(2)	6.1(19)	0.7(18)

C9	25(2)	35(3)	42(3)	5(2)	1(2)	-1(2)
C10	34(3)	43(3)	47(3)	11(2)	-2(2)	-2(2)
C11	36(3)	54(3)	40(3)	1(2)	-8(2)	-6(2)
C12	34(3)	45(3)	45(3)	-6(2)	4(2)	-10(2)
C13	23(2)	29(2)	45(3)	2(2)	7(2)	-1.5(18)
C14	18(2)	33(2)	31(2)	-3.9(19)	1.0(17)	2.1(18)
C15	41(3)	33(3)	38(3)	-4(2)	7(2)	-2(2)
C16	44(3)	43(3)	40(3)	-18(2)	6(2)	1(2)
C17	25(2)	55(3)	25(2)	-3(2)	3.0(18)	4(2)
C18	31(3)	45(3)	34(3)	-2(2)	8(2)	-4(2)
C19	33(3)	36(3)	31(2)	-7(2)	5.5(19)	-1(2)
C20	25(2)	34(2)	25(2)	-4.4(18)	-1.3(17)	1.9(19)
C21	28(3)	32(3)	48(3)	-9(2)	3(2)	8(2)
C22	28(3)	34(3)	47(3)	-6(2)	-5(2)	-2(2)
C23	25(2)	41(3)	27(2)	-1.6(19)	-4.5(18)	-1(2)
C24	31(3)	36(3)	47(3)	-7(2)	6(2)	6(2)
C25	27(2)	31(3)	48(3)	-4(2)	5(2)	1(2)
C26	32(3)	45(3)	28(2)	-1(2)	9(2)	1(2)
C27	40(3)	56(3)	36(3)	-2(2)	7(2)	6(3)
C28	50(4)	74(4)	41(3)	-15(3)	12(3)	-2(3)
C29	30(3)	112(6)	25(3)	-7(3)	2(2)	9(3)
C30	47(4)	96(5)	44(3)	0(3)	0(3)	35(4)
C31	45(3)	63(4)	37(3)	-2(3)	5(2)	22(3)
C32	24(2)	35(3)	51(3)	-2(2)	13(2)	3(2)
C34	42(3)	38(3)	60(4)	1(3)	-12(3)	9(2)
C35	21(3)	79(5)	99(6)	-44(4)	-1(3)	5(3)
C36	47(4)	57(4)	97(6)	-16(4)	31(4)	-19(3)
C37	39(3)	39(3)	56(3)	0(2)	23(3)	-10(2)
Br5	40.2(3)	51.6(3)	39.4(3)	-0.5(2)	-11.9(2)	-0.1(2)
Br6	39.5(3)	60.5(4)	29.9(3)	-2.8(2)	10.8(2)	-2.7(3)
Br7	19.0(3)	143.6(8)	57.2(4)	-31.5(4)	3.4(3)	7.8(4)
Br8	63.5(5)	111.2(7)	34.8(3)	-6.8(4)	-13.7(3)	5.1(4)
N4	20.7(19)	42(2)	34(2)	0.5(17)	5.9(16)	1.4(16)
N5	28(2)	54(3)	41(2)	5(2)	16.0(18)	2.1(19)
N6	35(2)	41(3)	56(3)	-5(2)	4(2)	8.8(19)
C38	17(2)	27(2)	36(2)	-0.7(18)	7.4(18)	-1.1(17)
C39	28(2)	31(2)	31(2)	1.3(19)	9.0(19)	5.8(19)
C40	27(2)	32(2)	29(2)	0.0(19)	2.4(18)	1.3(19)

C41	18(2)	32(2)	30(2)	-0.3(18)	0.1(17)	1.2(17)
C42	22(2)	26(2)	25(2)	-4.2(17)	4.1(17)	-2.8(17)
C43	22(2)	26(2)	30(2)	-3.0(18)	2.4(17)	0.4(17)
C44	33(3)	53(3)	27(2)	4(2)	10(2)	5(2)
C45	17(2)	34(2)	32(2)	-3.3(19)	5.2(17)	-0.8(17)
C46	23(2)	28(2)	35(2)	-2.6(19)	6.4(18)	1.5(18)
C47	22(2)	32(2)	39(3)	-5(2)	2.9(19)	1.2(18)
C48	20(2)	42(3)	32(2)	-4(2)	-2.4(18)	1.2(19)
C49	32(3)	40(3)	38(3)	6(2)	1(2)	0(2)
C50	24(2)	34(3)	37(3)	2(2)	-0.9(19)	-3.9(19)
C51	14(2)	34(2)	30(2)	-1.2(18)	0.7(17)	0.6(17)
C52	23(2)	37(3)	32(2)	-3(2)	2.1(18)	-5.3(19)
C53	22(2)	40(3)	35(3)	1(2)	5.1(19)	-6.9(19)
C54	28(2)	42(3)	28(2)	-1(2)	2.4(19)	1(2)
C55	31(2)	36(3)	33(2)	-6(2)	5(2)	-2(2)
C56	25(2)	33(2)	37(3)	-3(2)	6.9(19)	-3.3(19)
C57	20(2)	43(3)	23(2)	0.3(19)	0.9(17)	3.3(19)
C58	27(3)	47(3)	52(3)	-5(2)	6(2)	6(2)
C59	39(3)	65(4)	58(4)	-7(3)	11(3)	23(3)
C60	19(2)	85(4)	30(3)	-11(3)	-1.4(19)	6(3)
C61	26(3)	69(4)	43(3)	-13(3)	4(2)	-8(3)
C62	23(2)	52(3)	39(3)	-13(2)	1(2)	-2(2)
C63	23(2)	42(3)	30(2)	0(2)	3.4(18)	2.6(19)
C64	41(3)	50(3)	34(3)	0(2)	2(2)	3(2)
C65	38(3)	64(4)	42(3)	8(3)	-1(2)	9(3)
C66	42(3)	74(4)	27(3)	-1(3)	-5(2)	2(3)
C67	71(5)	65(4)	43(3)	-19(3)	-4(3)	16(3)
C68	56(4)	60(4)	40(3)	-11(3)	-4(3)	18(3)
C69	18(2)	36(3)	42(3)	-6(2)	8.3(19)	5.4(18)
C71	49(4)	46(3)	54(3)	-8(3)	-8(3)	24(3)
C72	22(3)	57(4)	92(5)	-37(4)	-4(3)	9(3)
C73	30(3)	49(3)	89(5)	-22(3)	26(3)	-7(3)
C74	26(2)	33(3)	55(3)	-9(2)	19(2)	-3(2)
Br9	99.2(6)	100.3(6)	37.8(3)	21.3(4)	2.5(4)	-3.9(5)
Br10	43.9(4)	80.6(5)	74.5(5)	3.9(4)	33.8(3)	-5.3(3)
Br11	38.0(4)	145.1(9)	79.7(5)	21.4(6)	-15.7(4)	-28.2(5)
Br12	58.0(4)	46.6(3)	31.9(3)	-3.4(2)	14.2(2)	4.3(3)
N7	28(2)	35(2)	37(2)	-3.9(17)	7.6(17)	-2.1(17)

N8	31(2)	42(2)	41(2)	-5.3(19)	12.8(18)	-1.8(18)
N9	34(2)	39(2)	38(2)	-0.6(18)	1.9(18)	-0.6(18)
C75	27(2)	27(2)	37(3)	-4.6(19)	6.0(19)	1.6(18)
C76	34(3)	29(2)	33(2)	-5.8(19)	9(2)	0.6(19)
C77	34(3)	32(2)	32(2)	-7.6(19)	9(2)	-2(2)
C78	32(3)	27(2)	37(3)	-5.4(19)	7(2)	-4.1(19)
C79	31(2)	31(2)	32(2)	-5.3(19)	10.2(19)	-1.6(19)
C80	33(3)	27(2)	36(3)	-3.7(19)	9(2)	-1.4(19)
C81	34(3)	39(3)	36(3)	-5(2)	12(2)	-5(2)
C82	29(2)	35(3)	32(2)	-3(2)	7.1(19)	-2.5(19)
C83	35(3)	36(3)	36(3)	-2(2)	8(2)	-6(2)
C84	37(3)	39(3)	38(3)	-9(2)	9(2)	-5(2)
C85	32(3)	48(3)	30(2)	-2(2)	12(2)	5(2)
C86	47(3)	35(3)	39(3)	0(2)	18(2)	-3(2)
C87	45(3)	37(3)	37(3)	-6(2)	15(2)	-9(2)
C88	28(2)	42(3)	30(2)	-4(2)	9.4(19)	-3(2)
C89	35(3)	47(3)	41(3)	0(2)	11(2)	-8(2)
C90	33(3)	62(4)	54(3)	-1(3)	9(2)	-17(3)
C91	34(3)	78(4)	46(3)	4(3)	-1(2)	-17(3)
C92	39(3)	65(4)	49(3)	12(3)	-4(3)	-8(3)
C93	34(3)	57(3)	42(3)	5(3)	5(2)	-13(2)
C94	31(2)	35(3)	30(2)	-5.4(19)	7.3(19)	-6(2)
C95	33(3)	37(3)	37(3)	1(2)	7(2)	-2(2)
C96	28(3)	43(3)	52(3)	-3(2)	9(2)	1(2)
C97	25(2)	59(3)	43(3)	-8(2)	16(2)	-7(2)
C98	40(3)	43(3)	42(3)	6(2)	11(2)	-7(2)
C99	39(3)	39(3)	36(3)	-1(2)	10(2)	-6(2)
C100	27(2)	34(3)	34(2)	-1(2)	6.0(19)	-2.8(19)
C101	31(3)	41(3)	35(3)	1(2)	7(2)	3(2)
C102	37(3)	55(3)	37(3)	-6(2)	10(2)	-2(2)
C103	48(3)	60(4)	37(3)	9(3)	-1(2)	-5(3)
C104	54(4)	47(3)	54(4)	7(3)	-8(3)	5(3)
C105	43(3)	37(3)	47(3)	-2(2)	8(2)	4(2)
C106	26(2)	36(3)	37(3)	4(2)	5.9(19)	-1.7(19)
C108	50(3)	46(3)	32(3)	0(2)	-1(2)	-4(3)
C109	42(3)	70(4)	42(3)	13(3)	-6(3)	-4(3)
C1	41(3)	69(4)	62(4)	12(3)	6(3)	15(3)
C111	41(3)	51(3)	47(3)	4(3)	10(2)	8(3)

Table 4. Bond Lengths for **4e**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C11	1.897(5)	C48	C49	1.377(7)
Br2	C17	1.897(5)	C49	C50	1.387(7)
Br3	C23	1.908(5)	C51	C52	1.390(7)
Br4	C29	1.901(5)	C51	C56	1.394(7)
N1	N2	1.372(6)	C52	C53	1.389(7)
N1	C1	1.390(6)	C53	C54	1.372(7)
N1	C32	1.424(7)	C54	C55	1.387(7)
N2	C7	1.311(7)	C55	C56	1.385(7)
N3	C32	1.376(7)	C57	C58	1.384(7)
N3	C34	1.378(7)	C57	C62	1.377(7)
C1	C2	1.394(7)	C58	C59	1.399(8)
C1	C6	1.412(7)	C59	C60	1.369(9)
C2	C3	1.406(7)	C60	C61	1.364(9)
C2	C7	1.437(7)	C61	C62	1.375(7)
C3	C4	1.398(7)	C63	C64	1.382(7)
C3	C26	1.483(7)	C63	C68	1.399(8)
C4	C5	1.422(7)	C64	C65	1.396(8)
C4	C20	1.495(7)	C65	C66	1.368(9)
C5	C6	1.404(6)	C66	C67	1.384(9)
C5	C14	1.494(7)	C67	C68	1.373(9)
C6	C8	1.485(7)	C69	C74	1.351(7)

C8	C9	1.389(7)	C71	C72	1.387(10)
C8	C13	1.382(7)	C72	C73	1.357(10)
C9	C10	1.387(7)	C73	C74	1.349(9)
C10	C11	1.381(8)	Br9	C103	1.898(6)
C11	C12	1.369(8)	Br10	C97	1.914(5)
C12	C13	1.391(7)	Br11	C91	1.907(6)
C14	C15	1.389(7)	Br12	C85	1.897(5)
C14	C19	1.392(7)	N7	N8	1.369(6)
C15	C16	1.374(8)	N7	C75	1.381(6)
C16	C17	1.371(8)	N7	C106	1.422(7)
C17	C18	1.379(7)	N8	C81	1.314(7)
C18	C19	1.377(7)	N9	C106	1.320(7)
C20	C21	1.387(7)	N9	C108	1.343(7)
C20	C25	1.395(7)	C75	C76	1.403(7)
C21	C22	1.392(7)	C75	C80	1.421(7)
C22	C23	1.372(7)	C76	C77	1.418(7)
C23	C24	1.375(7)	C76	C81	1.415(7)
C24	C25	1.379(7)	C77	C78	1.390(7)
C26	C27	1.383(8)	C77	C82	1.482(7)
C26	C31	1.387(8)	C78	C79	1.433(7)
C27	C28	1.394(8)	C78	C88	1.498(7)
C28	C29	1.371(10)	C79	C80	1.393(7)
C29	C30	1.369(10)	C79	C94	1.503(7)

C30	C31	1.387(8)	C80	C100	1.467(7)
C32	C37	1.334(7)	C82	C83	1.396(7)
C34	C35	1.403(10)	C82	C87	1.405(7)
C35	C36	1.388(11)	C83	C84	1.380(7)
C36	C37	1.359(10)	C84	C85	1.382(8)
Br5	C48	1.902(5)	C85	C86	1.392(8)
Br6	C54	1.896(5)	C86	C87	1.379(7)
Br7	C60	1.893(5)	C88	C89	1.383(7)
Br8	C66	1.904(5)	C88	C93	1.389(8)
N4	N5	1.373(6)	C89	C90	1.389(8)
N4	C38	1.379(6)	C90	C91	1.381(9)
N4	C69	1.429(6)	C91	C92	1.374(9)
N5	C44	1.311(7)	C92	C93	1.400(8)
N6	C69	1.353(7)	C94	C95	1.394(7)
N6	C71	1.372(7)	C94	C99	1.391(7)
C38	C39	1.399(7)	C95	C96	1.388(7)
C38	C43	1.414(7)	C96	C97	1.370(8)
C39	C40	1.412(7)	C97	C98	1.371(8)
C39	C44	1.421(7)	C98	C99	1.391(7)
C40	C41	1.393(7)	C100	C101	1.393(7)
C40	C63	1.485(7)	C100	C105	1.406(7)
C41	C42	1.430(6)	C101	C102	1.377(7)
C41	C57	1.497(6)	C102	C103	1.393(9)

C42	C43	1.396(6)	C103	C104	1.365(9)
C42	C51	1.495(6)	C104	C105	1.391(8)
C43	C45	1.494(6)	C106	C111	1.382(8)
C45	C46	1.389(7)	C108	C109	1.376(9)
C45	C50	1.392(7)	C109	C110	1.379(10)
C46	C47	1.398(7)	C110	C111	1.396(9)
C47	C48	1.383(7)			

Table 5. Bond Angles for **4e**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	N1	C1	111.2(4)	C56	C51	C42	120.2(4)
N2	N1	C32	117.6(4)	C53	C52	C51	120.7(5)
C1	N1	C32	130.9(4)	C54	C53	C52	119.5(5)
C7	N2	N1	106.2(4)	C53	C54	Br6	119.4(4)
C32	N3	C34	115.6(5)	C53	C54	C55	121.3(5)
N1	C1	C2	106.2(4)	C55	C54	Br6	119.3(4)
N1	C1	C6	131.2(5)	C56	C55	C54	118.8(5)
C2	C1	C6	122.6(4)	C55	C56	C51	121.0(5)
C1	C2	C3	121.8(4)	C58	C57	C41	120.5(4)
C1	C2	C7	104.6(4)	C62	C57	C41	121.5(4)
C3	C2	C7	133.5(5)	C62	C57	C58	117.9(5)
C2	C3	C26	119.4(4)	C57	C58	C59	120.9(6)
C4	C3	C2	116.9(4)	C60	C59	C58	119.1(6)

C4	C3	C26	123.7(4)	C59	C60	Br7	120.0(4)
C3	C4	C5	120.9(4)	C61	C60	Br7	119.3(5)
C3	C4	C20	120.1(4)	C61	C60	C59	120.7(5)
C5	C4	C20	119.0(4)	C60	C61	C62	119.8(6)
C4	C5	C14	119.0(4)	C61	C62	C57	121.6(5)
C6	C5	C4	122.4(4)	C64	C63	C40	122.9(5)
C6	C5	C14	118.6(4)	C64	C63	C68	117.9(5)
C1	C6	C8	122.3(4)	C68	C63	C40	119.2(5)
C5	C6	C1	115.4(4)	C63	C64	C65	121.2(5)
C5	C6	C8	122.3(4)	C66	C65	C64	118.9(6)
N2	C7	C2	111.8(5)	C65	C66	Br8	119.3(5)
C9	C8	C6	121.9(4)	C65	C66	C67	121.5(5)
C13	C8	C6	119.2(4)	C67	C66	Br8	119.2(5)
C13	C8	C9	118.8(5)	C68	C67	C66	118.8(6)
C10	C9	C8	120.7(5)	C67	C68	C63	121.6(6)
C11	C10	C9	119.0(5)	N6	C69	N4	117.8(4)
C10	C11	Br1	118.9(4)	C74	C69	N4	116.1(5)
C12	C11	Br1	119.5(4)	C74	C69	N6	126.1(5)
C12	C11	C10	121.5(5)	N6	C71	C72	120.7(6)
C11	C12	C13	118.9(5)	C73	C72	C71	119.0(6)
C8	C13	C12	121.1(5)	C74	C73	C72	122.1(6)
C15	C14	C5	119.8(4)	C73	C74	C69	116.2(6)
C15	C14	C19	118.6(4)	N8	N7	C75	111.1(4)

C19	C14	C5	121.6(4)	N8	N7	C106	117.7(4)
C16	C15	C14	121.0(5)	C75	N7	C106	130.7(4)
C17	C16	C15	119.3(5)	C81	N8	N7	106.3(4)
C16	C17	Br2	119.0(4)	C106	N9	C108	116.6(5)
C16	C17	C18	121.3(5)	N7	C75	C76	105.9(4)
C18	C17	Br2	119.6(4)	N7	C75	C80	131.9(5)
C19	C18	C17	119.1(5)	C76	C75	C80	122.0(5)
C18	C19	C14	120.7(5)	C75	C76	C77	121.5(4)
C21	C20	C4	121.8(4)	C75	C76	C81	104.9(4)
C21	C20	C25	117.8(4)	C81	C76	C77	133.5(5)
C25	C20	C4	120.5(4)	C76	C77	C82	117.9(4)
C20	C21	C22	121.5(5)	C78	C77	C76	117.6(4)
C23	C22	C21	118.7(5)	C78	C77	C82	124.5(5)
C22	C23	Br3	119.2(4)	C77	C78	C79	119.9(5)
C22	C23	C24	121.4(5)	C77	C78	C88	119.7(4)
C24	C23	Br3	119.4(4)	C79	C78	C88	120.5(4)
C23	C24	C25	119.2(5)	C78	C79	C94	118.2(4)
C24	C25	C20	121.3(5)	C80	C79	C78	123.7(4)
C27	C26	C3	120.0(5)	C80	C79	C94	118.2(4)
C27	C26	C31	118.6(5)	C75	C80	C100	122.1(4)
C31	C26	C3	121.4(5)	C79	C80	C75	115.2(4)
C26	C27	C28	121.6(6)	C79	C80	C100	122.6(4)
C29	C28	C27	118.2(6)	N8	C81	C76	111.8(5)

C28	C29	Br4	118.7(5)	C83	C82	C77	121.5(4)
C30	C29	Br4	119.9(5)	C83	C82	C87	117.8(5)
C30	C29	C28	121.5(5)	C87	C82	C77	120.4(4)
C29	C30	C31	120.0(6)	C84	C83	C82	121.4(5)
C26	C31	C30	120.1(6)	C83	C84	C85	119.3(5)
N3	C32	N1	117.4(4)	C84	C85	Br12	119.6(4)
C37	C32	N1	116.0(5)	C84	C85	C86	121.3(5)
C37	C32	N3	126.6(5)	C86	C85	Br12	119.1(4)
N3	C34	C35	120.0(6)	C87	C86	C85	118.6(5)
C36	C35	C34	120.0(6)	C86	C87	C82	121.6(5)
C37	C36	C35	120.3(6)	C89	C88	C78	121.6(5)
C32	C37	C36	117.5(6)	C89	C88	C93	118.1(5)
N5	N4	C38	111.3(4)	C93	C88	C78	120.3(5)
N5	N4	C69	117.2(4)	C88	C89	C90	121.8(6)
C38	N4	C69	131.6(4)	C91	C90	C89	118.7(5)
C44	N5	N4	106.2(4)	C90	C91	Br11	119.9(4)
C69	N6	C71	115.8(5)	C92	C91	Br11	118.7(5)
N4	C38	C39	105.8(4)	C92	C91	C90	121.4(5)
N4	C38	C43	132.2(4)	C91	C92	C93	118.8(6)
C39	C38	C43	122.0(4)	C88	C93	C92	121.1(5)
C38	C39	C40	121.5(4)	C95	C94	C79	120.7(4)
C38	C39	C44	105.2(4)	C99	C94	C79	120.9(5)
C40	C39	C44	133.3(5)	C99	C94	C95	118.4(5)

C39	C40	C63	118.6(4)	C96	C95	C94	121.3(5)
C41	C40	C39	117.2(4)	C97	C96	C95	118.4(5)
C41	C40	C63	124.2(4)	C96	C97	Br10	118.7(4)
C40	C41	C42	120.9(4)	C96	C97	C98	122.5(5)
C40	C41	C57	119.4(4)	C98	C97	Br10	118.7(4)
C42	C41	C57	119.7(4)	C97	C98	C99	118.6(5)
C41	C42	C51	118.5(4)	C94	C99	C98	120.8(5)
C43	C42	C41	122.0(4)	C101	C100	C80	122.7(5)
C43	C42	C51	119.5(4)	C101	C100	C105	117.6(5)
C38	C43	C45	122.2(4)	C105	C100	C80	119.7(4)
C42	C43	C38	116.3(4)	C102	C101	C100	122.0(5)
C42	C43	C45	121.6(4)	C101	C102	C103	118.8(5)
N5	C44	C39	111.5(4)	C102	C103	Br9	119.2(5)
C46	C45	C43	120.2(4)	C104	C103	Br9	119.7(5)
C46	C45	C50	119.1(4)	C104	C103	C102	121.0(5)
C50	C45	C43	120.7(4)	C103	C104	C105	119.9(6)
C45	C46	C47	120.8(5)	C104	C105	C100	120.6(5)
C48	C47	C46	118.3(4)	N9	C106	N7	116.1(4)
C47	C48	Br5	119.0(4)	N9	C106	C111	125.2(5)
C49	C48	Br5	119.0(4)	C111	C106	N7	118.7(5)
C49	C48	C47	122.0(4)	N9	C108	C109	123.2(6)
C48	C49	C50	118.9(5)	C108	C109	C110	119.0(6)
C49	C50	C45	120.8(5)	C109	C110	C111	118.8(6)

C52	C51	C42	121.1(4)	C106	C111	C110	117.1(6)	
C52	C51	C56	118.7(4)					

Table 6. Torsion Angles for **4e**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Br1	C11	C12	C13	177.8(4)	C43	C38	C39	C40	0.2(7)
Br2	C17	C18	C19	-179.0(4)	C43	C38	C39	C44	-178.5(4)
Br3	C23	C24	C25	177.5(4)	C43	C42	C51	C52	116.9(5)
Br4	C29	C30	C31	177.6(6)	C43	C42	C51	C56	-62.5(6)
N1	N2	C7	C2	-0.3(6)	C43	C45	C46	C47	176.9(4)
N1	C1	C2	C3	-179.1(4)	C43	C45	C50	C49	-176.8(5)
N1	C1	C2	C7	-1.2(5)	C44	C39	C40	C41	177.5(5)
N1	C1	C6	C5	179.9(5)	C44	C39	C40	C63	-3.2(8)
N1	C1	C6	C8	2.2(8)	C45	C46	C47	C48	-0.4(7)
N1	C32	C37	C36	-179.6(5)	C46	C45	C50	C49	1.2(7)
N2	N1	C1	C2	1.2(6)	C46	C47	C48	Br5	-177.8(3)
N2	N1	C1	C6	-177.2(5)	C46	C47	C48	C49	2.0(7)
N2	N1	C32	N3	-123.4(5)	C47	C48	C49	C50	-1.9(8)
N2	N1	C32	C37	54.5(7)	C48	C49	C50	C45	0.3(8)
N3	C32	C37	C36	-1.9(9)	C50	C45	C46	C47	-1.1(7)
N3	C34	C35	C36	-1.3(10)	C51	C42	C43	C38	-178.5(4)
C1	N1	N2	C7	-0.6(6)	C51	C42	C43	C45	0.4(7)
C1	N1	C32	N3	49.2(8)	C51	C52	C53	C54	0.8(7)
C1	N1	C32	C37	-132.9(6)	C52	C51	C56	C55	0.8(7)

C1	C2	C3	C4	-1.1(7)	C52	C53	C54	Br6	-179.8(4)
C1	C2	C3	C26	179.7(5)	C52	C53	C54	C55	0.8(7)
C1	C2	C7	N2	1.0(6)	C53	C54	C55	C56	-1.6(8)
C1	C6	C8	C9	-120.4(5)	C54	C55	C56	C51	0.8(7)
C1	C6	C8	C13	57.8(6)	C56	C51	C52	C53	-1.6(7)
C2	C1	C6	C5	1.7(7)	C57	C41	C42	C43	179.2(4)
C2	C1	C6	C8	-176.0(4)	C57	C41	C42	C51	-1.5(6)
C2	C3	C4	C5	1.4(7)	C57	C58	C59	C60	-1.1(9)
C2	C3	C4	C20	-178.7(4)	C58	C57	C62	C61	-0.1(8)
C2	C3	C26	C27	56.9(7)	C58	C59	C60	Br7	-178.8(5)
C2	C3	C26	C31	-122.5(6)	C58	C59	C60	C61	0.3(9)
C3	C2	C7	N2	178.5(5)	C59	C60	C61	C62	0.7(9)
C3	C4	C5	C6	-0.2(7)	C60	C61	C62	C57	-0.8(9)
C3	C4	C5	C14	179.4(4)	C62	C57	C58	C59	1.0(8)
C3	C4	C20	C21	75.3(6)	C63	C40	C41	C42	-177.9(4)
C3	C4	C20	C25	-106.0(6)	C63	C40	C41	C57	1.5(7)
C3	C26	C27	C28	179.8(5)	C63	C64	C65	C66	0.0(9)
C3	C26	C31	C30	179.4(6)	C64	C63	C68	C67	1.5(10)
C4	C3	C26	C27	-122.3(6)	C64	C65	C66	Br8	-178.9(5)
C4	C3	C26	C31	58.3(8)	C64	C65	C66	C67	1.8(10)
C4	C5	C6	C1	-1.4(7)	C65	C66	C67	C68	-2.0(11)
C4	C5	C6	C8	176.3(4)	C66	C67	C68	C63	0.3(12)
C4	C5	C14	C15	-109.3(5)	C68	C63	C64	C65	-1.6(9)

C4	C5	C14	C19	69.6(6)	C69	N4	N5	C44	-178.9(5)
C4	C20	C21	C22	175.9(5)	C69	N4	C38	C39	178.3(5)
C4	C20	C25	C24	-178.0(5)	C69	N4	C38	C43	-1.7(9)
C5	C4	C20	C21	-104.8(6)	C69	N6	C71	C72	1.3(8)
C5	C4	C20	C25	73.8(6)	C71	N6	C69	N4	177.4(4)
C5	C6	C8	C9	62.1(7)	C71	N6	C69	C74	-3.9(8)
C5	C6	C8	C13	-119.7(5)	C71	C72	C73	C74	-3.7(9)
C5	C14	C15	C16	-179.0(5)	C72	C73	C74	C69	1.4(8)
C5	C14	C19	C18	178.9(5)	Br9	C103	C104	C105	176.3(5)
C6	C1	C2	C3	-0.5(8)	Br10	C97	C98	C99	179.9(4)
C6	C1	C2	C7	177.3(5)	Br11	C91	C92	C93	-179.7(5)
C6	C5	C14	C15	70.3(6)	Br12	C85	C86	C87	-176.7(4)
C6	C5	C14	C19	-110.8(5)	N7	N8	C81	C76	-0.9(6)
C6	C8	C9	C10	177.0(5)	N7	C75	C76	C77	177.4(4)
C6	C8	C13	C12	-176.9(5)	N7	C75	C76	C81	0.0(5)
C7	C2	C3	C4	-178.2(5)	N7	C75	C80	C79	-178.8(5)
C7	C2	C3	C26	2.5(9)	N7	C75	C80	C100	-0.2(8)
C8	C9	C10	C11	0.2(9)	N7	C106	C111	C110	179.4(5)
C9	C8	C13	C12	1.4(7)	N8	N7	C75	C76	-0.6(5)
C9	C10	C11	Br1	-177.6(4)	N8	N7	C75	C80	175.5(5)
C9	C10	C11	C12	0.6(9)	N8	N7	C106	N9	125.5(5)
C10	C11	C12	C13	-0.4(9)	N8	N7	C106	C111	-52.2(7)
C11	C12	C13	C8	-0.6(8)	N9	C106	C111	C110	1.9(9)

C13	C8	C9	C10	-1.2(8)	N9	C108	C109	C110	0.7(10)
C14	C5	C6	C1	179.0(4)	C75	N7	N8	C81	0.9(6)
C14	C5	C6	C8	-3.3(7)	C75	N7	C106	N9	-46.1(7)
C14	C15	C16	C17	-1.0(8)	C75	N7	C106	C111	136.2(6)
C15	C14	C19	C18	-2.2(7)	C75	C76	C77	C78	2.1(7)
C15	C16	C17	Br2	178.9(4)	C75	C76	C77	C82	-175.6(4)
C15	C16	C17	C18	-0.1(8)	C75	C76	C81	N8	0.6(6)
C16	C17	C18	C19	0.0(8)	C75	C80	C100	C101	118.5(6)
C17	C18	C19	C14	1.1(8)	C75	C80	C100	C105	-62.1(7)
C19	C14	C15	C16	2.1(8)	C76	C75	C80	C79	-3.2(7)
C20	C4	C5	C6	180.0(4)	C76	C75	C80	C100	175.4(4)
C20	C4	C5	C14	-0.5(7)	C76	C77	C78	C79	-2.3(7)
C20	C21	C22	C23	1.8(8)	C76	C77	C78	C88	178.9(4)
C21	C20	C25	C24	0.7(8)	C76	C77	C82	C83	119.6(5)
C21	C22	C23	Br3	-179.5(4)	C76	C77	C82	C87	-54.3(7)
C21	C22	C23	C24	1.4(8)	C77	C76	C81	N8	-176.3(5)
C22	C23	C24	C25	-3.5(8)	C77	C78	C79	C80	-0.2(7)
C23	C24	C25	C20	2.4(8)	C77	C78	C79	C94	179.3(4)
C25	C20	C21	C22	-2.8(8)	C77	C78	C88	C89	116.8(6)
C26	C3	C4	C5	-179.4(5)	C77	C78	C88	C93	-62.0(7)
C26	C3	C4	C20	0.4(7)	C77	C82	C83	C84	-174.6(5)
C26	C27	C28	C29	-0.2(10)	C77	C82	C87	C86	174.6(5)
C27	C26	C31	C30	0.0(9)	C78	C77	C82	C83	-57.9(7)

C27	C28	C29	Br4	-178.4(5)	C78	C77	C82	C87	128.2(6)
C27	C28	C29	C30	1.9(11)	C78	C79	C80	C75	3.0(7)
C28	C29	C30	C31	-2.7(12)	C78	C79	C80	C100	-175.6(4)
C29	C30	C31	C26	1.7(11)	C78	C79	C94	C95	-65.1(6)
C31	C26	C27	C28	-0.7(9)	C78	C79	C94	C99	117.1(5)
C32	N1	N2	C7	173.5(5)	C78	C88	C89	C90	-179.2(5)
C32	N1	C1	C2	-171.8(5)	C78	C88	C93	C92	180.0(5)
C32	N1	C1	C6	9.8(9)	C79	C78	C88	C89	-62.0(7)
C32	N3	C34	C35	-0.9(9)	C79	C78	C88	C93	119.3(5)
C34	N3	C32	N1	-179.7(5)	C79	C80	C100	C101	-63.0(7)
C34	N3	C32	C37	2.6(9)	C79	C80	C100	C105	116.4(6)
C34	C35	C36	C37	2.0(10)	C79	C94	C95	C96	-178.2(5)
C35	C36	C37	C32	-0.5(10)	C79	C94	C99	C98	178.4(5)
Br5	C48	C49	C50	177.9(4)	C80	C75	C76	C77	0.8(7)
Br6	C54	C55	C56	179.0(4)	C80	C75	C76	C81	-176.6(4)
Br7	C60	C61	C62	179.8(4)	C80	C79	C94	C95	114.5(5)
Br8	C66	C67	C68	178.8(6)	C80	C79	C94	C99	-63.3(6)
N4	N5	C44	C39	-0.1(6)	C80	C100	C101	C102	176.9(5)
N4	C38	C39	C40	-179.9(4)	C80	C100	C105	C104	-176.8(5)
N4	C38	C39	C44	1.4(5)	C81	C76	C77	C78	178.5(5)
N4	C38	C43	C42	179.9(5)	C81	C76	C77	C82	0.9(8)
N4	C38	C43	C45	1.0(8)	C82	C77	C78	C79	175.2(4)
N4	C69	C74	C73	-178.7(5)	C82	C77	C78	C88	-3.6(7)

N5	N4	C38	C39	-1.6(5)	C82	C83	C84	C85	1.2(8)
N5	N4	C38	C43	178.4(5)	C83	C82	C87	C86	0.5(8)
N5	N4	C69	N6	125.4(5)	C83	C84	C85	Br12	176.7(4)
N5	N4	C69	C74	-53.5(6)	C83	C84	C85	C86	-1.8(8)
N6	C69	C74	C73	2.6(8)	C84	C85	C86	C87	1.8(8)
N6	C71	C72	C73	2.2(9)	C85	C86	C87	C82	-1.1(8)
C38	N4	N5	C44	1.0(6)	C87	C82	C83	C84	-0.5(8)
C38	N4	C69	N6	-54.5(7)	C88	C78	C79	C80	178.5(5)
C38	N4	C69	C74	126.7(6)	C88	C78	C79	C94	-2.0(7)
C38	C39	C40	C41	-0.8(7)	C88	C89	C90	C91	-0.2(9)
C38	C39	C40	C63	178.5(4)	C89	C88	C93	C92	1.2(8)
C38	C39	C44	N5	-0.9(6)	C89	C90	C91	Br11	-179.5(5)
C38	C43	C45	C46	-66.2(6)	C89	C90	C91	C92	0.0(10)
C38	C43	C45	C50	111.7(5)	C90	C91	C92	C93	0.8(10)
C39	C38	C43	C42	-0.2(7)	C91	C92	C93	C88	-1.4(10)
C39	C38	C43	C45	-179.0(4)	C93	C88	C89	C90	-0.4(8)
C39	C40	C41	C42	1.4(7)	C94	C79	C80	C75	-176.6(4)
C39	C40	C41	C57	-179.3(4)	C94	C79	C80	C100	4.8(7)
C39	C40	C63	C64	119.5(6)	C94	C95	C96	C97	1.0(8)
C39	C40	C63	C68	-59.0(7)	C95	C94	C99	C98	0.6(8)
C40	C39	C44	N5	-179.4(5)	C95	C96	C97	Br10	-179.6(4)
C40	C41	C42	C43	-1.5(7)	C95	C96	C97	C98	-2.0(8)
C40	C41	C42	C51	177.8(4)	C96	C97	C98	C99	2.2(9)

C40	C41	C57	C58	111.5(5)	C97	C98	C99	C94	-1.5(8)
C40	C41	C57	C62	-71.2(6)	C99	C94	C95	C96	-0.4(7)
C40	C63	C64	C65	179.9(5)	C100	C101	C102	C103	0.2(8)
C40	C63	C68	C67	-180.0(6)	C101	C100	C105	C104	2.6(8)
C41	C40	C63	C64	-61.3(7)	C101	C102	C103	Br9	-176.1(4)
C41	C40	C63	C68	120.3(6)	C101	C102	C103	C104	2.1(9)
C41	C42	C43	C38	0.8(7)	C102	C103	C104	C105	-2.0(10)
C41	C42	C43	C45	179.7(4)	C103	C104	C105	C100	-0.5(9)
C41	C42	C51	C52	-62.3(6)	C105	C100	C101	C102	-2.5(8)
C41	C42	C51	C56	118.2(5)	C106	N7	N8	C81	-172.3(4)
C41	C57	C58	C59	178.3(5)	C106	N7	C75	C76	171.5(5)
C41	C57	C62	C61	-177.3(5)	C106	N7	C75	C80	-12.4(9)
C42	C41	C57	C58	-69.1(6)	C106	N9	C108	C109	1.2(8)
C42	C41	C57	C62	108.1(5)	C108	N9	C106	N7	180.0(5)
C42	C43	C45	C46	114.9(5)	C108	N9	C106	C111	-2.5(8)
C42	C43	C45	C50	-67.1(6)	C108	C109	C110	C111	-1.3(10)
C42	C51	C52	C53	178.9(4)	C109	C110	C111	C106	0.1(9)
C42	C51	C56	C55	-179.7(4)					

Table 7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **4e**.

Atom	x	y	z	U(eq)
H7	8441	8369	6508	49
H9	8621	7788	9061	41
H10	9543	7869	9833	51

H12	10293	9164	9325	50
H13	9364	9083	8556	39
H15	7435	9060	8863	45
H16	6945	9065	9636	51
H18	6279	7641	9408	44
H19	6766	7635	8632	40
H21	5928	7579	7478	44
H22	4576	7529	7539	45
H24	4586	8979	7891	46
H25	5946	9016	7880	43
H27	7230	7700	6444	53
H28	6421	7658	5622	66
H30	5301	8899	5944	76
H31	6087	8930	6771	58
H34	11149	7694	8866	59
H35	12114	8295	8781	81
H36	11836	8902	8141	78
H37	10581	8940	7622	52
H44	10476	6776	9925	45
H46	9408	5979	7825	34
H47	8466	5970	7049	38
H49	9302	7290	6652	45
H50	10238	7295	7423	39
H52	12244	7245	7797	37
H53	12766	7169	7033	39
H55	11626	5863	6734	40
H56	11129	5931	7507	38
H58	12767	5894	8501	50
H59	14137	5842	8481	65
H61	14384	7273	8879	56
H62	13041	7318	8921	46
H64	12692	6073	9721	51
H65	13519	6158	10534	59
H67	12561	7501	10699	74
H68	11749	7415	9893	64
H71	7663	7307	7546	62
H72	6730	6715	7694	71
H73	7030	6197	8397	65

H74	8284	6193	8908	44
H81	10049	5063	6230	43
H83	7656	4388	5707	43
H84	7580	4378	4811	46
H86	8858	5649	4898	47
H87	8929	5656	5794	47
H89	6608	4308	6637	49
H90	5296	4314	6186	59
H92	5633	5693	5671	63
H93	6960	5672	6112	54
H95	6821	5600	7378	42
H96	5766	5570	7840	49
H98	6406	4184	8309	50
H99	7469	4216	7851	45
H101	8389	5457	8358	43
H102	8601	5294	9242	51
H104	9702	4017	8998	65
H105	9496	4181	8108	51
H108	10828	5583	8949	52
H109	11911	5071	9201	63
H110	12253	4495	8610	69
H111	11442	4438	7775	56

Table 8. Solvent masks information for **4e.**

Number	X	Y	Z	Volume	Electron count Content
1	-0.009	0.119	0.869	9	-1
2	0.500	0.000	0.500	1506	548
3	0.500	0.500	1.000	1506	548
4	-0.009	0.381	0.369	8	-1
5	0.008	0.619	0.631	8	-1
6	0.008	0.881	0.131	8	-1

X-Ray Crystallographic Data of A'

Table 1. Crystal Data and Summary of X-ray Data Collection for **A'**

	A'
formula	$C_{36}H_{44}Cl_2F_{12}N_6P_2Rh_2$
fw	1127.43
T (K)	296(2)
crystsyst	Triclinic
space group	P -1
a (Å)	8.0891(10)
b (Å)	11.6008(15)
c (Å)	11.6973(15)
α (deg)	93.667(2)
β (deg)	97.710(2)
γ (deg)	99.109(2)
V (Å^3)	1070.0(2)
Z	1
D_{calc} (g·cm^{-3})	1.750
μ (mm^{-1})	1.059
F(000)	564
cryst size (mm)	0.220 x 0.210 x 0.180
max. 2θ (deg)	52.996
no. of reflns collected	7.17
no. of indepreflns/R_{int}	4433/0.0350
no. of params	271
goodness-of-fit on F^2	1.070
R_1, wR_2 [I> 2σ(I)]	0.0586, 0.1636
R_1, wR_2 (all data)	0.0619, 0.1666
largest diff peak and hole (e Å^{-3})	1.846, −2.085

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **A'**. Ueq is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Rh(1)	4215(1)	2784(1)	1965(1)	28(1)
P(1)	831(2)	7581(2)	3352(2)	68(1)
N(1)	4998(5)	1186(3)	2362(3)	34(1)
N(2)	2867(5)	1566(4)	631(3)	38(1)
N(3)	3145(5)	456(3)	717(3)	36(1)
Cl(1)	6489(2)	3066(1)	844(1)	44(1)
F(1)	1259(19)	8860(9)	3292(13)	233(5)
F(2)	-1039(7)	7701(10)	3090(7)	161(4)
F(3)	708(11)	7628(11)	4643(5)	187(5)
F(4)	424(18)	6267(10)	3414(15)	244(6)
F(5)	2669(8)	7461(14)	3614(9)	261(8)
F(6)	1061(10)	7635(12)	2096(6)	183(5)
C(1)	6170(7)	1048(5)	3242(4)	42(1)
C(2)	6605(8)	-9(5)	3457(5)	50(1)
C(3)	5839(8)	-980(5)	2731(5)	53(1)
C(4)	4646(7)	-874(5)	1801(5)	46(1)
C(5)	4274(6)	228(4)	1658(4)	35(1)
C(6)	2276(7)	-262(5)	-207(4)	45(1)
C(7)	1420(7)	409(5)	-900(4)	48(1)
C(8)	1844(7)	1551(5)	-353(4)	45(1)
C(9)	3610(6)	3262(5)	3639(4)	40(1)
C(10)	4984(6)	4085(4)	3375(4)	39(1)
C(11)	4361(7)	4638(4)	2384(4)	40(1)
C(12)	2655(6)	4126(4)	2009(4)	40(1)
C(13)	2186(6)	3265(5)	2789(4)	42(1)
C(14)	3620(9)	2501(6)	4634(5)	58(2)
C(15)	6724(7)	4399(6)	4060(5)	53(1)
C(16)	5339(9)	5605(5)	1854(6)	60(2)
C(17)	1535(9)	4472(6)	1011(5)	58(2)
C(18)	475(8)	2564(7)	2753(6)	66(2)

Table 3. Bond lengths [A] and angles [deg] for **A'**.

Rh(1)-N(2)	2.096(4)	C(4)-H(4)	0.9300
Rh(1)-N(1)	2.112(4)	C(6)-C(7)	1.358(8)

Rh(1)-C(10)	2.120(4)	C(6)-H(6)	0.9300
Rh(1)-C(13)	2.140(4)	C(7)-C(8)	1.404(8)
Rh(1)-C(9)	2.141(4)	C(7)-H(7)	0.9300
Rh(1)-C(11)	2.156(5)	C(8)-H(8)	0.9300
Rh(1)-C(12)	2.156(4)	C(9)-C(13)	1.418(7)
Rh(1)-Cl(1)	2.3912(12)	C(9)-C(10)	1.427(8)
P(1)-F(1)	1.478(11)	C(9)-C(14)	1.505(7)
P(1)-F(5)	1.507(7)	C(10)-C(11)	1.431(7)
P(1)-F(6)	1.509(6)	C(10)-C(15)	1.502(7)
P(1)-F(4)	1.516(11)	C(11)-C(12)	1.413(7)
P(1)-F(3)	1.525(6)	C(11)-C(16)	1.485(8)
P(1)-F(2)	1.532(6)	C(12)-C(13)	1.437(8)
N(1)-C(1)	1.338(6)	C(12)-C(17)	1.495(7)
N(1)-C(5)	1.343(6)	C(13)-C(18)	1.484(8)
N(2)-C(8)	1.322(6)	C(14)-H(14A)	0.9600
N(2)-N(3)	1.349(6)	C(14)-H(14B)	0.9600
N(3)-C(6)	1.361(6)	C(14)-H(14C)	0.9600
N(3)-C(5)	1.400(6)	C(15)-H(15A)	0.9600
C(1)-C(2)	1.357(8)	C(15)-H(15B)	0.9600
C(1)-H(1)	0.9300	C(15)-H(15C)	0.9600
C(2)-C(3)	1.375(8)	C(16)-H(16A)	0.9600
C(2)-H(2)	0.9300	C(16)-H(16B)	0.9600
C(3)-C(4)	1.380(8)	C(16)-H(16C)	0.9600
C(3)-H(3)	0.9300	C(17)-H(17A)	0.9600
C(4)-C(5)	1.374(7)	C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600	F(6)-P(1)-F(2)	92.2(4)
C(18)-H(18A)	0.9600	F(4)-P(1)-F(2)	93.0(7)
C(18)-H(18B)	0.9600	F(3)-P(1)-F(2)	90.0(4)
N(2)-Rh(1)-N(1)	75.81(15)	C(1)-N(1)-C(5)	117.3(4)
N(2)-Rh(1)-C(10)	166.10(18)	C(1)-N(1)-Rh(1)	125.7(3)
N(1)-Rh(1)-C(10)	111.41(17)	C(5)-N(1)-Rh(1)	117.0(3)
N(2)-Rh(1)-C(13)	100.69(18)	C(8)-N(2)-N(3)	106.1(4)
N(1)-Rh(1)-C(13)	116.91(18)	C(8)-N(2)-Rh(1)	138.9(4)
C(10)-Rh(1)-C(13)	65.54(19)	N(3)-N(2)-Rh(1)	114.9(3)
N(2)-Rh(1)-C(9)	130.26(19)	N(2)-N(3)-C(6)	110.8(4)
N(1)-Rh(1)-C(9)	96.94(17)	N(2)-N(3)-C(5)	118.4(4)
C(10)-Rh(1)-C(9)	39.1(2)	C(6)-N(3)-C(5)	130.8(4)
C(13)-Rh(1)-C(9)	38.68(18)	N(1)-C(1)-C(2)	122.8(5)

N(2)-Rh(1)-C(11)	134.75(18)	N(1)-C(1)-H(1)	118.6
N(1)-Rh(1)-C(11)	149.44(17)	C(2)-C(1)-H(1)	118.6
C(10)-Rh(1)-C(11)	39.10(19)	C(1)-C(2)-C(3)	119.0(5)
C(13)-Rh(1)-C(11)	64.7(2)	C(1)-C(2)-H(2)	120.5
C(9)-Rh(1)-C(11)	64.8(2)	C(3)-C(2)-H(2)	120.5
N(2)-Rh(1)-C(12)	102.98(17)	C(2)-C(3)-C(4)	120.1(5)
N(1)-Rh(1)-C(12)	155.87(19)	C(2)-C(3)-H(3)	120.0
C(10)-Rh(1)-C(12)	65.39(18)	C(4)-C(3)-H(3)	120.0
C(13)-Rh(1)-C(12)	39.1(2)	C(5)-C(4)-C(3)	116.8(5)
C(9)-Rh(1)-C(12)	65.00(18)	C(5)-C(4)-H(4)	121.6
C(11)-Rh(1)-C(12)	38.2(2)	C(3)-C(4)-H(4)	121.6
N(2)-Rh(1)-Cl(1)	88.27(12)	N(1)-C(5)-C(4)	124.0(5)
N(1)-Rh(1)-Cl(1)	86.72(11)	N(1)-C(5)-N(3)	113.8(4)
C(10)-Rh(1)-Cl(1)	103.71(15)	C(4)-C(5)-N(3)	122.1(4)
C(13)-Rh(1)-Cl(1)	156.06(16)	C(7)-C(6)-N(3)	107.1(5)
C(9)-Rh(1)-Cl(1)	141.10(14)	C(7)-C(6)-H(6)	126.4
C(11)-Rh(1)-Cl(1)	93.17(15)	N(3)-C(6)-H(6)	126.4
C(12)-Rh(1)-Cl(1)	117.41(15)	C(6)-C(7)-C(8)	105.5(4)
F(1)-P(1)-F(5)	92.2(8)	C(6)-C(7)-H(7)	127.2
F(1)-P(1)-F(6)	79.1(7)	C(8)-C(7)-H(7)	127.2
F(5)-P(1)-F(6)	88.0(5)	N(2)-C(8)-C(7)	110.4(5)
F(1)-P(1)-F(4)	179.0(8)	N(2)-C(8)-H(8)	124.8
F(5)-P(1)-F(4)	86.9(8)	C(7)-C(8)-H(8)	124.8
F(6)-P(1)-F(4)	100.7(9)	C(13)-C(9)-C(10)	108.3(4)
F(1)-P(1)-F(3)	96.4(8)	C(13)-C(9)-C(14)	124.4(5)
F(5)-P(1)-F(3)	89.8(5)	C(10)-C(9)-C(14)	127.3(5)
F(6)-P(1)-F(3)	174.9(7)	C(13)-C(9)-Rh(1)	70.6(2)
F(4)-P(1)-F(3)	83.7(7)	C(10)-C(9)-Rh(1)	69.6(2)
F(1)-P(1)-F(2)	87.9(7)	C(14)-C(9)-Rh(1)	125.3(4)
F(5)-P(1)-F(2)	179.8(4)	C(9)-C(10)-C(11)	107.4(4)
C(9)-C(10)-C(15)	126.8(5)	C(18)-C(13)-Rh(1)	127.0(4)
C(11)-C(10)-C(15)	125.6(5)	C(9)-C(14)-H(14A)	109.3
C(9)-C(10)-Rh(1)	71.3(3)	C(9)-C(14)-H(14B)	109.6
C(11)-C(10)-Rh(1)	71.8(3)	H(14A)-C(14)-H(14B)	109.5
C(15)-C(10)-Rh(1)	126.3(3)	C(9)-C(14)-H(14C)	109.6
C(12)-C(11)-C(10)	108.6(5)	H(14A)-C(14)-H(14C)	109.5
C(12)-C(11)-C(16)	125.7(5)	H(14B)-C(14)-H(14C)	109.5
C(10)-C(11)-C(16)	125.6(5)	C(10)-C(15)-H(15A)	109.6

C(12)-C(11)-Rh(1)	70.9(3)	C(10)-C(15)-H(15B)	109.4
C(10)-C(11)-Rh(1)	69.1(3)	H(15A)-C(15)-H(15B)	109.5
C(16)-C(11)-Rh(1)	126.8(4)	C(10)-C(15)-H(15C)	109.4
C(11)-C(12)-C(13)	107.7(4)	H(15A)-C(15)-H(15C)	109.5
C(11)-C(12)-C(17)	125.4(5)	H(15B)-C(15)-H(15C)	109.5
C(13)-C(12)-C(17)	126.9(5)	C(11)-C(16)-H(16A)	109.6
C(11)-C(12)-Rh(1)	70.9(3)	C(11)-C(16)-H(16B)	109.5
C(13)-C(12)-Rh(1)	69.9(3)	H(16A)-C(16)-H(16B)	109.5
C(17)-C(12)-Rh(1)	126.9(4)	C(11)-C(16)-H(16C)	109.3
C(9)-C(13)-C(12)	108.0(5)	H(16A)-C(16)-H(16C)	109.5
C(9)-C(13)-C(18)	126.2(5)	H(16B)-C(16)-H(16C)	109.5
C(12)-C(13)-C(18)	125.7(5)	C(12)-C(17)-H(17A)	109.4
C(9)-C(13)-Rh(1)	70.7(2)	C(12)-C(17)-H(17B)	109.6
C(12)-C(13)-Rh(1)	71.1(3)	H(17A)-C(17)-H(17B)	109.5
C(13)-C(18)-H(18B)	109.5	C(12)-C(17)-H(17C)	109.4
H(18A)-C(18)-H(18B)	109.5	H(17A)-C(17)-H(17C)	109.5
C(13)-C(18)-H(18C)	109.3	H(17B)-C(17)-H(17C)	109.5
H(18A)-C(18)-H(18C)	109.5	C(13)-C(18)-H(18A)	109.6
H(18B)-C(18)-H(18C)	109.5		

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **A'**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Rh(1)	28(1)	31(1)	26(1)	-1(1)	-1(1)	9(1)
P(1)	36(1)	120(2)	51(1)	24(1)	-2(1)	15(1)
N(1)	33(2)	38(2)	31(2)	5(2)	1(2)	10(2)
N(2)	35(2)	39(2)	36(2)	-5(2)	-4(2)	4(2)
N(3)	34(2)	36(2)	36(2)	-4(2)	3(2)	5(2)
Cl(1)	42(1)	48(1)	45(1)	3(1)	13(1)	11(1)
F(1)	277(14)	134(8)	281(14)	4(9)	67(11)	-1(9)
F(2)	56(3)	292(12)	152(6)	84(7)	16(3)	51(5)
F(3)	141(6)	360(15)	64(3)	21(6)	16(4)	55(8)
F(4)	237(13)	134(8)	364(19)	66(11)	45(13)	17(8)
F(5)	66(4)	510(20)	250(11)	267(14)	29(5)	79(8)
F(6)	113(5)	377(15)	76(4)	67(6)	19(3)	65(7)
C(1)	43(3)	47(3)	35(2)	2(2)	0(2)	10(2)
C(2)	52(3)	53(3)	47(3)	13(2)	-3(2)	20(3)
C(3)	61(4)	42(3)	60(3)	14(2)	9(3)	17(3)

C(4)	50(3)	39(2)	50(3)	2(2)	10(2)	10(2)
C(5)	31(2)	36(2)	40(2)	2(2)	9(2)	6(2)
C(6)	40(3)	48(3)	45(3)	-14(2)	9(2)	-1(2)
C(7)	39(3)	64(3)	34(2)	-11(2)	-8(2)	5(2)
C(8)	38(3)	59(3)	34(2)	1(2)	-6(2)	9(2)
C(9)	42(3)	50(3)	29(2)	-3(2)	5(2)	17(2)
C(10)	44(3)	41(2)	31(2)	-7(2)	-1(2)	14(2)
C(11)	51(3)	32(2)	37(2)	-5(2)	2(2)	15(2)
C(12)	41(3)	44(2)	38(2)	-2(2)	0(2)	21(2)
C(13)	34(2)	55(3)	39(2)	-1(2)	9(2)	18(2)
C(14)	68(4)	76(4)	38(3)	16(3)	16(2)	26(3)
C(15)	47(3)	58(3)	48(3)	-12(3)	-14(2)	12(3)
C(16)	78(4)	37(2)	63(4)	5(3)	8(3)	4(3)
C(17)	63(4)	64(3)	52(3)	7(3)	-7(3)	35(3)
C(18)	40(3)	89(5)	71(4)	7(4)	9(3)	11(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **A'**.

	x	y	z	U(eq)
H(1)	6710	1704	3727	50
H(2)	7408	-75	4087	60
H(3)	6125	-1710	2867	64
H(4)	4118	-1517	1295	55
H(6)	2270	-1062	-339	55
H(7)	704	164	-1593	57
H(8)	1458	2204	-641	54
H(14A)	2981	2791	5191	87
H(14B)	4764	2519	4993	87
H(14C)	3119	1710	4355	87
H(15A)	6744	5034	4634	80
H(15B)	7527	4634	3550	80
H(15C)	7014	3731	4435	80
H(16A)	4714	5732	1129	90
H(16B)	6408	5400	1726	90
H(16C)	5527	6308	2367	90
H(17A)	1045	5128	1263	88
H(17B)	651	3826	720	88
H(17C)	2193	4687	408	88

H(18A)	566	1858	3125	100
H(18B)	-43	2368	1963	100
H(18C)	-206	3015	3150	100

Table 6. Torsion angles [deg] for **A'**.

C(8)-N(2)-N(3)-C(6)	-0.8(5)	Rh(1)-C(10)-C(11)-C(16)	-121.0(5)
Rh(1)-N(2)-N(3)-C(6)	-177.4(3)	C(9)-C(10)-C(11)-Rh(1)	-62.8(3)
C(8)-N(2)-N(3)-C(5)	176.5(4)	C(15)-C(10)-C(11)-Rh(1)	122.0(5)
Rh(1)-N(2)-N(3)-C(5)	-0.1(5)	C(10)-C(11)-C(12)-C(13)	1.5(5)
C(5)-N(1)-C(1)-C(2)	-1.8(7)	C(16)-C(11)-C(12)-C(13)	-177.4(5)
Rh(1)-N(1)-C(1)-C(2)	179.3(4)	Rh(1)-C(11)-C(12)-C(13)	60.5(3)
N(1)-C(1)-C(2)-C(3)	1.3(9)	C(10)-C(11)-C(12)-C(17)	178.9(5)
C(1)-C(2)-C(3)-C(4)	-0.1(9)	C(16)-C(11)-C(12)-C(17)	0.0(8)
C(2)-C(3)-C(4)-C(5)	-0.5(8)	Rh(1)-C(11)-C(12)-C(17)	-122.2(5)
C(1)-N(1)-C(5)-C(4)	1.1(7)	C(10)-C(11)-C(12)-Rh(1)	-59.0(3)
Rh(1)-N(1)-C(5)-C(4)	-179.9(4)	C(16)-C(11)-C(12)-Rh(1)	122.1(5)
C(1)-N(1)-C(5)-N(3)	-176.1(4)	C(10)-C(9)-C(13)-C(12)	-2.0(5)
Rh(1)-N(1)-C(5)-N(3)	2.9(5)	C(14)-C(9)-C(13)-C(12)	178.3(4)
C(3)-C(4)-C(5)-N(1)	0.0(8)	Rh(1)-C(9)-C(13)-C(12)	-61.6(3)
C(3)-C(4)-C(5)-N(3)	177.0(5)	C(10)-C(9)-C(13)-C(18)	-178.1(5)
N(2)-N(3)-C(5)-N(1)	-1.8(6)	C(14)-C(9)-C(13)-C(18)	2.2(8)
C(6)-N(3)-C(5)-N(1)	174.9(5)	Rh(1)-C(9)-C(13)-C(18)	122.3(6)
N(2)-N(3)-C(5)-C(4)	-179.1(4)	C(10)-C(9)-C(13)-Rh(1)	59.6(3)
C(6)-N(3)-C(5)-C(4)	-2.4(8)	C(14)-C(9)-C(13)-Rh(1)	-120.1(5)
N(2)-N(3)-C(6)-C(7)	-0.1(6)	C(11)-C(12)-C(13)-C(9)	0.3(5)
C(5)-N(3)-C(6)-C(7)	-176.9(5)	C(17)-C(12)-C(13)-C(9)	-177.0(5)
N(3)-C(6)-C(7)-C(8)	0.8(6)	Rh(1)-C(12)-C(13)-C(9)	61.4(3)
N(3)-N(2)-C(8)-C(7)	1.4(6)	C(11)-C(12)-C(13)-C(18)	176.4(5)
Rh(1)-N(2)-C(8)-C(7)	176.7(4)	C(17)-C(12)-C(13)-C(18)	-0.9(8)
C(6)-C(7)-C(8)-N(2)	-1.4(7)	Rh(1)-C(12)-C(13)-C(18)	-122.5(5)
C(13)-C(9)-C(10)-C(11)	2.9(5)	C(11)-C(12)-C(13)-Rh(1)	-61.1(3)
C(14)-C(9)-C(10)-C(11)	-177.4(5)	C(17)-C(12)-C(13)-Rh(1)	121.6(5)
Rh(1)-C(9)-C(10)-C(11)	63.2(3)	C(15)-C(10)-C(11)-C(16)	1.0(8)
C(13)-C(9)-C(10)-C(15)	178.0(5)		
C(14)-C(9)-C(10)-C(15)	-2.3(8)		
Rh(1)-C(9)-C(10)-C(15)	-121.8(5)		
C(13)-C(9)-C(10)-Rh(1)	-60.3(3)		
C(14)-C(9)-C(10)-Rh(1)	119.5(5)		

C(9)-C(10)-C(11)-C(12)	-2.7(5)
C(15)-C(10)-C(11)-C(12)	-177.9(4)
Rh(1)-C(10)-C(11)-C(12)	60.1(3)
C(9)-C(10)-C(11)-C(16)	176.2(5)

X-Ray Crystallographic Data of B.

Table 1. Crystal Data and Summary of X-ray Data Collection for **B**

	B
formula	$C_{18}H_{21}ClN_3Rh$
fw	417.74
T (K)	296.15
crystsyst	Orthorhombic
space group	Pnma
a (Å)	15.8057(15)
b (Å)	15.6386(16)
c (Å)	7.5003(7)
α (deg)	90
β (deg)	90
γ (deg)	90
V (Å^3)	1853.9(3)
Z	4
D_{calc} (g·cm^{-3})	1.497
μ (mm^{-1})	1.067
F(000)	848.0
cryst size (mm)	0.22 × 0.21 × 0.18
max. 2θ (deg)	52.998
no. of reflns collected	9232
no. of indepreflns/R_{int}	1726/0.0550
no. of params	144
goodness-of-fit on F^2	1.055
R_1, wR_2 [I> 2σ(I)]	0.0607, 0.1794
R_1, wR_2 (all data)	0.0836, 0.1936
largest diff peak and hole (e Å^{-3})	1.42, −0.68

Table 2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **B**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
Rh1	4472.8(4)	2500	3711.0(10)	44.4(4)
Cl1	5106(3)	2500	6618(6)	42.1(12)
N1	2992(6)	3179(5)	5483(13)	48(2)
C3	3723(6)	3529(6)	4658(16)	52(3)
C1	3660(7)	4434(6)	4733(19)	67(3)
C2	2890(8)	4644(5)	5605(19)	75(4)
N2	2477(6)	3869(6)	6068(14)	62(3)
C9	4466(4)	2041(5)	982(10)	50.4(16)
C7	2725(7)	618(4)	5767(16)	57(4)
C8	2101(6)	1123(6)	6540(18)	78(5)
C5	2166(5)	2009(6)	6477(15)	59(3)
C4	2854(5)	2390(4)	5639(12)	48(3)
N3	3477(5)	1885(5)	4866(12)	48(3)
C6	3413(6)	999(5)	4929(13)	59(3)
C10	5217(5)	1765(5)	1809(10)	56.2(17)
C11	5691(7)	2500	2320(16)	69(3)
C14	6570(13)	2500	3220(30)	112(5)
C13	5546(7)	856(7)	2070(20)	96(3)
C12	3805(7)	1498(6)	171(12)	94(3)
Cl1A	5126(4)	2892(4)	6547(8)	42.1(12)

Table 3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **B**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
Rh1	28.1(5)	78.1(6)	27.2(5)	0	1.2(2)	0
Cl1	42.2(14)	46(2)	37.7(13)	0	-4.0(11)	0
N1	43(4)	57(4)	44(4)	-3(3)	2(3)	8(3)
C3	49(6)	58(6)	48(6)	-1(5)	-1(5)	6(5)
C1	68(5)	65(4)	68(5)	-3(4)	3(4)	1(4)
C2	75(4)	75(4)	75(4)	0(2)	1(2)	-1(2)
N2	55(4)	68(4)	62(4)	-6(4)	-1(4)	7(4)
C9	50(4)	75(4)	26(3)	-8(3)	8(3)	-2(3)
C7	66(8)	39(5)	66(7)	-4(5)	14(6)	-8(6)

C8	61(11)	96(12)	77(13)	6(9)	21(9)	-10(9)
C5	36(7)	90(9)	52(9)	4(6)	12(6)	0(6)
C4	35(4)	71(7)	38(5)	-3(6)	-2(4)	5(6)
N3	39(6)	69(7)	36(6)	1(5)	4(5)	8(6)
C6	56(5)	63(5)	57(5)	3(4)	4(4)	1(4)
C10	49(4)	78(4)	42(4)	0(3)	14(3)	13(3)
C11	30(5)	132(10)	45(6)	0	2(4)	0
C14	110(6)	114(6)	111(6)	0	0(2)	0
C13	95(4)	96(4)	96(4)	1(2)	3(2)	6.9(19)
C12	113(8)	116(7)	54(5)	-15(5)	-1(6)	-52(6)
Cl1A	42.2(14)	46(2)	37.7(13)	0	-4.0(11)	0

Table 4. Bond Lengths for **B**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Rh1	Cl1	2.399(4)	C2	N2	1.4200
Rh1	C3	2.121(8)	C9	C9[1]	1.435(16)
Rh1	C9[1]	2.169(7)	C9	C10	1.408(11)
Rh1	C9	2.169(7)	C9	C12	1.478(10)
Rh1	N3	2.037(6)	C7	C8	1.3900
Rh1	C10	2.177(7)	C7	C6	1.3900
Rh1	C10[1]	2.177(7)	C8	C5	1.3900
Rh1	C11	2.190(11)	C5	C4	1.3900
Rh1	Cl1A[1]	2.443(6)	C4	N3	1.3900
Rh1	Cl1A	2.443(6)	N3	C6	1.3900
N1	C3	1.4200	C10	C11	1.425(11)
N1	N2	1.4200	C10	C13	1.525(13)
N1	C4	1.259(11)	C11	C10[1]	1.425(11)
C3	C1	1.4200	C11	C14	1.54(2)

C1	C2	1.4200	Cl1A	Cl1A[1]	1.225(14)

Table 5. Bond Angles for **B**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C3	Rh1	Cl1	85.9(3)	N2	N1	C3	108.0
C3	Rh1	C9	124.4(4)	C4	N1	C3	124.0(7)
C3	Rh1	C9[1]	93.6(4)	C4	N1	N2	128.0(7)
C3	Rh1	C10	157.2(4)	N1	C3	Rh1	108.0(5)
C3	Rh1	C10[1]	96.9(4)	C1	C3	Rh1	144.0(5)
C3	Rh1	C11	130.6(3)	C1	C3	N1	108.0
C9[1]	Rh1	Cl1	149.3(2)	C3	C1	C2	108.0
C9	Rh1	Cl1	149.3(2)	C1	C2	N2	108.0
C9	Rh1	C9[1]	38.6(4)	N1	N2	C2	108.0
C9[1]	Rh1	C10	63.8(3)	C9[1]	C9	Rh1	70.7(2)
C9	Rh1	C10[1]	63.8(3)	C9[1]	C9	C12	125.1(5)
C9[1]	Rh1	C10[1]	37.8(3)	C10	C9	Rh1	71.4(4)
C9	Rh1	C10	37.8(3)	C10	C9	C9[1]	107.9(5)
C9[1]	Rh1	C11	63.6(3)	C10	C9	C12	126.9(8)
C9	Rh1	C11	63.6(3)	C12	C9	Rh1	125.6(5)
C9[1]	Rh1	Cl1A[1]	155.1(2)	C8	C7	C6	120.0
C9[1]	Rh1	Cl1A	137.8(3)	C5	C8	C7	120.0
C9	Rh1	Cl1A	155.1(2)	C8	C5	C4	120.0
C9	Rh1	Cl1A[1]	137.8(3)	N1	C4	C5	126.7(6)

N3	Rh1	Cl1	86.3(3)	N1	C4	N3	113.3(6)
N3	Rh1	C3	77.5(4)	N3	C4	C5	120.0
N3	Rh1	C9[1]	123.6(3)	C4	N3	Rh1	117.2(4)
N3	Rh1	C9	104.0(3)	C4	N3	C6	120.0
N3	Rh1	C10	116.5(3)	C6	N3	Rh1	122.8(4)
N3	Rh1	C10[1]	160.9(3)	N3	C6	C7	120.0
N3	Rh1	C11	151.8(2)	C9	C10	Rh1	70.8(4)
C10	Rh1	Cl1	111.7(2)	C9	C10	C11	108.3(7)
C10[1]	Rh1	Cl1	111.7(2)	C9	C10	C13	129.0(8)
C10	Rh1	C10[1]	63.8(4)	C11	C10	Rh1	71.4(5)
C10[1]	Rh1	C11	38.1(3)	C11	C10	C13	122.6(8)
C10	Rh1	C11	38.1(3)	C13	C10	Rh1	126.4(7)
C10[1]	Rh1	Cl1A[1]	118.3(3)	C10[1]	C11	Rh1	70.5(5)
C10[1]	Rh1	Cl1A	102.1(3)	C10	C11	Rh1	70.5(5)
C10	Rh1	Cl1A	118.3(3)	C10	C11	C10[1]	107.6(10)
C10	Rh1	Cl1A[1]	102.1(3)	C10	C11	C14	126.2(5)
C11	Rh1	Cl1	93.8(3)	C10[1]	C11	C14	126.2(5)
C11	Rh1	Cl1A	92.5(3)	C14	C11	Rh1	125.7(11)
C11	Rh1	Cl1A[1]	92.5(3)	Cl1A[1]	Cl1A	Rh1	75.48(16)
Cl1A	Rh1	Cl1A[1]	29.0(3)				

Table 6. Torsion Angles for B.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Rh1	C3	C1	C2	177.1(13)	C9	C10	C11	Rh1	61.5(5)

Rh1	C9	C10	C11	-61.9(6)	C9	C10	C11	C10[1]	0.5(11)
Rh1	C9	C10	C13	121.8(10)	C9	C10	C11	C14	-178.0(13)
Rh1	N3	C6	C7	178.8(8)	C7	C8	C5	C4	0.0
Rh1	C10	C11	C10[1]	-61.0(7)	C8	C7	C6	N3	0.0
Rh1	C10	C11	C14	120.5(14)	C8	C5	C4	N1	180.0(11)
N1	C3	C1	C2	0.0	C8	C5	C4	N3	0.0
N1	C4	N3	Rh1	1.1(9)	C5	C4	N3	Rh1	-178.9(7)
N1	C4	N3	C6	-180.0(10)	C5	C4	N3	C6	0.0
C3	N1	N2	C2	0.0	C4	N1	C3	Rh1	1.9(11)
C3	N1	C4	C5	177.9(8)	C4	N1	C3	C1	-179.9(12)
C3	N1	C4	N3	-2.1(12)	C4	N1	N2	C2	179.9(13)
C3	C1	C2	N2	0.0	C4	N3	C6	C7	0.0
C1	C2	N2	N1	0.0	C6	C7	C8	C5	0.0
N2	N1	C3	Rh1	-178.2(8)	C13	C10	C11	Rh1	-121.9(9)
N2	N1	C3	C1	0.0	C13	C10	C11	C10[1]	177.1(8)
N2	N1	C4	C5	-1.9(16)	C13	C10	C11	C14	-1.4(18)
N2	N1	C4	N3	178.1(8)	C12	C9	C10	Rh1	-121.0(8)
C9[1]	C9	C10	Rh1	61.6(2)	C12	C9	C10	C11	177.0(8)
C9[1]	C9	C10	C11	-0.3(7)	C12	C9	C10	C13	0.7(14)
C9[1]	C9	C10	C13	-176.6(9)					

Table 7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **B**.

Atom	x	y	z	U(eq)
H1	4054	4821	4290	81

H2	2691	5193	5832	90
AH7	2682	25	5809	68
H8	1641	868	7100	93
H5	1748	2347	6994	71
H6	3830	661	4412	71
H14A	6795	1930	3224	167
H14B	6512	2699	4423	167
H14C	6947	2871	2579	167
H13A	5076	468	2028	144
H13B	5826	808	3198	144
H13C	5937	718	1130	144
H12A	3842	1549	-1102	142
H12B	3256	1683	561	142
H12C	3890	912	509	142

Table 8. Atomic Occupancy for **B**.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
Cl1	0.462(6)	N1	0.5	C3	0.5
C1	0.5	H1	0.5	C2	0.5
H2	0.5	N2	0.5	C7	0.5
H7	0.5	C8	0.5	H8	0.5
C5	0.5	H5	0.5	C4	0.5
N3	0.5	C6	0.5	H6	0.5
H14A	0.5	H14B	0.5	H14C	0.5
Cl1A	0.269(3)				

X-Ray Crystallographic Data of C

Table 1. Crystal Data and Summary of X-ray Data Collection for **C**

	C
formula	$C_{33}H_{32}ClN_2Rh$
fw	594.96
T (K)	293(2)
crystsyst	Orthorhombic
space group	$Pca2_1$
a (Å)	17.2309(13)
b (Å)	11.2062(8)
c (Å)	14.3729(13)
α (deg)	90
β (deg)	90
γ (deg)	90
V (Å^3)	2775.3(4)
Z	4
D_{calc} (g·cm^{-3})	1.424
μ (mm^{-1})	0.736
F(000)	1224.0
cryst size (mm)	0.25 × 0.22 × 0.18
max. 2θ (deg)	50.018
no. of reflns collected	9639
no. of indepreflns/R_{int}	4520/0.1415
no. of params	318
goodness-of-fit on F^2	1.041
R_1, wR_2 [I> 2σ(I)]	0.0797, 0.1829
R_1, wR_2 (all data)	0.1141, 0.2122
largest diff peak and hole (e Å^{-3})	1.08, −0.58

Table 2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **C**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Rh1	-1414.0(5)	-8418.8(8)	-728.8(13)	47.8(4)
Cl1	-814(3)	-9463(4)	551(4)	71.5(12)
N1	-2505(9)	-8621(12)	-54(9)	62(4)
N2	-3033(6)	-6775(12)	-589(13)	66(5)
C3	-976(7)	-7786(9)	-2043(10)	74(5)
C4	-1750(6)	-8192(12)	-2166(9)	62(4)
C5	-1765(7)	-9439(12)	-1991(12)	92(6)
C1	-999(9)	-9804(10)	-1760(12)	87(7)
C2	-512(6)	-8783(14)	-1793(11)	80(5)
C6	-621(19)	-10980(30)	-1540(20)	147(11)
C7	309(16)	-8730(30)	-1630(20)	139(10)
C8	-698(15)	-6582(18)	-2281(19)	93(8)
C9	-2388(16)	-7510(20)	-2577(19)	126(9)
C10	-2390(20)	-10250(30)	-2050(30)	171(13)
C11	-3116(9)	-7893(17)	-117(11)	61(4)
C12	-2668(11)	-9698(19)	305(14)	79(5)
C13	-3382(13)	-10010(20)	693(17)	95(6)
C14	-3929(13)	-9230(20)	640(18)	98(6)
C15	-3838(12)	-8140(20)	278(16)	87(6)
C16	-3688(9)	-6423(16)	-1048(11)	61(4)

C17	-3519(10)	-5360(20)	-1387(15)	79(5)
C18	-2789(11)	-4984(19)	-1020(13)	86(6)
C19	-2477(9)	-5909(14)	-550(13)	64(5)
C20	-1779(8)	-5941(13)	-25(11)	53(4)
C21	-1252(9)	-6830(14)	-15(11)	51(4)
C25	-1425(8)	-2513(8)	1275(10)	83(6)
C26	-946(7)	-2844(10)	542(10)	93(7)
C27	-1032(6)	-3959(10)	130(8)	87(6)
C22	-1597(6)	-4742(7)	452(8)	49(4)
C23	-2076(6)	-4411(9)	1186(8)	62(4)
C24	-1990(7)	-3296(10)	1597(8)	82(6)
C28	-518(9)	-6720(12)	565(13)	51(4)
C29	186(11)	-6600(15)	155(15)	73(5)
C30	834(11)	-6444(16)	712(15)	77(5)
C31	783(11)	-6390(16)	1656(13)	69(5)
C32	73(9)	-6530(14)	2054(15)	62(5)
C33	-570(9)	-6685(12)	1540(12)	49(4)

Table 3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **C**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
Rh1	51.5(6)	43.2(6)	48.8(6)	-3.5(7)	5.0(8)	1.8(5)
Cl1	83(3)	49(2)	83(3)	8(2)	-9(3)	3(2)
N1	71(9)	71(9)	44(8)	-6(7)	16(7)	-7(7)
N2	34(5)	79(9)	84(13)	-34(9)	1(8)	12(6)
C3	95(14)	61(11)	65(11)	-12(9)	14(10)	1(10)

C4	59(9)	82(12)	45(9)	6(8)	3(8)	27(9)
C5	94(8)	92(8)	90(8)	-11(6)	5(6)	-20(6)
C1	103(9)	79(8)	79(9)	-7(6)	5(6)	13(6)
C2	78(7)	86(8)	77(8)	4(6)	-2(6)	6(6)
C6	155(12)	142(12)	146(12)	-3(7)	1(7)	11(7)
C7	133(12)	145(12)	138(12)	-1(7)	5(7)	6(7)
C8	99(10)	91(10)	88(10)	6(6)	6(6)	-9(6)
C9	127(10)	131(10)	120(10)	-7(7)	-2(7)	9(7)
C10	173(14)	171(14)	168(15)	-5(7)	-1(7)	-6(7)
C11	50(6)	75(7)	58(6)	-13(5)	-8(5)	-6(6)
C12	78(7)	82(8)	78(7)	-3(6)	-6(6)	-9(6)
C13	97(8)	98(8)	91(8)	-3(6)	-3(6)	-16(6)
C14	96(8)	107(9)	91(8)	-3(6)	-4(6)	-11(6)
C15	78(7)	98(8)	84(8)	-11(6)	3(6)	-4(6)
C16	50(6)	76(7)	57(7)	-17(5)	-15(5)	9(5)
C17	75(7)	86(8)	76(7)	-8(6)	-15(6)	11(6)
C18	84(8)	85(8)	88(8)	-8(6)	-5(6)	8(6)
C19	54(8)	58(9)	80(13)	-25(9)	-25(9)	15(8)
C20	48(8)	43(8)	68(10)	-1(7)	-2(7)	18(7)
C21	50(8)	58(9)	44(9)	-2(7)	3(7)	-4(8)
C25	82(8)	75(8)	90(8)	-4(6)	-13(6)	-8(6)
C26	71(12)	50(11)	160(20)	17(13)	-23(14)	-9(10)
C27	82(13)	86(14)	94(15)	12(13)	13(12)	15(12)
C22	40(7)	42(8)	67(10)	4(8)	-7(7)	8(7)
C23	63(9)	41(8)	83(12)	-1(8)	12(9)	7(8)
C24	101(15)	61(12)	82(14)	-4(9)	3(12)	13(11)
C28	48(8)	38(8)	66(11)	-5(8)	14(8)	16(6)
C29	64(7)	83(7)	70(7)	1(6)	3(6)	-2(6)
C30	67(7)	83(8)	82(8)	4(6)	1(6)	-6(6)
C31	56(10)	82(13)	68(12)	2(9)	-18(9)	-8(9)
C32	47(9)	65(11)	75(12)	3(9)	8(9)	1(8)
C33	44(8)	49(9)	54(9)	-8(7)	6(7)	2(6)

Table 4. Bond Lengths for **C**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Rh1	Cl1	2.412(5)	C11	C15	1.40(3)

Rh1	N1	2.128(14)	C12	C13	1.40(3)
Rh1	C3	2.154(13)	C13	C14	1.29(3)
Rh1	C4	2.160(13)	C14	C15	1.34(3)
Rh1	C5	2.227(15)	C16	C17	1.32(3)
Rh1	C1	2.262(15)	C17	C18	1.43(2)
Rh1	C2	2.218(14)	C18	C19	1.35(2)
Rh1	C21	2.073(16)	C19	C20	1.42(2)
N1	C11	1.34(2)	C20	C21	1.35(2)
N1	C12	1.34(2)	C20	C22	1.541(17)
N2	C11	1.43(2)	C21	C28	1.52(2)
N2	C16	1.366(19)	C25	C26	1.3900
N2	C19	1.37(2)	C25	C24	1.3900
C3	C4	1.4200	C26	C27	1.3900
C3	C2	1.4200	C27	C22	1.3900
C3	C8	1.47(2)	C22	C23	1.3900
C4	C5	1.4200	C23	C24	1.3900
C4	C9	1.46(3)	C28	C29	1.35(2)
C5	C1	1.4200	C28	C33	1.40(2)
C5	C10	1.42(3)	C29	C30	1.39(3)
C1	C2	1.4200	C30	C31	1.36(3)
C1	C6	1.51(3)	C31	C32	1.36(2)
C2	C7	1.44(3)	C32	C33	1.34(2)

Table 5. Bond Angles for **C**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Rh1	Cl1	88.8(4)	C10	C5	C4	129.1(18)
N1	Rh1	C3	138.1(5)	C10	C5	C1	122.8(18)
N1	Rh1	C4	102.2(5)	C5	C1	Rh1	70.2(5)
N1	Rh1	C5	94.4(5)	C5	C1	C6	134.7(16)
N1	Rh1	C1	120.3(5)	C2	C1	Rh1	69.8(6)
N1	Rh1	C2	156.0(5)	C2	C1	C5	108.0
C3	Rh1	Cl1	132.7(4)	C2	C1	C6	117.3(16)
C3	Rh1	C4	38.4(2)	C6	C1	Rh1	127.0(16)
C3	Rh1	C5	63.2(3)	C3	C2	Rh1	68.6(5)
C3	Rh1	C1	62.6(3)	C3	C2	C7	124.3(16)
C3	Rh1	C2	37.9(2)	C1	C2	Rh1	73.2(6)
C4	Rh1	Cl1	154.3(3)	C1	C2	C3	108.0
C4	Rh1	C5	37.7(2)	C1	C2	C7	127.6(16)
C4	Rh1	C1	62.6(3)	C7	C2	Rh1	124.8(16)
C4	Rh1	C2	63.3(3)	N1	C11	N2	119.2(14)
C5	Rh1	Cl1	119.2(4)	N1	C11	C15	123.6(18)
C5	Rh1	C1	36.9(2)	C15	C11	N2	117.2(17)
C1	Rh1	Cl1	91.8(3)	N1	C12	C13	124(2)
C2	Rh1	Cl1	97.8(3)	C14	C13	C12	117(2)
C2	Rh1	C5	62.2(3)	C13	C14	C15	124(2)
C2	Rh1	C1	36.9(2)	C14	C15	C11	116(2)

C21	Rh1	Cl1	89.0(5)	C17	C16	N2	104.8(15)
C21	Rh1	N1	89.1(5)	C16	C17	C18	109.0(18)
C21	Rh1	C3	96.0(5)	C19	C18	C17	108.0(18)
C21	Rh1	C4	114.1(6)	N2	C19	C20	126.7(16)
C21	Rh1	C5	151.6(6)	C18	C19	N2	104.2(15)
C21	Rh1	C1	150.6(6)	C18	C19	C20	128.6(17)
C21	Rh1	C2	113.9(6)	C19	C20	C22	112.8(12)
C11	N1	Rh1	126.9(11)	C21	C20	C19	126.5(15)
C11	N1	C12	114.2(15)	C21	C20	C22	120.2(13)
C12	N1	Rh1	117.1(13)	C20	C21	Rh1	122.6(12)
C16	N2	C11	113.5(13)	C20	C21	C28	120.4(14)
C19	N2	C11	132.3(15)	C28	C21	Rh1	116.9(10)
C19	N2	C16	113.3(15)	C26	C25	C24	120.0
C4	C3	Rh1	71.0(6)	C27	C26	C25	120.0
C4	C3	C2	108.0	C22	C27	C26	120.0
C4	C3	C8	124.8(14)	C27	C22	C20	123.0(9)
C2	C3	Rh1	73.5(6)	C27	C22	C23	120.0
C2	C3	C8	126.6(14)	C23	C22	C20	116.7(9)
C8	C3	Rh1	128.2(13)	C22	C23	C24	120.0
C3	C4	Rh1	70.6(6)	C23	C24	C25	120.0
C3	C4	C5	108.0	C29	C28	C21	121.0(17)
C3	C4	C9	126.2(15)	C29	C28	C33	119.3(17)
C5	C4	Rh1	73.7(6)	C33	C28	C21	119.7(14)

C5	C4	C9	124.8(15)	C28	C29	C30	118.9(19)	
C9	C4	Rh1	130.6(14)	C31	C30	C29	122.0(19)	
C4	C5	Rh1	68.6(5)	C32	C31	C30	118.2(18)	
C1	C5	Rh1	72.9(5)	C33	C32	C31	121.8(19)	
C1	C5	C4	108.0	C32	C33	C28	119.9(16)	
C10	C5	Rh1	125.9(19)					

Table 6. Torsion Angles for **C**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Rh1	N1	C11	N2	-8(2)	C10	C5	C1	C2	178(2)
Rh1	N1	C11	C15	173.9(14)	C10	C5	C1	C6	1(3)
Rh1	N1	C12	C13	-173.9(17)	C11	N1	C12	C13	-8(3)
Rh1	C3	C4	C5	-64.7(6)	C11	N2	C16	C17	176.4(16)
Rh1	C3	C4	C9	126.6(18)	C11	N2	C19	C18	-169.2(18)
Rh1	C3	C2	C1	63.1(6)	C11	N2	C19	C20	3(3)
Rh1	C3	C2	C7	-118(2)	C12	N1	C11	N2	-172.7(16)
Rh1	C4	C5	C1	-62.6(5)	C12	N1	C11	C15	9(2)
Rh1	C4	C5	C10	120(3)	C12	C13	C14	C15	-3(4)
Rh1	C5	C1	C2	-59.9(5)	C13	C14	C15	C11	5(4)
Rh1	C5	C1	C6	123(2)	C16	N2	C11	N1	146.4(16)
Rh1	C1	C2	C3	-60.1(5)	C16	N2	C11	C15	-36(2)
Rh1	C1	C2	C7	121(2)	C16	N2	C19	C18	-1(2)
Rh1	C21	C28	C29	71.5(17)	C16	N2	C19	C20	171.3(16)
Rh1	C21	C28	C33	-111.5(13)	C16	C17	C18	C19	8(2)

N1	C11	C15	C14	-8(3)	C17	C18	C19	N2	-4(2)
N1	C12	C13	C14	5(3)	C17	C18	C19	C20	-176.1(18)
N2	C11	C15	C14	174.0(19)	C18	C19	C20	C21	-138(2)
N2	C16	C17	C18	-8(2)	C18	C19	C20	C22	33(3)
N2	C19	C20	C21	51(3)	C19	N2	C11	N1	-46(3)
N2	C19	C20	C22	-138.0(16)	C19	N2	C11	C15	132(2)
C3	C4	C5	Rh1	62.6(5)	C19	N2	C16	C17	6(2)
C3	C4	C5	C1	0.0	C19	C20	C21	Rh1	-4(2)
C3	C4	C5	C10	-178(3)	C19	C20	C21	C28	178.2(16)
C4	C3	C2	Rh1	-63.1(6)	C19	C20	C22	C27	-104.1(14)
C4	C3	C2	C1	0.0	C19	C20	C22	C23	70.1(15)
C4	C3	C2	C7	179(2)	C20	C21	C28	C29	-111.0(18)
C4	C5	C1	Rh1	59.9(5)	C20	C21	C28	C33	66(2)
C4	C5	C1	C2	0.0	C20	C22	C23	C24	-174.4(11)
C4	C5	C1	C6	-177(3)	C21	C20	C22	C27	67.6(17)
C5	C1	C2	Rh1	60.1(5)	C21	C20	C22	C23	-118.1(14)
C5	C1	C2	C3	0.0	C21	C28	C29	C30	176.9(15)
C5	C1	C2	C7	-179(2)	C21	C28	C33	C32	-176.8(14)
C2	C3	C4	Rh1	64.7(6)	C25	C26	C27	C22	0.0
C2	C3	C4	C5	0.0	C26	C25	C24	C23	0.0
C2	C3	C4	C9	-168.7(19)	C26	C27	C22	C20	174.1(11)
C6	C1	C2	Rh1	-122.2(19)	C26	C27	C22	C23	0.0
C6	C1	C2	C3	178(2)	C27	C22	C23	C24	0.0

C6	C1	C2	C7	-1(3)	C22	C20	C21	Rh1	-174.9(10)
C8	C3	C4	Rh1	-123.9(17)	C22	C20	C21	C28	8(2)
C8	C3	C4	C5	171.4(19)	C22	C23	C24	C25	0.0
C8	C3	C4	C9	3(2)	C24	C25	C26	C27	0.0
C8	C3	C2	Rh1	125.8(17)	C28	C29	C30	C31	-1(3)
C8	C3	C2	C1	-171.2(19)	C29	C28	C33	C32	0(2)
C8	C3	C2	C7	7(3)	C29	C30	C31	C32	2(3)
C9	C4	C5	Rh1	-128.5(17)	C30	C31	C32	C33	-2(3)
C9	C4	C5	C1	168.9(19)	C31	C32	C33	C28	1(2)
C9	C4	C5	C10	-9(3)	C33	C28	C29	C30	0(2)
C10	C5	C1	Rh1	-122(2)					

Table 7. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **C**.

Atom	x	y	z	U(eq)
H6A	-145	-10847	-1213	221
H6B	-514	-11401	-2111	221
H6C	-964	-11453	-1163	221
H7A	418	-8130	-1172	209
H7B	571	-8535	-2200	209
H7C	488	-9491	-1410	209
H8A	-1050	-6220	-2715	139
H8B	-191	-6637	-2555	139
H8C	-672	-6105	-1727	139
H9A	-2872	-7799	-2334	189
H9B	-2381	-7614	-3241	189
H9C	-2328	-6684	-2428	189
H10A	-2508	-10561	-1446	256
H10B	-2261	-10889	-2464	256
H10C	-2843	-9838	-2289	256
H12	-2279	-10273	295	95

H13	-3459	-10749	976	114
H14	-441	-9440	867	118
H15	-4235	-7580	290	104
H16	-4152	-6841	-1109	73
H17	-3826	-4926	-1798	95
H18	-2567	-4234	-1093	103
H25	-1368	-1767	1551	99
H26	-568	-2321	326	112
H27	-711	-4181	-361	105
H23	-2454	-4934	1401	74
H24	-2311	-3074	2088	98
H29	233	-6622	-489	87
H30	1319	-6373	433	93
H31	1222	-6261	2019	82
H32	32	-6517	2699	75
H33	-1050	-6770	1829	59