

Unforeseen 1,2-Aryl Shift in Tetraarylpyrrolo[3,2-*b*]pyrroles Triggered by Oxidative Aromatic Coupling

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1. General remarks

All reagents and solvents were purchased from commercial sources and were used as received unless otherwise noted. Reagent grade solvents (CH_2Cl_2 , hexanes) were distilled prior to use. DMF was dried over magnesium sulfate, then distilled and stored under argon. Transformations with moisture and oxygen sensitive compounds were performed under a stream of argon. The reaction progress was monitored by means of thin layer chromatography (TLC), which was performed on aluminium foil plates, covered with Silica gel 60 F₂₅₄ (Merck) or Aluminium oxide 60 F₂₅₄ (neutral, Merck). Products purification was done by means of column chromatography with Kieselgel 60 (Merck) or Aluminium oxide (Fluka). Occasionally, dry column vacuum chromatography (DCVC) for purification of products obtained was performed using Silica gel Type D 5F. The identity and purity of prepared compounds were proved by ^1H NMR and ^{13}C NMR spectrometry as well as by MS-spectrometry (*via* EI-MS or ESI-MS). NMR spectra were measured on Bruker AM 500 MHz, Bruker AM 600 MHz, Varian 600 MHz, Varian 400 MHz or Varian 200 MHz instruments with TMS as internal standard. All chemical shifts are given in ppm. All melting points for crystalline products were measured with automated melting point apparatus EZ-MELT and were given without correction. The absorbance and fluorescence spectra were measured in toluene on Perkin –Elmer Lambda 25 UV/VIS and Hitachi F-7000 respectively.

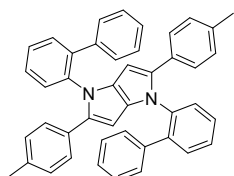
Linear optical measurements

Steady-state fluorescence measurements were performed with dilute solutions (10^{-6}M , optical density<0.1) contained in standard 1 cm quartz cuvettes at room temperature. Compounds were dissolved in toluene unless otherwise noted. Emission spectra were obtained, for each compound, under excitation at $\lambda=330\text{ nm}$. Fluorescence quantum yields were measured by using quinine hemisulphate monohydrate in 0.5M sulfuric acid as a standard.

2. Experimental section

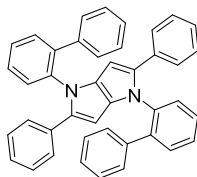
General procedure for the synthesis of Tetrarylpyrrolopyrroles (4a-g)

In a 25 mL round-bottom flask equipped with a reflux condenser and magnetic stir bar, 6 mL glacial acetic acid was placed followed by the addition of aldehyde (6 mmol), 2-aminobiphenyl (6 mmol), and TsOH (0.6 mmol). The mixture was stirred at 90 °C for 30 min. After that time butane-2,3-dione (3 mmol) was slowly added via syringe and the resulting mixture was stirred at 90 °C for 3 h. The reaction mixture was then cooled to room temperature. The precipitate of the obtained dye was then filtered off and washed with cooled glacial acetic acid. Recrystallization from AcOEt and drying under vacuum afforded pure product.



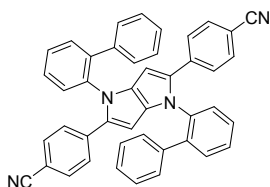
4a

1,4-di([1,1'-biphenyl]-2-yl)-2,5-bis(4-methylphenyl)-1,4-dihydropyrrolo[3,2-b]pyrrole (4a)- Off-white solid. Yield 650 mg (18%). R_f = 0.48 (SiO₂, DCM/hexanes, 1:4). Mixture of atropisomers, ratio A:B = 6:1. Apparent peaks overlapping. ¹H NMR (500 MHz, CDCl₃) δ 7.73 (dd, J = 7.8, 1.3 Hz, 12H, A), 7.58 (dd, J = 7.8, 1.3 Hz, 2H, B), 7.48 (dt, J = 7.7, 1.7 Hz, 12H, A), 7.46 – 7.43 (m, 2H, B), 7.43 – 7.39 (m, 12H, A), 7.39 – 7.36 (m, 2H, B), 7.34 (dd, J = 7.7, 1.6 Hz, 14H, A+B), 7.11 – 7.06 (m, 14H, A+B), 7.02 (dd, J = 8.2, 6.7 Hz, 28H, A+B), 6.79 (d, J = 7.9 Hz, 4H, B), 6.75 (d, J = 7.9 Hz, 24H, A), 6.69 (m, 4H, B), 6.62 (d, J = 8.2 Hz, 4H, B), 6.61–6.57 (m, 24H, A), 6.53 – 6.47 (m, 24H, A), 6.03 (s, 12H, A), 5.93 (s, 2H, B), 2.23 (s, 42H, A+B). ¹³C NMR (126 MHz, CDCl₃) δ 139.4, 138.9, 138.1, 138.0, 137.1, 136.6, 134.8, 134.7, 131.7, 131.1, 131.0, 130.9, 130.7, 128.3, 128.2, 128.0, 127.9, 127.8, 127.7, 127.5, 127.4, 127.2, 126.8, 126.55, 126.47, 92.8, 92.3, 21.0. HRMS (ESI-TOF) calcd for C₄₄H₃₄N₂: 590.2722 [M]⁺, found: 590.2729.



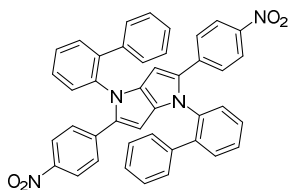
4b

1,4-di([1,1'-biphenyl]-2-yl)-2,5-diphenyl-1,4-dihydropyrrolo[3,2-b]pyrrole (4b)- Off-white solid. Yield 506 mg (30%). R_f = 0.48 (SiO₂, DCM/hexanes, 1:4). Mixture of atropisomers, ratio A:B = 6:1. ¹H NMR (500 MHz, CDCl₃) δ 7.78 (dd, J = 7.7, 1.3 Hz, 12H, A), 7.66 (dd, J = 7.9, 1.3 Hz, 2H, B), 7.54 – 7.49 (m, 14H, A+B), 7.49 – 7.46 (m, 2H, B), 7.45 – 7.41 (m, 14H, A+B), 7.35 (dd, J = 7.7, 1.6 Hz, 14H, A+B), 7.09 (d, J = 7.3 Hz, 14H, A+B), 7.03 (t, J = 7.6 Hz, 28H, A), 6.98 (dd, J = 6.4, 2.0 Hz, 16H, A+B), 6.97 – 6.92 (m, 24H, A), 6.73 (d, J = 7.9 Hz, 4H, B), 6.66 – 6.64 (m, 2H, B), 6.64 – 6.60 (m, 28H, A+B), 6.57 (dt, J = 7.1, 1.4 Hz, 24H, A), 6.10 (s, 12H, A), 6.01 (s, 2H, B). ¹³C NMR (126 MHz, CDCl₃) δ 139.4, 138.8, 137.8, 137.2, 133.6, 133.5, 132.0, 131.14, 131.07, 128.4, 128.1, 128.0, 127.9, 127.73, 127.69, 127.57, 127.51, 127.50, 127.3, 126.8, 126.6, 126.5, 125.3, 125.2, 93.0, 92.7. HRMS (EI) calcd for C₄₂H₃₀N₂: 562.2409 [M]⁺, found: 562.2402.



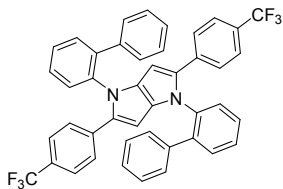
4c

*1,4-di([1,1'-biphenyl]-2-yl)-2,5-bis(4-cyanophenyl)-1,4-dihydropyrrolo[3,2-*b*]pyrrole (4c)*- Yellow solid. Yield 257 mg (14%). R_f = 0.34 (SiO₂, DCM/hexanes, 1:1). Mixture of atropisomers, ratio A:B = 5:1. ¹H NMR (500 MHz, CDCl₃) δ 7.76 (dd, J = 7.8, 1.4 Hz, 10H, A), 7.72 (dd, J = 7.8, 1.4 Hz, 2H, B), 7.57 (ddd, J = 7.7, 6.9, 1.6 Hz, 12H, A+B), 7.50 (td, J = 7.6, 1.5 Hz, 12H, A+B), 7.39 (dd, J = 7.7, 1.6 Hz, 12H, A+B), 7.26-7.24 (m, 4H, B), 7.22 (d, J = 8.4 Hz, 20H, A), 7.11 (t, J = 7.4 Hz, 12H, A+B), 7.02 (dd, J = 8.8, 6.5 Hz, 24H, A+B), 6.77 (d, J = 8.4 Hz, 4H, B), 6.69 (d, J = 8.4 Hz, 20H, A), 6.52 (d, J = 7.3 Hz, 24H, A+B), 6.19 (s, 10H, A), 6.13 (s, 2H, B). ¹³C NMR (126 MHz, CDCl₃) δ 139.2, 139.0, 138.23, 138.17, 137.4, 137.0, 136.8, 136.5, 136.2, 133.5, 133.4, 131.5, 131.4, 128.9, 128.7, 128.3, 128.2, 127.96, 127.90, 127.8, 127.6, 127.4, 127.3, 127.1, 126.9, 126.63, 126.61, 119.3, 108.4, 108.3, 94.3, 94.1. HRMS (ESI-TOF) calcd for C₄₄H₂₈N₄Na: 635.2212 [M+Na]⁺, found: 635.2202.



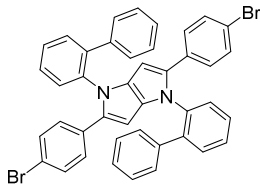
4d

*1,4-di([1,1'-biphenyl]-2-yl)-2,5-bis(4-nitrophenyl)-1,4-dihydropyrrolo[3,2-*b*]pyrrole (4d)*- Red solid. Yield 300 mg (15%). R_f = 0.43 (SiO₂, DCM/hexanes, 1:1). Mixture of atropisomers, ratio A:B = 9:2. ¹H NMR (500 MHz, CDCl₃) δ 7.85-7.81 (m, 22H, A+B), 7.78 (dd, J = 7.6, 1.5 Hz, 9H, A), 7.75 (dd, J = 7.6, 1.5 Hz, 2H, B), 7.59 (td, J = 7.6, 1.5 Hz, 11H, A+B), 7.52 (td, J = 7.7, 1.2 Hz, 11H, A+B), 7.42 – 7.37 (m, 11H, A+B), 7.12 (t, J = 7.5 Hz, 11H, A+B), 7.02 (td, J = 7.8, 1.8 Hz, 22H, A+B), 6.83 (d, J = 8.9 Hz, 4H, B), 6.74 (d, J = 8.9 Hz, 18H, A), 6.57 – 6.51 (m, 22H, A+B), 6.26 (s, 9H, A), 6.20 (s, 2H, B). ¹³C NMR (126 MHz, CDCl₃) δ 145.1, 145.0, 139.35, 139.33, 139.2, 139.0, 138.15, 138.07, 136.8, 136.7, 136.6, 136.3, 134.04, 134.02, 131.6, 131.5, 129.0, 128.8, 128.5, 128.4, 127.97, 127.95, 127.88, 127.6, 127.4, 127.3, 127.2, 127.1, 126.45, 126.42, 123.2, 94.9, 94.7. HRMS (ESI-TOF) calcd for C₄₂H₂₈N₄O₄Na: 675.2008 [M+Na]⁺, found: 675.2005.



4e

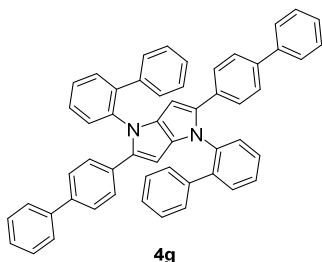
*1,4-di([1,1'-biphenyl]-2-yl)-2,5-bis(4-(trifluoromethyl)phenyl)-1,4-dihydropyrrolo[3,2-*b*]pyrrole (4e)*- Off-white solid. Yield 400 mg (19%). R_f = 0.61 (SiO₂, DCM/hexanes, 1:4). Mixture of atropisomers, ratio A:B = 5:1. ¹H NMR (500 MHz, CDCl₃) δ 7.78 (d, J = 7.8 Hz, 10H, A), 7.72 (d, J = 7.8 Hz, 2H, B), 7.55 (t, J = 7.0 Hz, 12H, A+B), 7.47 (t, J = 7.5 Hz, 12H, A+B), 7.40 – 7.33 (m, 12H, A+B), 7.21-7.17 (m, 24H, A+B), 7.10 (t, J = 7.2 Hz, 12H, A+B), 7.01 (t, J = 7.6 Hz, 24H, A+B), 6.79 (d, J = 8.1 Hz, 4H, B), 6.70 (d, J = 8.0 Hz, 20H, A), 6.55-6.49 (m, 24H, A+B), 6.18 (s, 10H, A), 6.11 (s, 2H, B). ¹³C NMR (126 MHz, CDCl₃) δ 139.3, 139.0, 138.46, 138.42, 137.28, 137.16, 136.69, 136.62, 136.60, 136.4, 136.0, 132.79, 132.77, 131.4, 131.3, 128.7, 128.5, 128.0, 127.8, 127.7, 127.6, 127.5, 127.3, 127.1, 126.9, 126.7, 126.6, 126.5, 125.4, 124.5(q), 123.3, 93.8, 93.5. HRMS (ESI-TOF) calcd for C₄₄H₂₈N₂F₆: 698.2157 [M]⁺, found: 698.2139.



4f

*1,4-di([1,1'-biphenyl]-2-yl)-2,5-bis(4-bromophenyl)-1,4-dihydropyrrolo[3,2-*b*]pyrrole (4f)*- Off-white solid. Yield 130 mg (6%). R_f = 0.56 (SiO₂, DCM/hexanes, 1:4). Mixture of atropisomers, ratio A:B = 5:1. ¹H NMR (600 MHz, CDCl₃) δ 7.74 (dd, J = 7.8, 1.3 Hz, 10H, A), 7.66 (dd, J = 7.8, 1.3 Hz, 2H, B), 7.51 (td, J = 7.6,

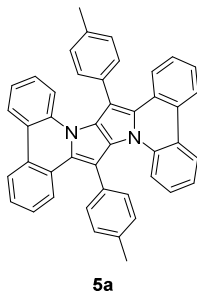
1.6 Hz, 10H, A), 7.50 – 7.48 (m, 2H, B), 7.44 (td, $J = 7.6$, 1.3 Hz, 12H, A+B), 7.42 – 7.39 (m, 2H, B), 7.35 (dd, $J = 7.7$, 1.6 Hz, 10H, A), 7.33 (d, $J = 1.4$ Hz, 2H, B), 7.11 – 7.08 (m, 14H, A+B), 7.07 – 7.05 (m, 22H, A+B), 7.03 (dd, $J = 8.3$, 7.0 Hz, 24H, A+B), 6.59 (d, $J = 7.1$ Hz, 4H, B), 6.58 – 6.53 (m, 24H, A+B), 6.45 (d, $J = 8.6$ Hz, 20H, A), 6.07 (s, 10H, A), 5.99 (s, 2H, B). ^{13}C NMR (151 MHz, CDCl_3) δ 139.3, 139.0, 138.61, 138.58, 137.3, 136.3, 135.8, 132.4, 132.3, 132.2, 131.3, 131.2, 130.6, 128.6, 128.35, 128.26, 128.2, 128.1, 127.84, 127.83, 127.81, 127.77, 127.71, 127.64, 127.59, 126.8, 126.7, 119.4, 119.2, 93.1, 92.8. HRMS (ESI-TOF) calcd for $\text{C}_{42}\text{H}_{28}\text{N}_2\text{Br}_2$: 718.0619 $[\text{M}]^+$, found: 718.0607.



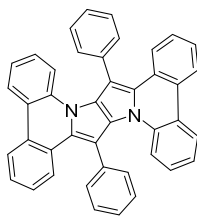
*1,4-di([1,1'-biphenyl]-2-yl)-2,5-di([1,1'-biphenyl]-4-yl)-1,4-dihydropyrrolo[3,2-*b*]pyrrole (4g)*- Yellow solid. Yield 350 mg (24%). $R_f = 0.40$ (SiO_2 , DCM/hexanes, 1:4). Mixture of atropisomers, ratio A:B = 11:2. ^1H NMR (500 MHz, CDCl_3) δ 7.82 (dd, $J = 7.9$, 1.4 Hz, 11H, A), 7.71 (dd, $J = 7.8$, 1.3 Hz, 2H, B), 7.57-7.53 (m, 39H, A), 7.46 (d, $J = 7.6$ Hz, 16H, A+B), 7.42 (t, $J = 7.7$ Hz, 33H, A), 7.39 – 7.35 (m, 16H, A+B), 7.34 – 7.30 (m, 16H, A+B), 7.22 (d, $J = 8.3$ Hz, 26H, A+B), 7.12 (t, $J = 7.4$ Hz, 16H, A+B), 7.04 (t, $J = 7.6$ Hz, 26H, A+B), 6.81 (d, $J = 8.3$ Hz, 4H, B), 6.70 (d, $J = 8.3$ Hz, 22H, A), 6.68-6.66 (m, 4H, B), 6.61 (d, $J = 7.2$ Hz, 22H, A), 6.17 (s, 11H, A), 6.08 (s, 2H, B). ^{13}C NMR (126 MHz, CDCl_3) δ 140.9, 139.5, 138.8, 138.0, 137.8, 137.0, 132.6, 132.5, 132.4, 132.3, 131.2, 128.7, 128.5, 128.22, 128.20, 128.0, 127.9, 127.75, 127.71, 127.62, 127.58, 127.4, 127.1, 127.0, 126.70, 126.66, 126.55, 126.22, 126.18, 93.1, 92.7. HRMS (ESI-TOF) calcd for $\text{C}_{54}\text{H}_{38}\text{N}_2$: 714.3035 $[\text{M}]^+$, found: 714.3029.

General procedure for the synthesis of rearranged π -expanded DHPPs (5a-g)

To a flask flushed with argon prior to use 50 mL round-bottom flask equipped with magnetic stir bar and septum, 15 mL of dry dichloroethane and 0.2 mmol of adequate TAPP **4** were placed. To dissolved substrate, 4 mmol of iron(III) chloride dissolved in 6 mL of dry nitromethane were added *via* syringe. Reaction was conducted at 80 °C for 16 hours. Then 20 mL of water was added and resulting mixture was stirred for another 15 minutes. Two phases were separated, water phase was extracted with methylene chloride (3 x 15 mL). Organic phases were combined and dried, solvent was evaporated and crude product was purified by means of flash column chromatography.

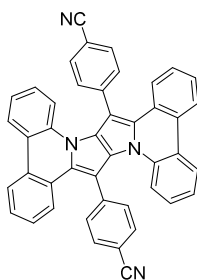


*9,18-bis(4-methylphenyl)-9,18-dihydrodibenzo[*e,g*]dibenzo[4,5:6,7]indolo[3,2-*b*]indole (5a)*- Yellow solid. Yield 82 mg (70%). $R_f = 0.51$ (SiO_2 , DCM/hexanes, 1:4). ^1H NMR (500 MHz, C_6D_6) δ 7.95 (dd, $J = 8.1$, 1.4 Hz, 4H), 7.86 (dd, $J = 8.3$, 1.3 Hz, 2H), 7.44 – 7.39 (m, 6H), 7.04 (d, $J = 7.7$ Hz, 4H), 7.03 – 6.99 (m, 2H), 6.95 – 6.90 (m, 4H), 6.85 (td, $J = 7.8$, 7.2, 1.4 Hz, 2H), 2.19 (s, 6H). ^{13}C NMR (126 MHz, C_6D_6) δ 137.3, 134.9, 133.9, 131.9, 129.9, 128.9, 128.8, 128.7, 126.95, 126.91, 125.7, 124.0, 123.2, 122.7, 122.5, 122.1, 119.9, 107.6, 21.0. HRMS (EI) calcd for $\text{C}_{44}\text{H}_{30}\text{N}_2$: 586.2409 $[\text{M}]^+$, found: 586.2402.



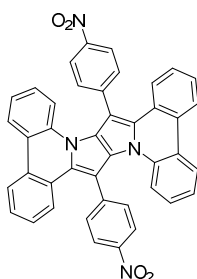
5b

9,18-diphenyl-9,18-dihydrodibenzo[e,g]dibenzo[4,5:6,7]indolo[3,2-b]indole (5b)- Yellow solid. Yield 60 mg (54%). $R_f = 0.51$ (SiO₂, DCM/hexanes, 1:4). ¹H NMR (600 MHz, C₆D₆) δ 7.93 (d, $J = 8.0$ Hz, 4H), 7.76 (dd, $J = 8.3, 1.2$ Hz, 2H), 7.49 – 7.45 (m, 4H), 7.30 (dd, $J = 8.3, 1.2$ Hz, 2H), 7.22 – 7.17 (m, 6H), 7.00 (ddd, $J = 8.5, 7.1, 1.4$ Hz, 2H), 6.93 – 6.90 (ddd, $J = 8.3, 7.0, 1.3$ Hz, 2H), 6.88 (ddd, $J = 8.3, 7.0, 1.3$ Hz, 2H), 6.80 (ddd, $J = 8.5, 7.1, 1.4$ Hz, 2H). HRMS (EI) calcd for C₄₂H₂₆N₂: 558.2096 [M]⁺, found: 558.2101.



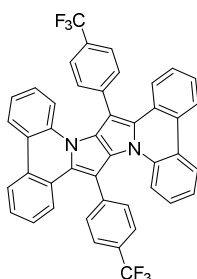
5c

9,18-bis(4-cyanophenyl)-9,18-dihydrodibenzo[e,g]dibenzo[4,5:6,7]indolo[3,2-b]indole (5c)- Yellow solid. Yield 72 mg (60%). $R_f = 0.38$ (SiO₂, DCM/hexanes, 1:1). ¹H NMR (600 MHz, C₆D₆) δ 7.93 (t, $J = 8.5$ Hz, 4H), 7.44 (dd, $J = 8.0, 1.1$ Hz, 2H), 7.10 – 7.07 (m, 4H), 7.07 – 7.04 (m, 2H), 7.01 (d, $J = 8.1$ Hz, 4H), 6.95 – 6.89 (m, 4H), 6.80 (dd, $J = 8.3, 1.1$ Hz, 2H), 6.64 (ddd, $J = 8.3, 7.1, 1.4$ Hz, 2H). HRMS (ESI-TOF) calcd for C₄₄H₂₄N₄: 608.2001 [M]⁺, found: 608.1985.



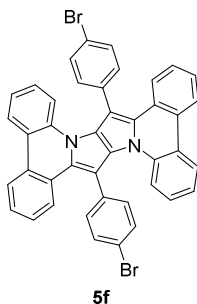
5d

9,18-bis(4-nitrophenyl)-9,18-dihydrodibenzo[e,g]dibenzo[4,5:6,7]indolo[3,2-b]indole (5d)- Red solid. Yield 86 mg (66%). $R_f = 0.47$ (SiO₂, DCM/hexanes, 1:1). ¹H NMR (500 MHz, CDCl₃) δ 8.41 (d, $J = 8.7$ Hz, 4H), 8.27 (dd, $J = 10.5, 8.4$ Hz, 4H), 7.83 (d, $J = 8.7$ Hz, 4H), 7.45 – 7.38 (m, 4H), 7.22 (ddd, $J = 8.2, 7.0, 1.4$ Hz, 2H), 7.19 – 7.14 (m, 2H), 6.91 (dd, $J = 8.4, 1.4$ Hz, 2H), 6.89 – 6.84 (m, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 147.4, 144.5, 132.85, 132.80, 129.3, 127.79, 127.77, 127.3, 127.2, 127.0, 126.8, 124.3, 123.64, 123.60, 123.5, 123.1, 122.0, 119.1, 105.0. HRMS (ESI-TOF) calcd for C₄₂H₂₄N₄O₄: 648.1798 [M]⁺, found: 648.1782.

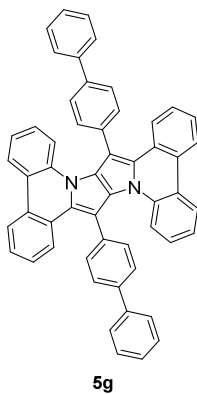


5e

9,18-bis(4-(trifluoromethyl)phenyl)-9,18-dihydrodibenzo[e,g]dibenzo[4,5:6,7]indolo[3,2-b]indole (5e)- Yellow solid. Yield 46 mg (33%). $R_f = 0.57$ (SiO₂, DCM/hexanes, 1:4). ¹H NMR (500 MHz, C₆D₆) δ 7.92 (t, $J = 8.7$ Hz, 4H), 7.59 (dd, $J = 8.3, 1.2$ Hz, 2H), 7.39 – 7.31 (m, 8H), 7.03 (ddd, $J = 8.3, 7.0, 1.2$ Hz, 2H), 6.94 – 6.88 (m, 4H), 6.84 (ddd, $J = 8.3, 7.0, 1.2$ Hz, 2H), 6.73 (ddd, $J = 8.5, 7.2, 1.4$ Hz, 2H). HRMS (ESI-TOF) calcd for C₄₄H₂₄N₂F₆: 694.1844 [M]⁺, found: 694.1830.



9,18-bis(4-bromophenyl)-9,18-dihydrodibenzo[e,g]dibenzo[4,5:6,7]indolo[3,2-b]indole (5f)- Yellow solid. Yield 91 mg (64%). $R_f = 0.51$ (SiO₂, DCM/hexanes, 1:4). ¹H NMR (500 MHz, C₆D₆) δ 7.97 (ddd, $J = 8.2, 4.8, 1.3$ Hz, 4H), 7.71 (dd, $J = 8.3, 1.2$ Hz, 2H), 7.37 – 7.33 (m, 4H), 7.18-7.16 (m, overlapped by solvent's peak, 6H), 7.07 (ddd, $J = 8.2, 7.0, 1.2$ Hz, 2H), 6.95 (td, $J = 8.0, 7.6, 1.2$ Hz, 2H), 6.91 (ddd, $J = 8.3, 7.0, 1.2$ Hz, 2H), 6.84 (ddd, $J = 8.5, 7.2, 1.4$ Hz, 2H). ¹³C NMR (126 MHz, C₆D₆) δ 136.5, 133.6, 133.4, 132.3, 128.9, 127.11, 127.06, 126.1, 123.7, 123.3, 123.1, 122.8, 121.99, 121.95, 119.5, 110.0, 106.1. HRMS (ESI-TOF) calcd for C₄₂H₂₄N₂Br₂: 714.0306 [M]⁺, found: 714.0281.



9,18-di([1,1'-biphenyl]-4-yl)-9,18-dihydrodibenzo[e,g]dibenzo[4,5:6,7]indolo[3,2-b]indole (5g)- Yellow solid. Yield 75 mg (53%). $R_f = 0.38$ (SiO₂, DCM/hexanes, 1:4). ¹H NMR (600 MHz, C₆D₆) δ 7.98 – 7.92 (m, 6H), 7.57 – 7.54 (m, 5H), 7.54 – 7.51 (m, 5H), 7.38 (dd, $J = 8.3, 1.2$ Hz, 2H), 7.25 – 7.22 (m, 4H), 7.16 – 7.12 (m, 4H), 7.02 (ddd, $J = 8.2, 7.0, 1.2$ Hz, 2H), 6.93 – 6.89 (m, 4H), 6.81 (ddd, $J = 8.5, 7.1, 1.4$ Hz, 2H). HRMS (ESI-TOF) calcd for C₅₄H₃₄N₂: 710.2722 [M]⁺, found: 710.2706.

3. X-Ray crystallography

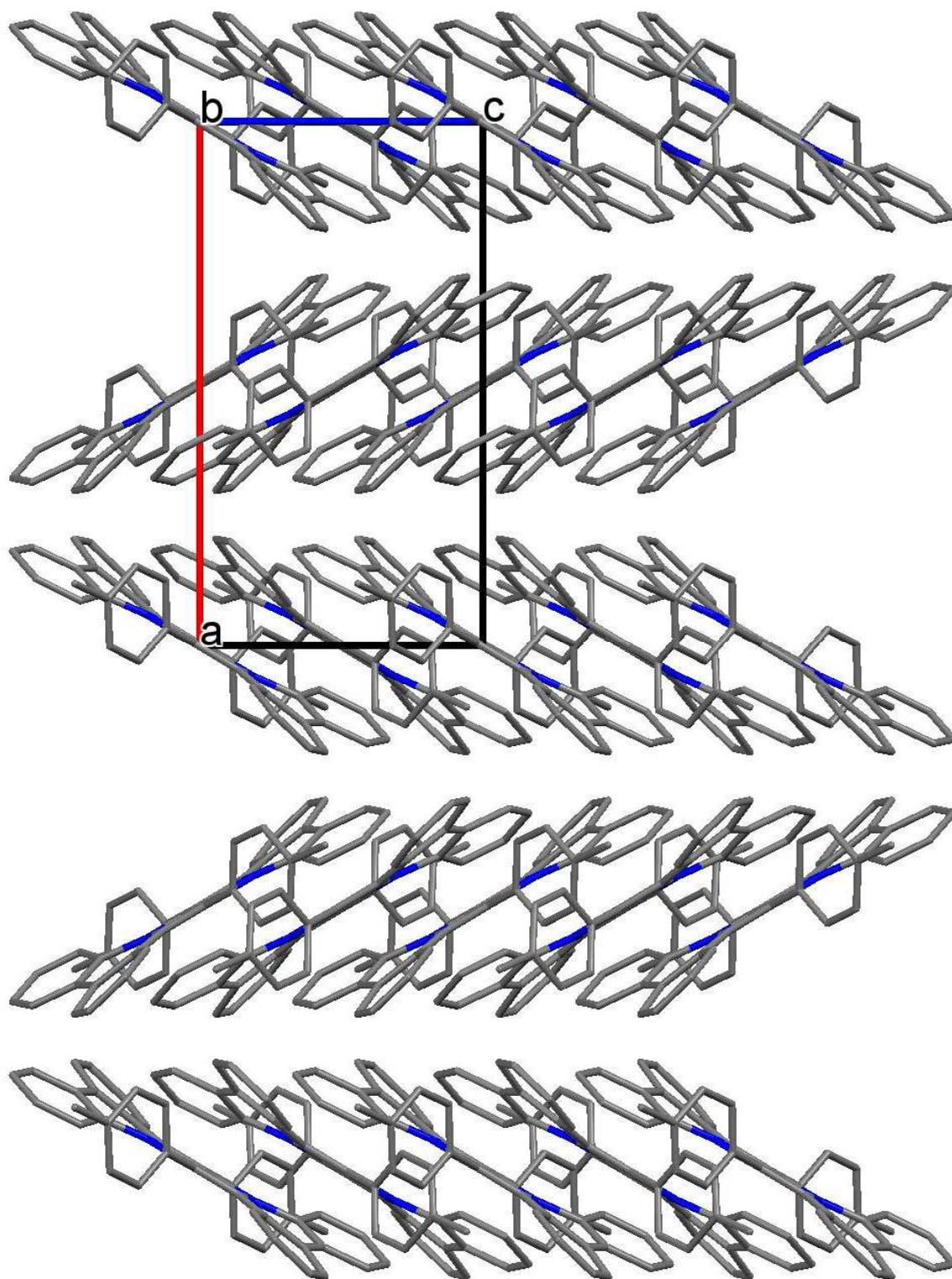


Figure S1. Crystal packing for compound **5a**.

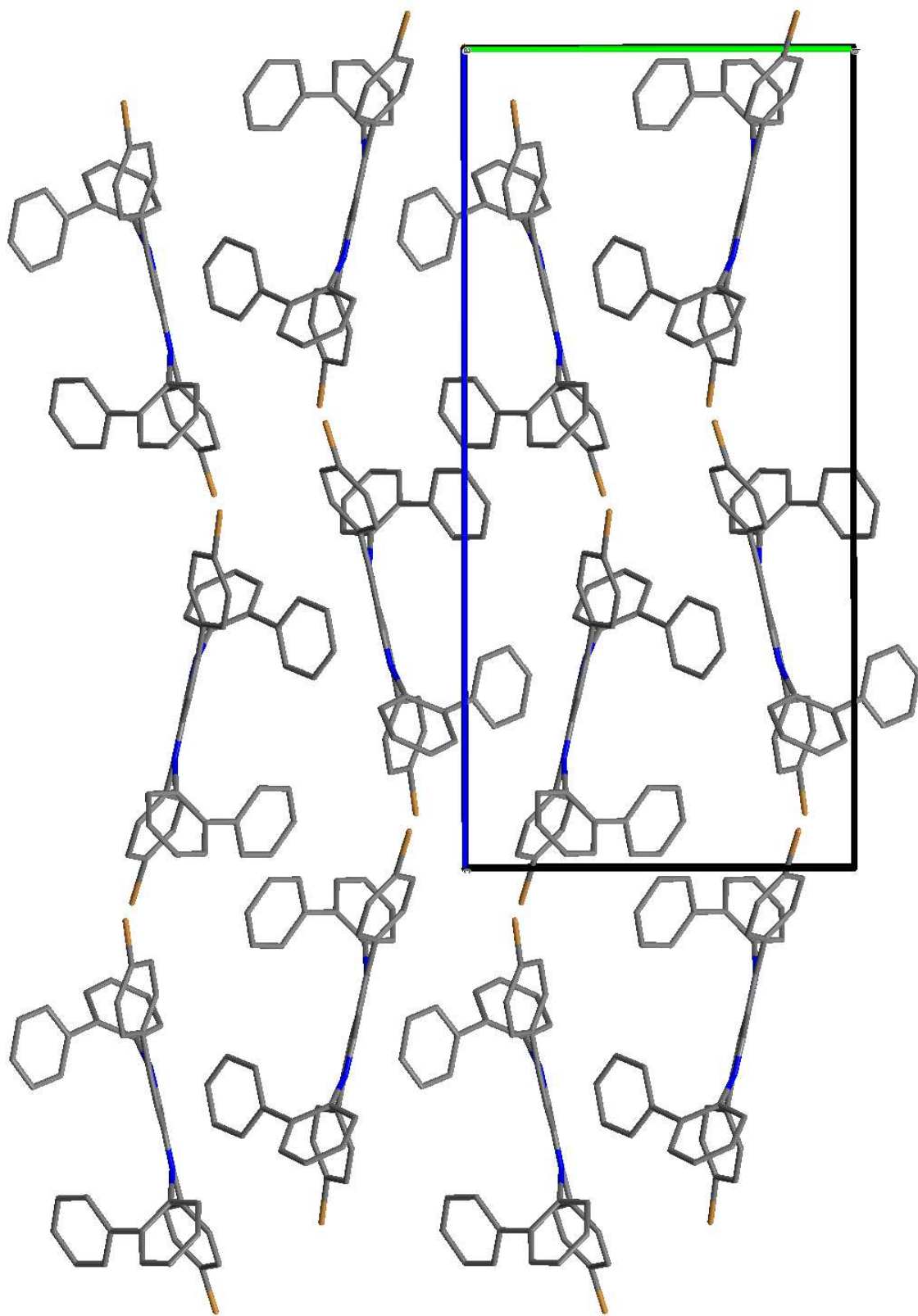
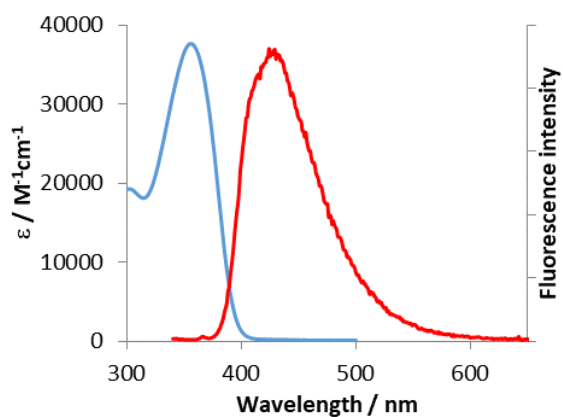


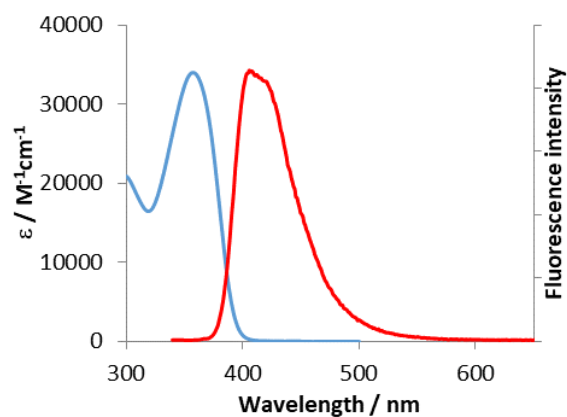
Figure S2. Crystal packing for compound **4f**.

4. Normalized absorption and emission spectra for synthesized compounds.

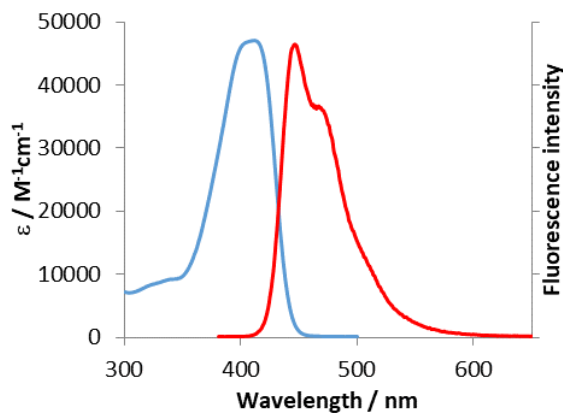
4a



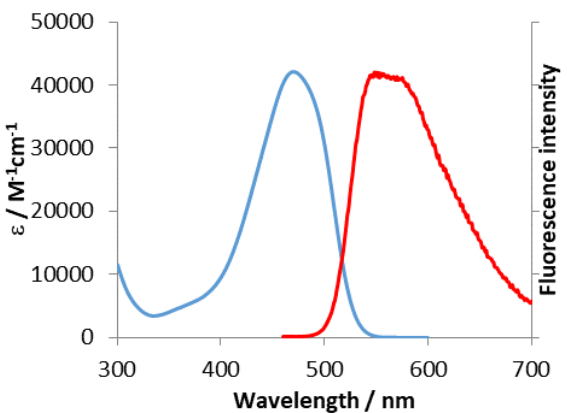
4b



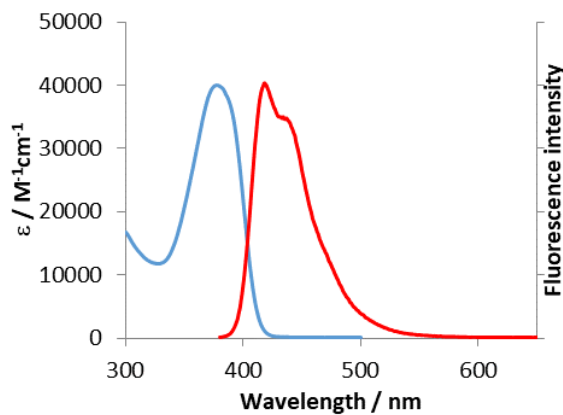
4c



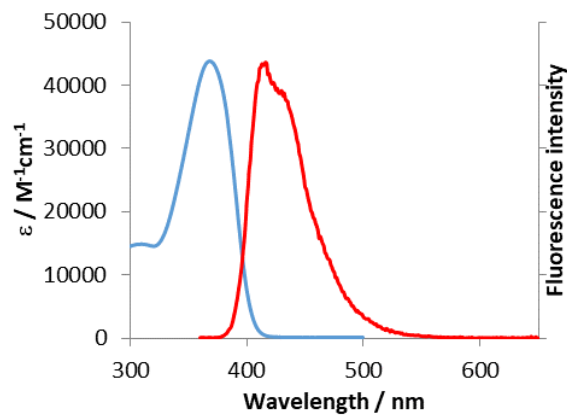
4d

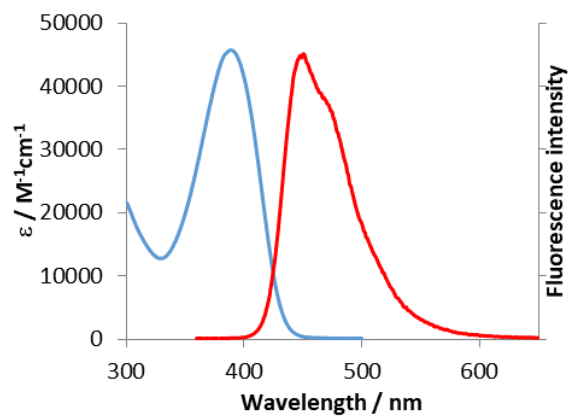
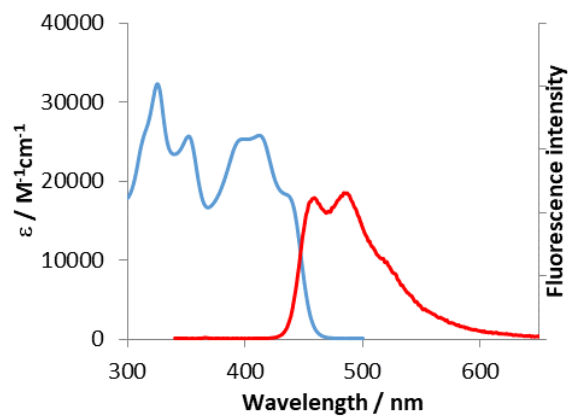
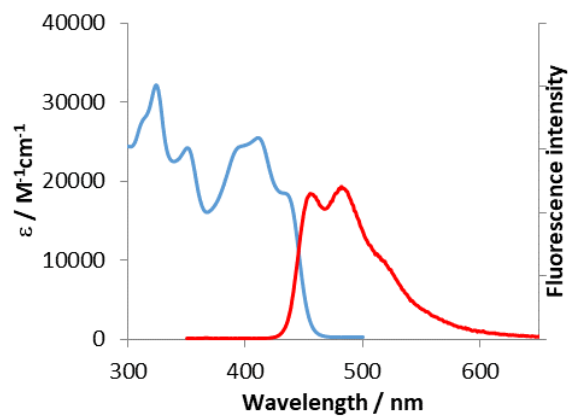
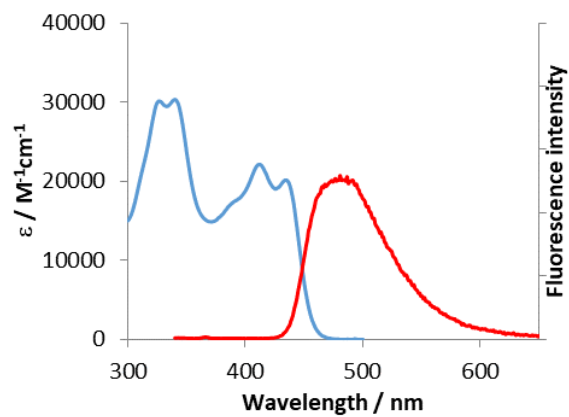
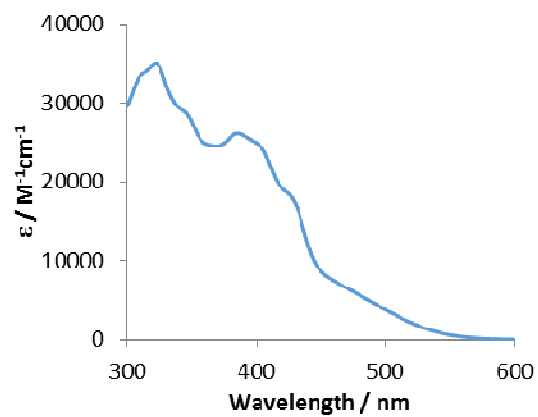
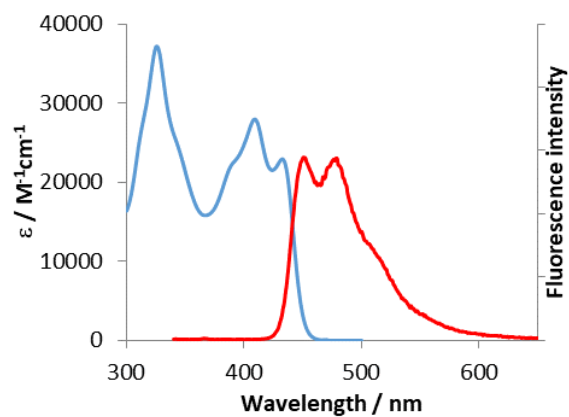


4e

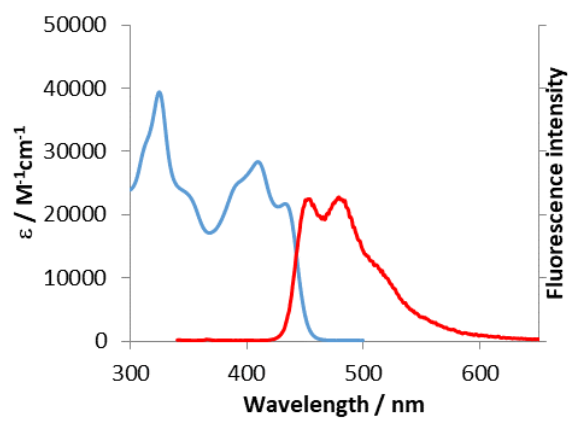


4f

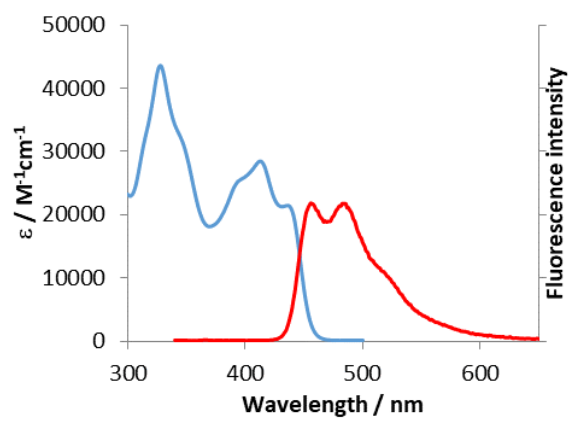


4g**5a****5b****5c****5d****5e**

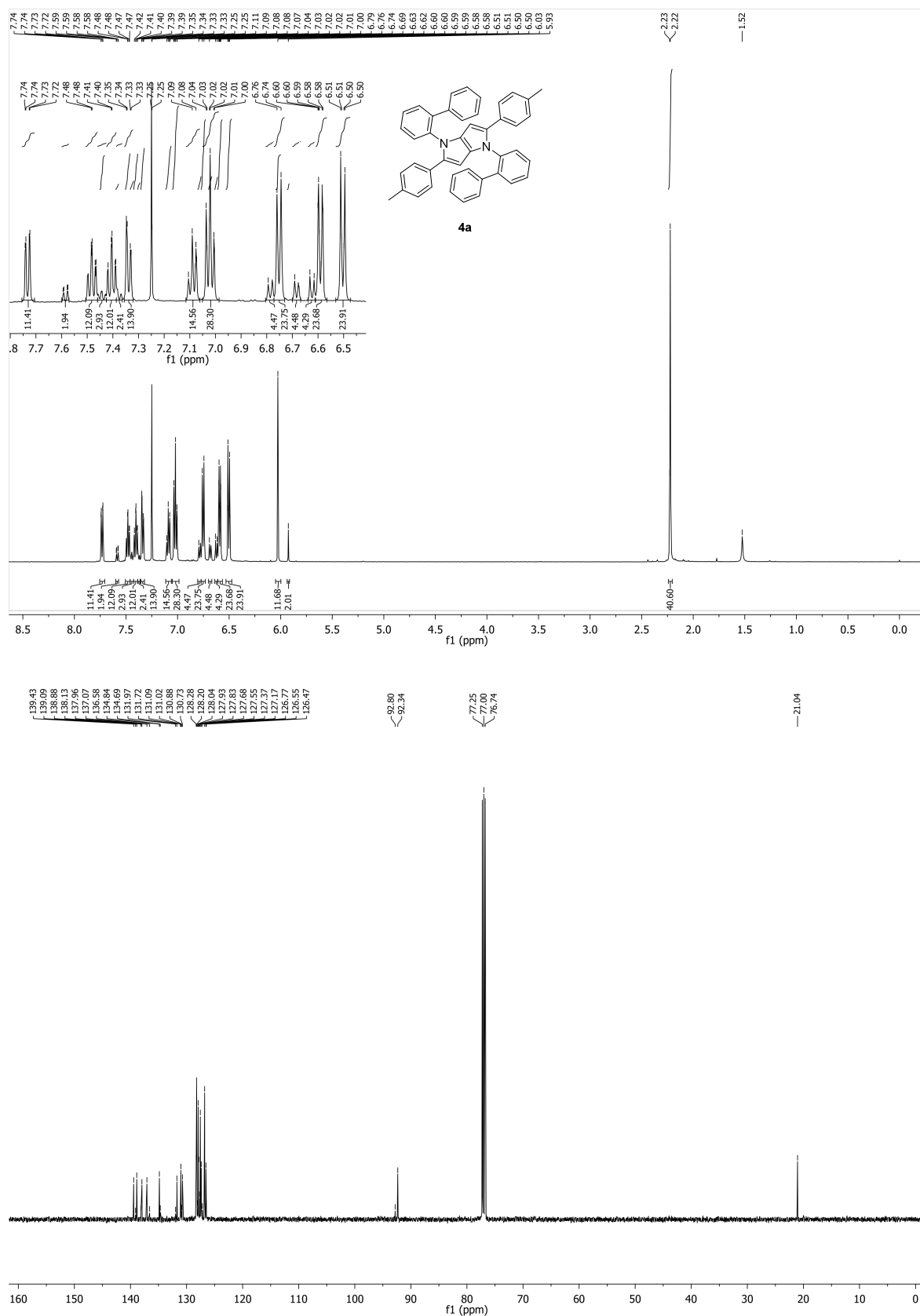
5f

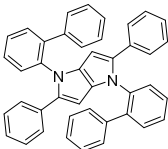


5g

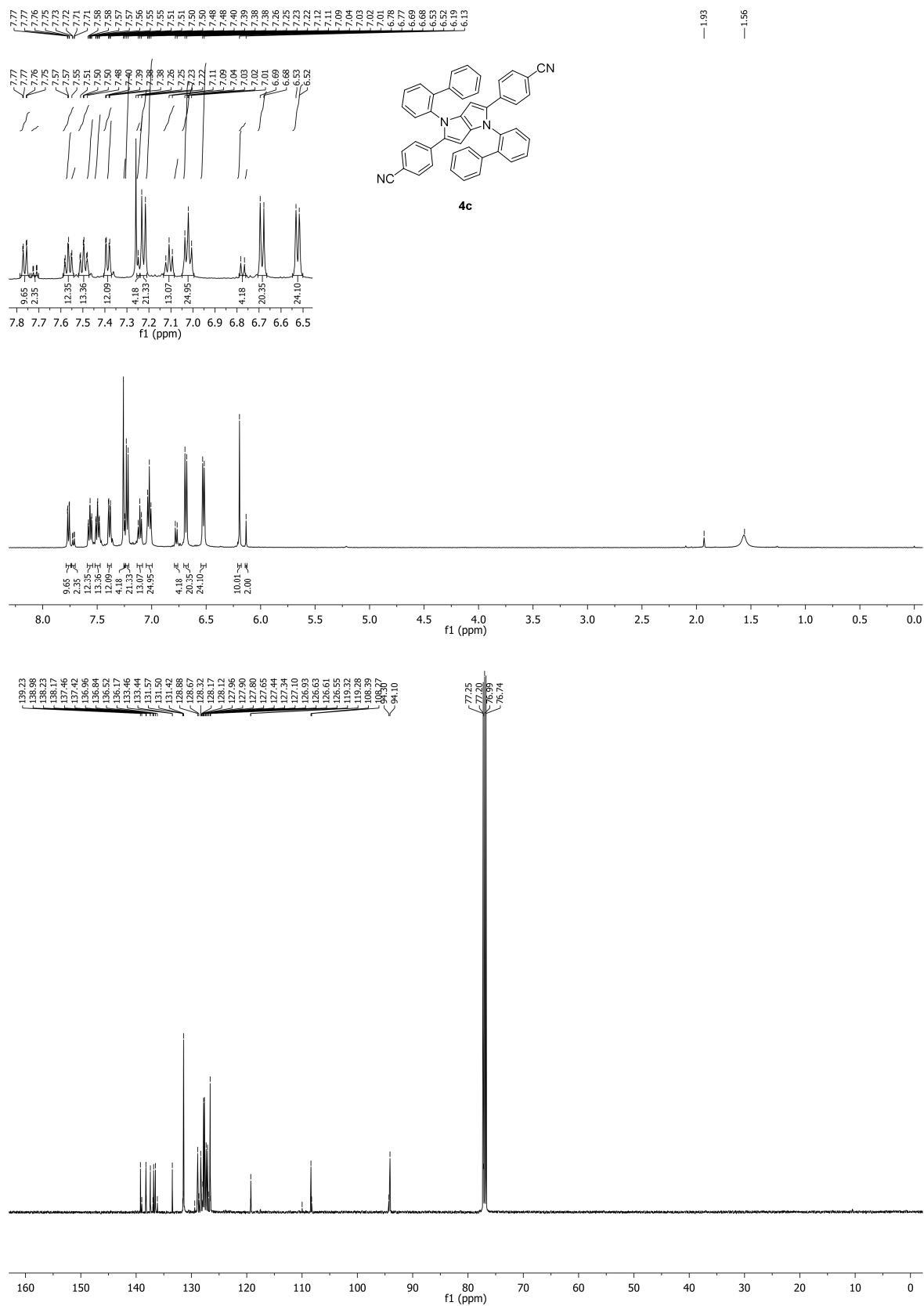


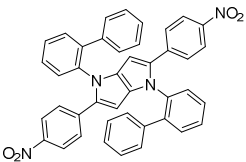
5. ^1H and ^{13}C NMR spectra for synthesized compounds



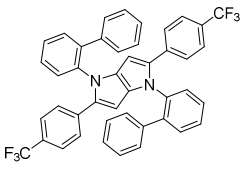


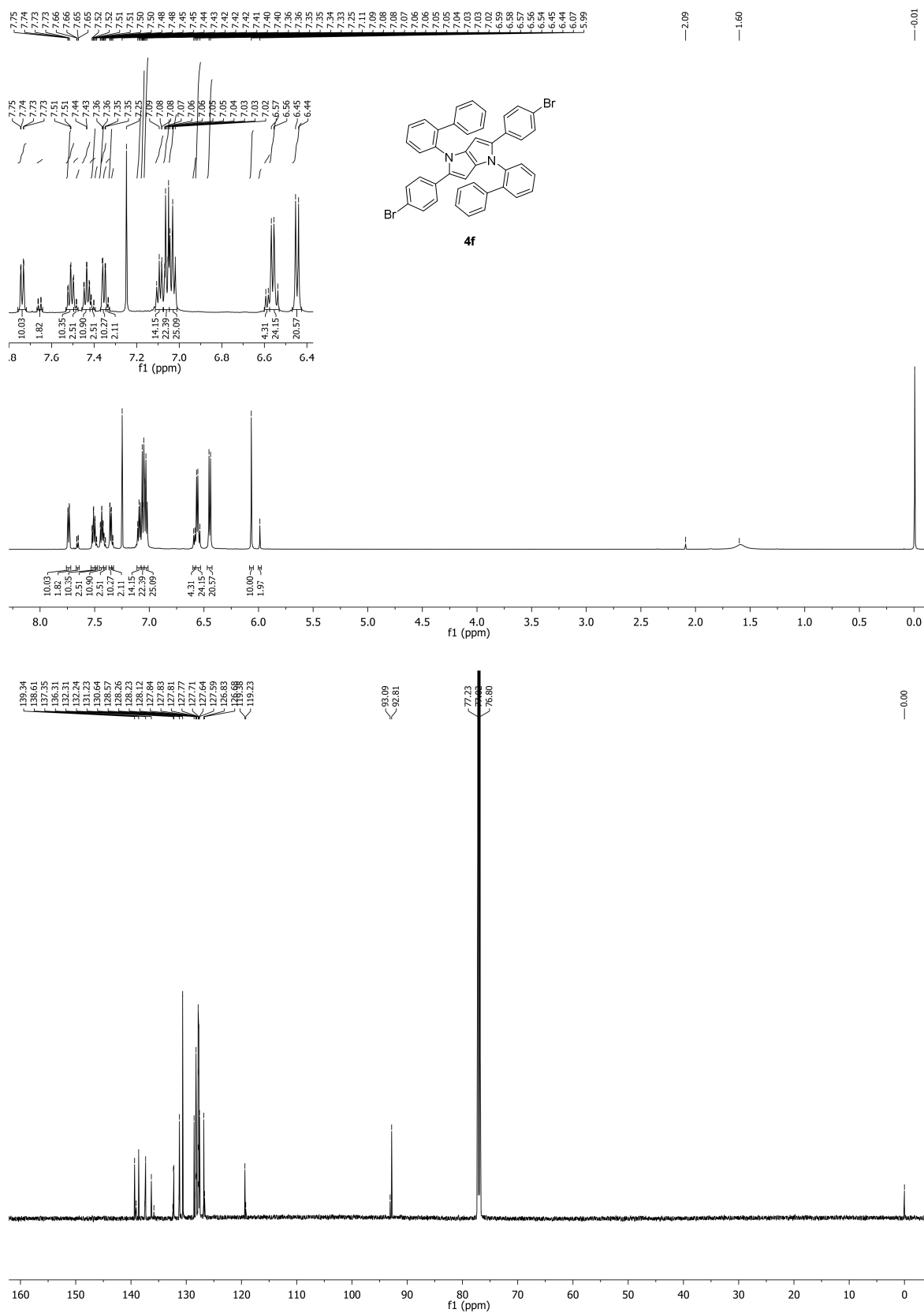
4b

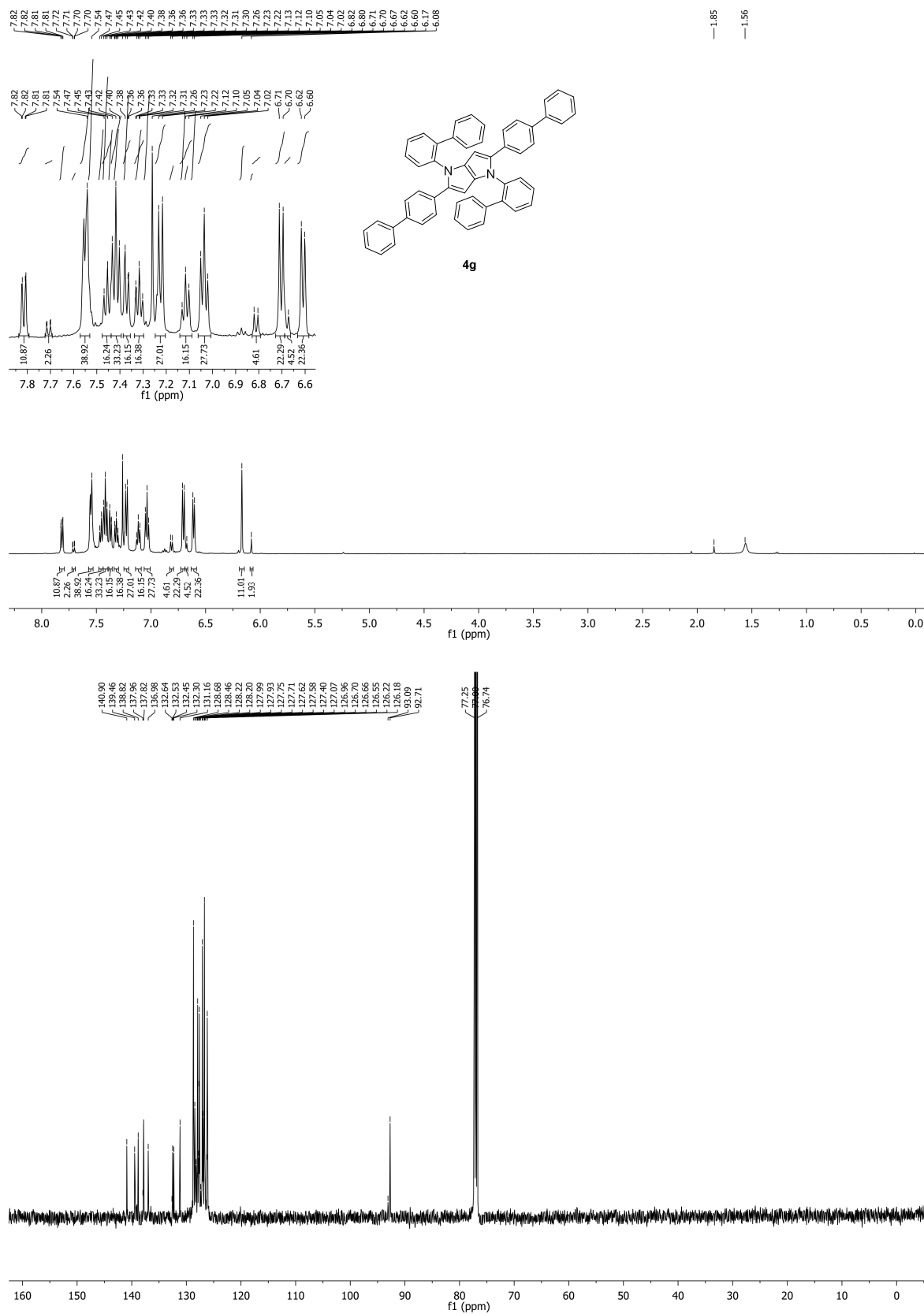


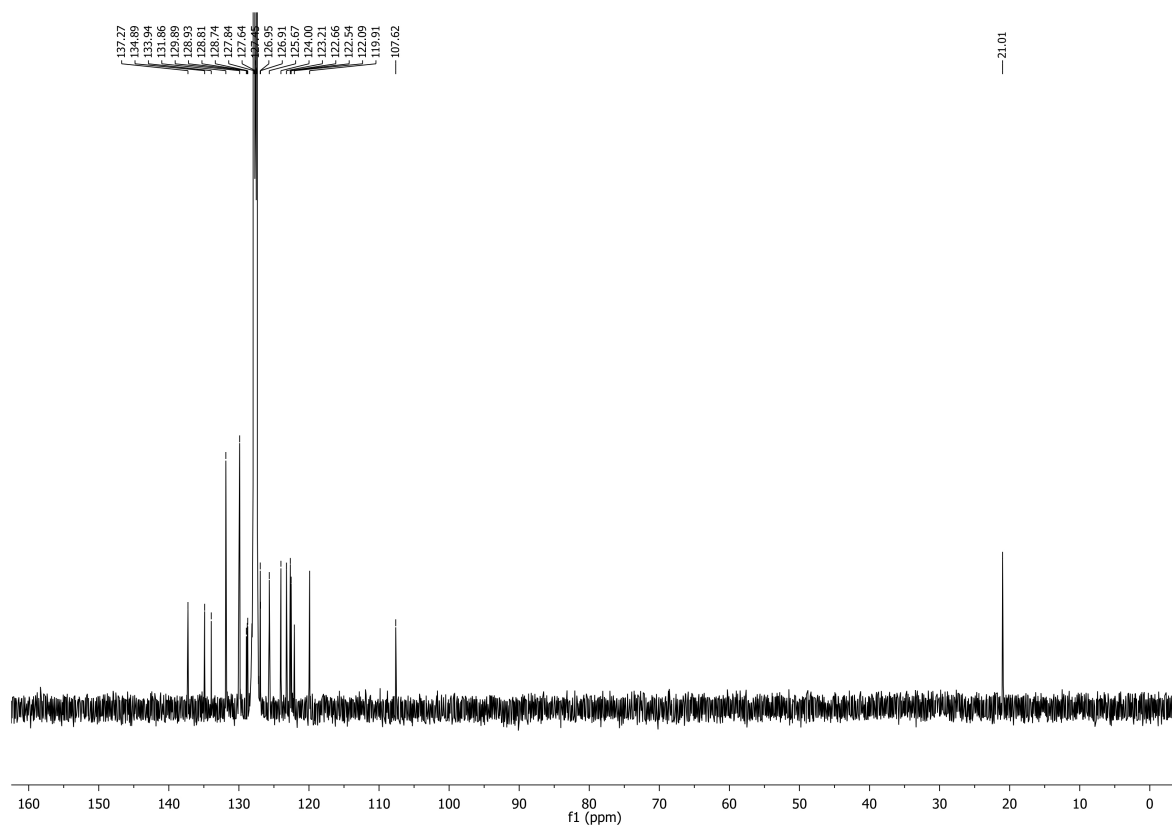
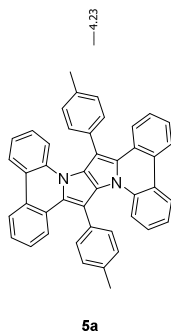
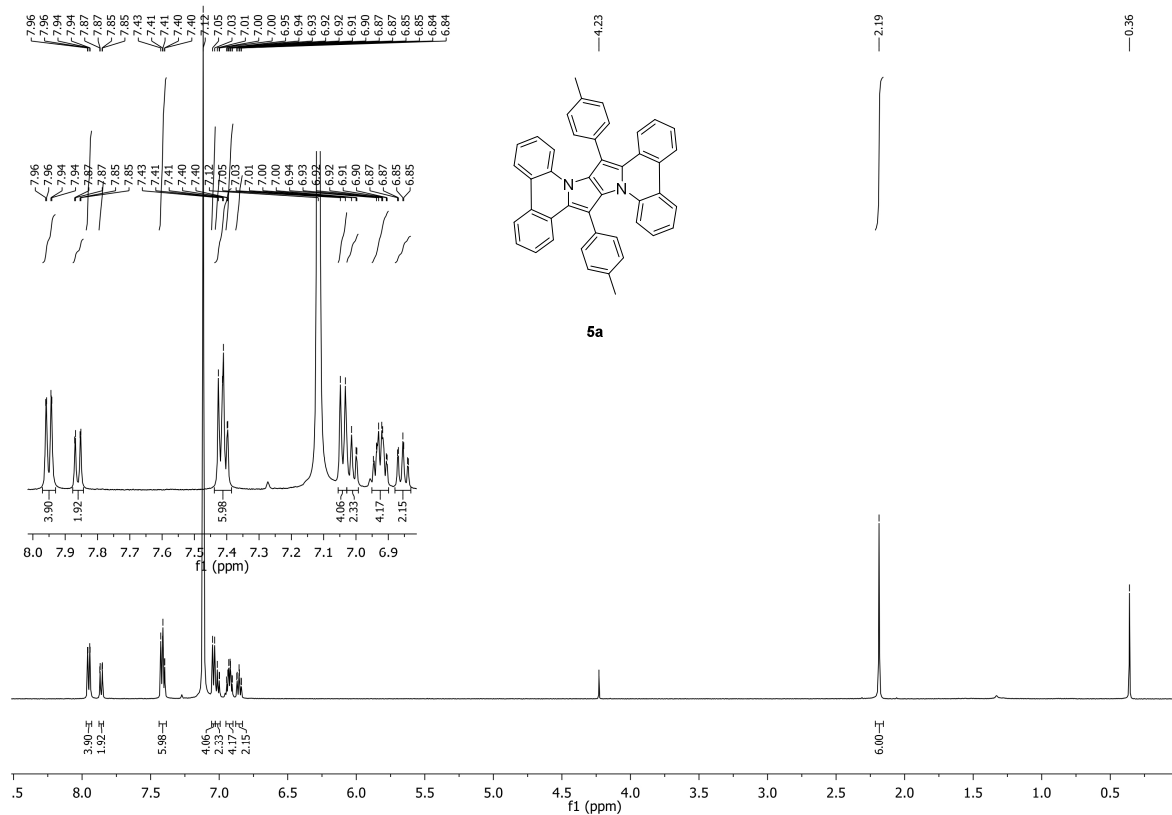


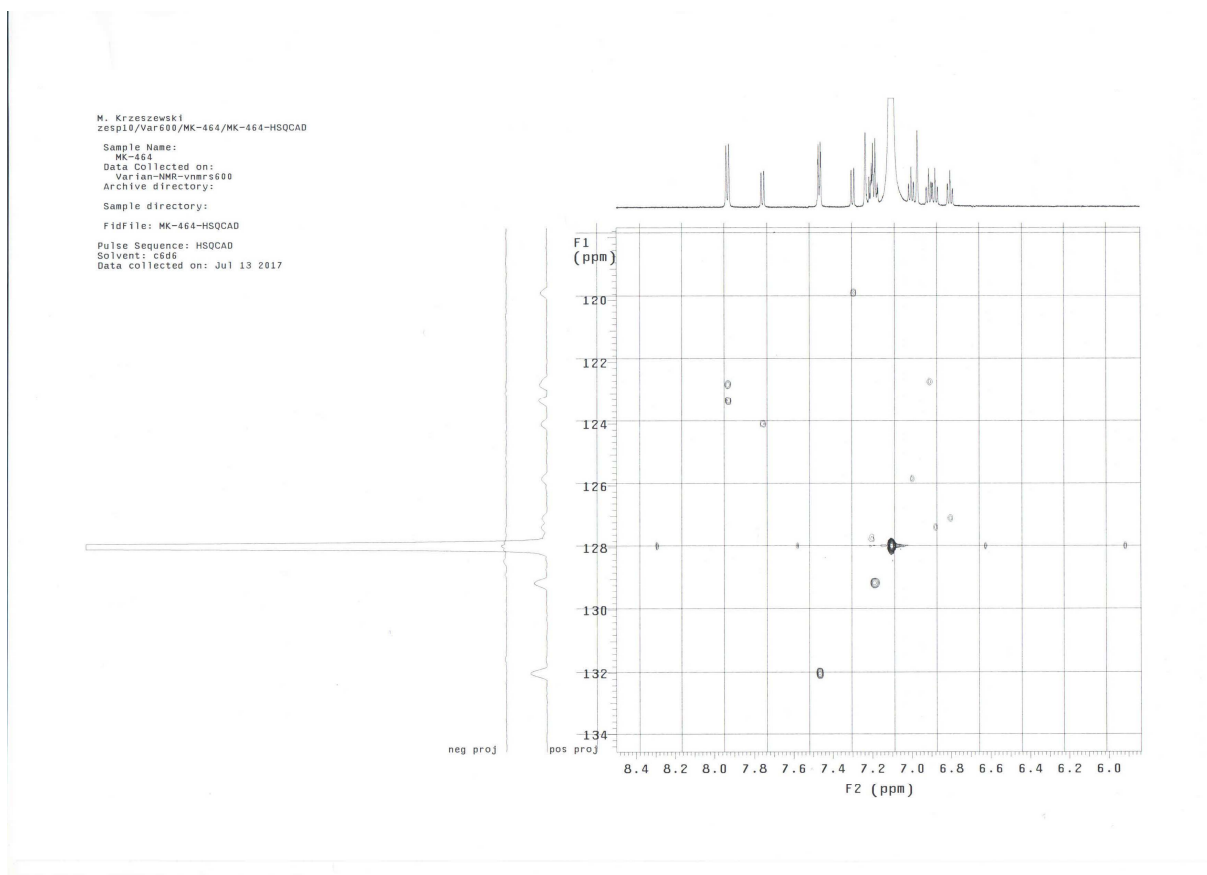
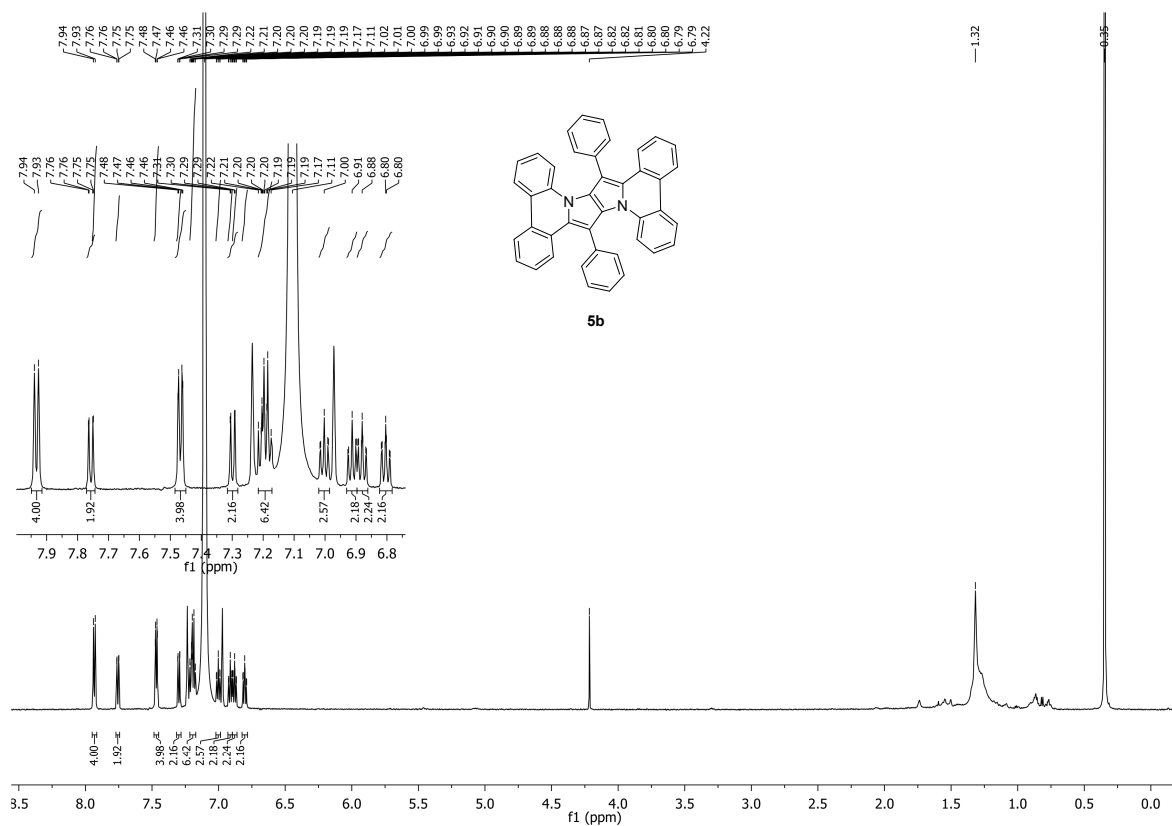
4d

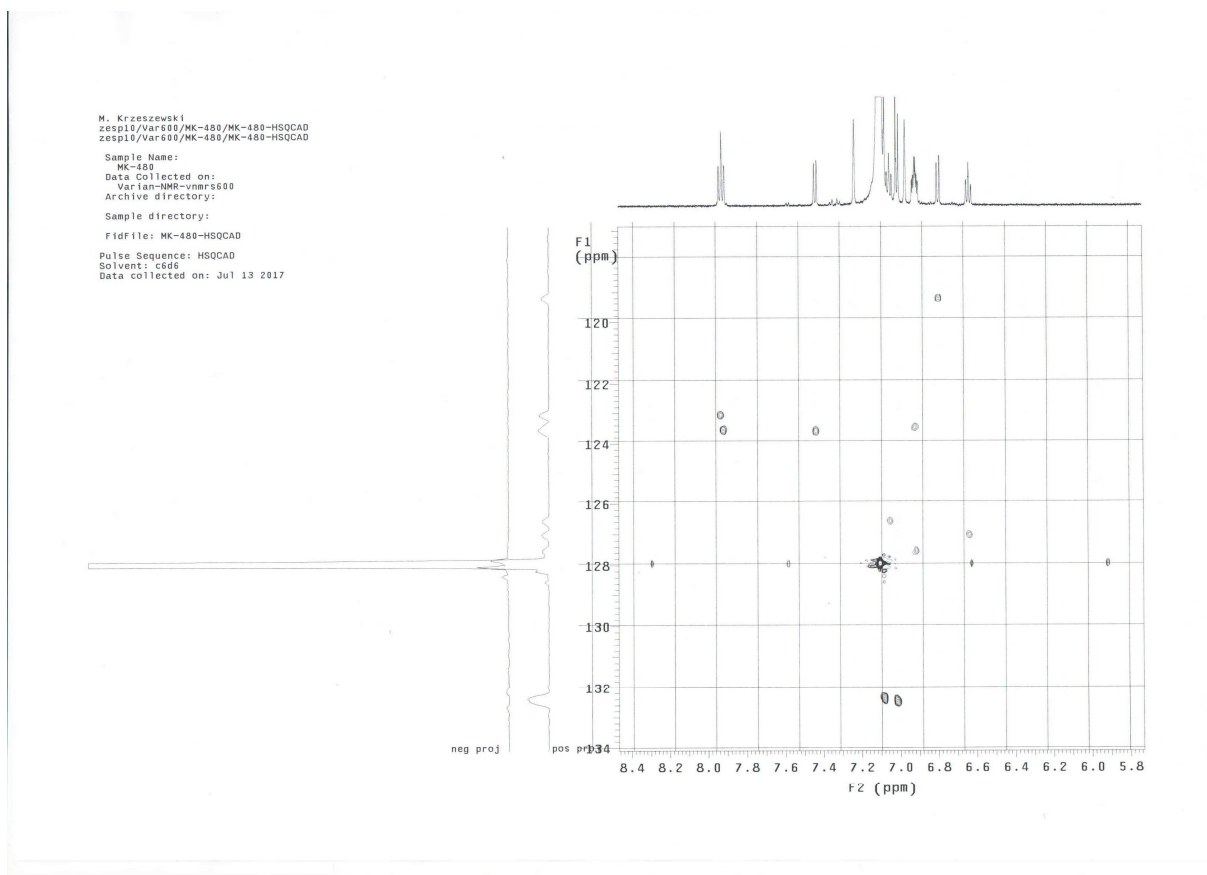
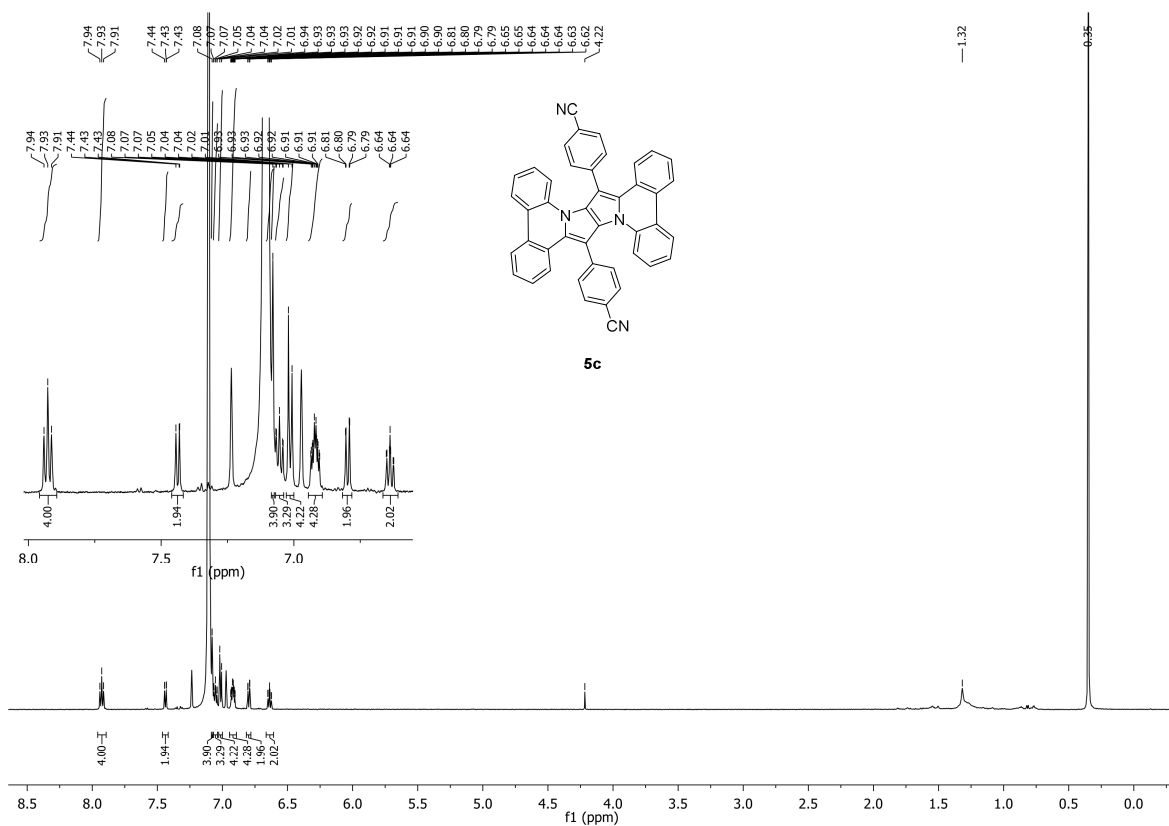


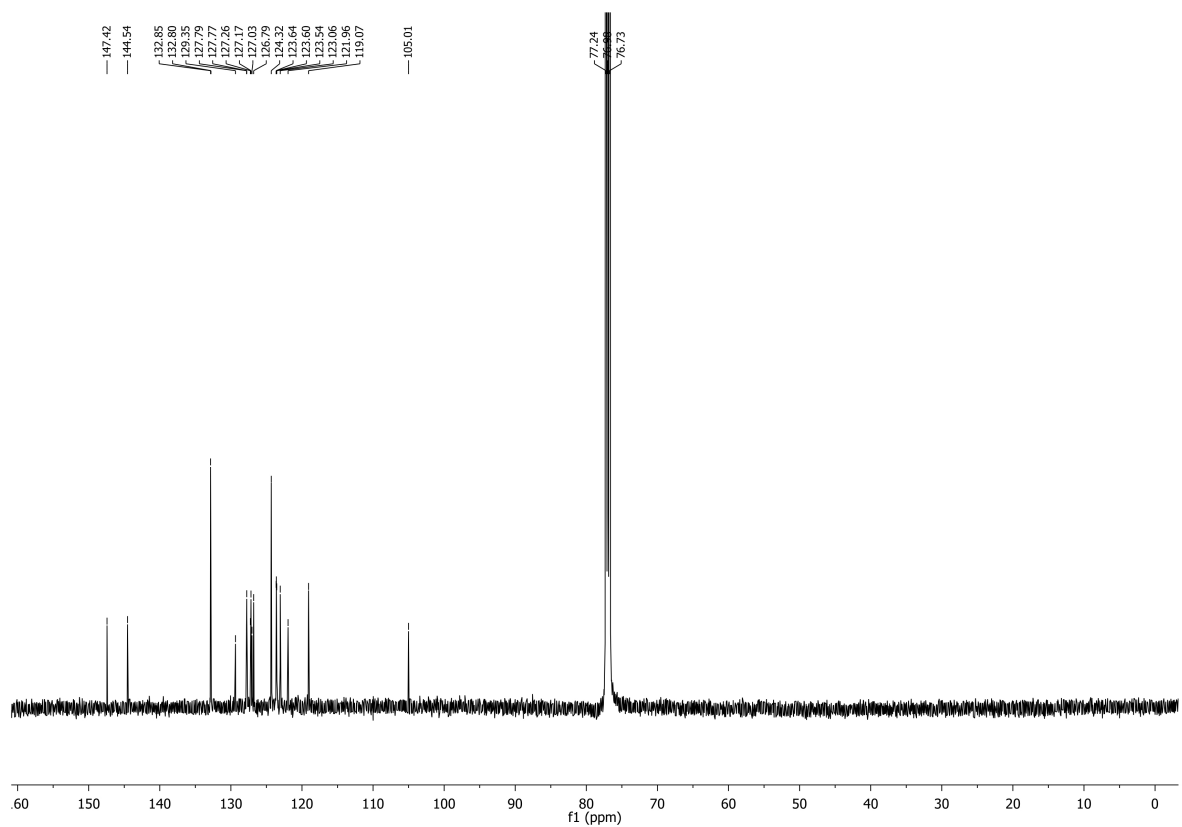
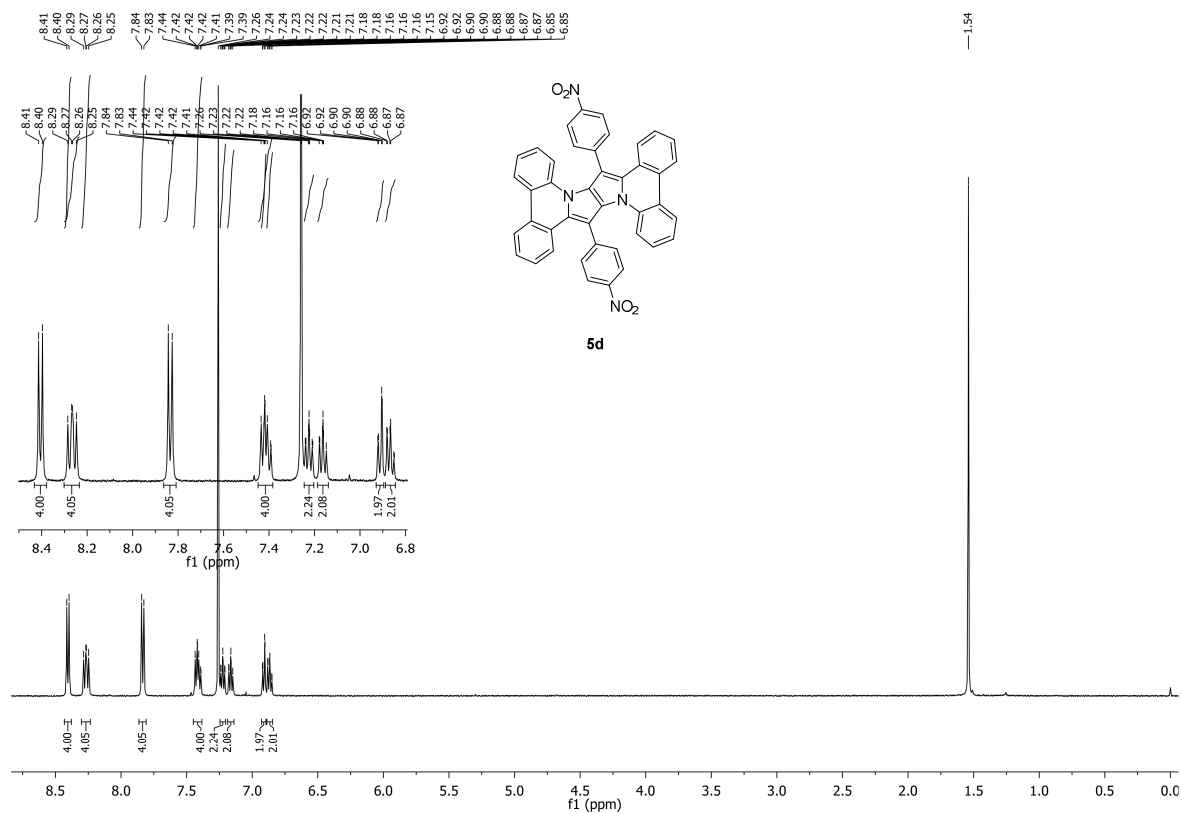


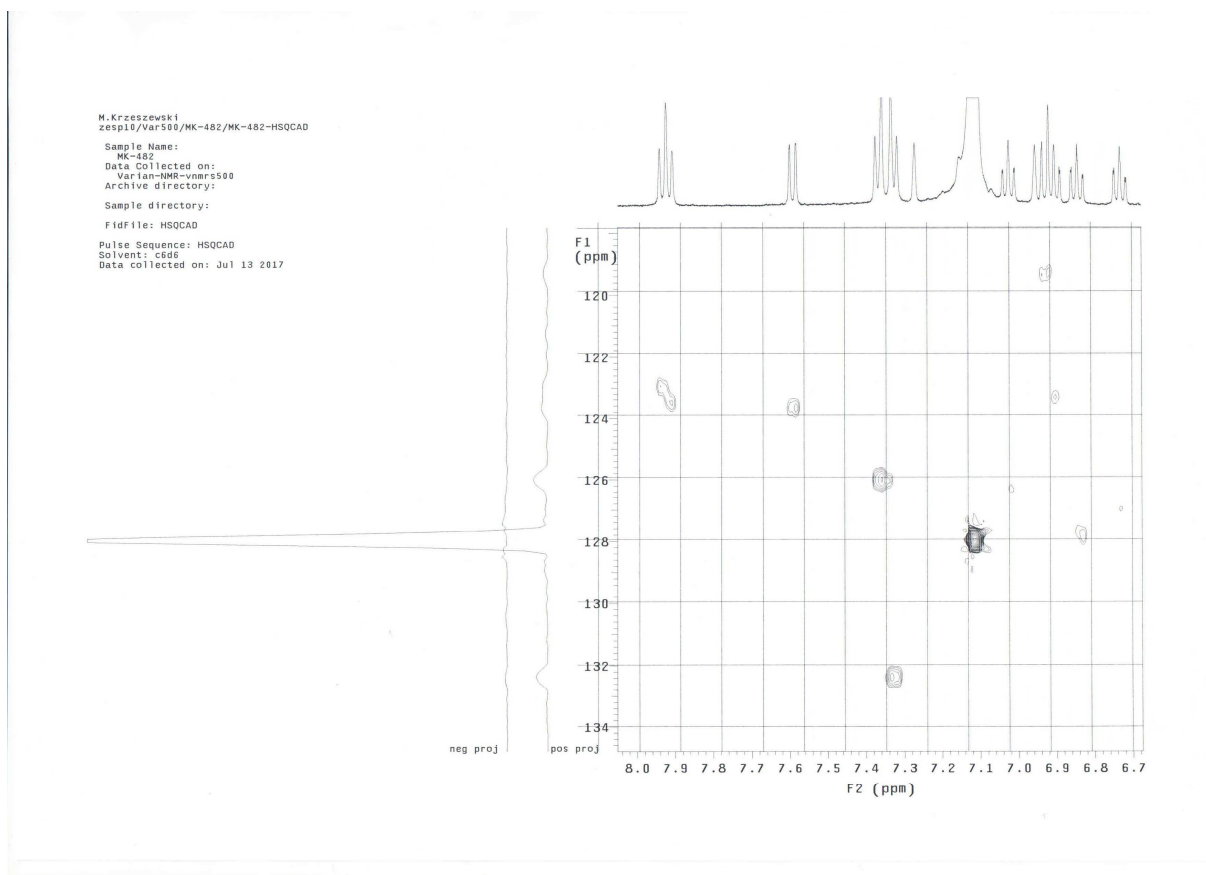
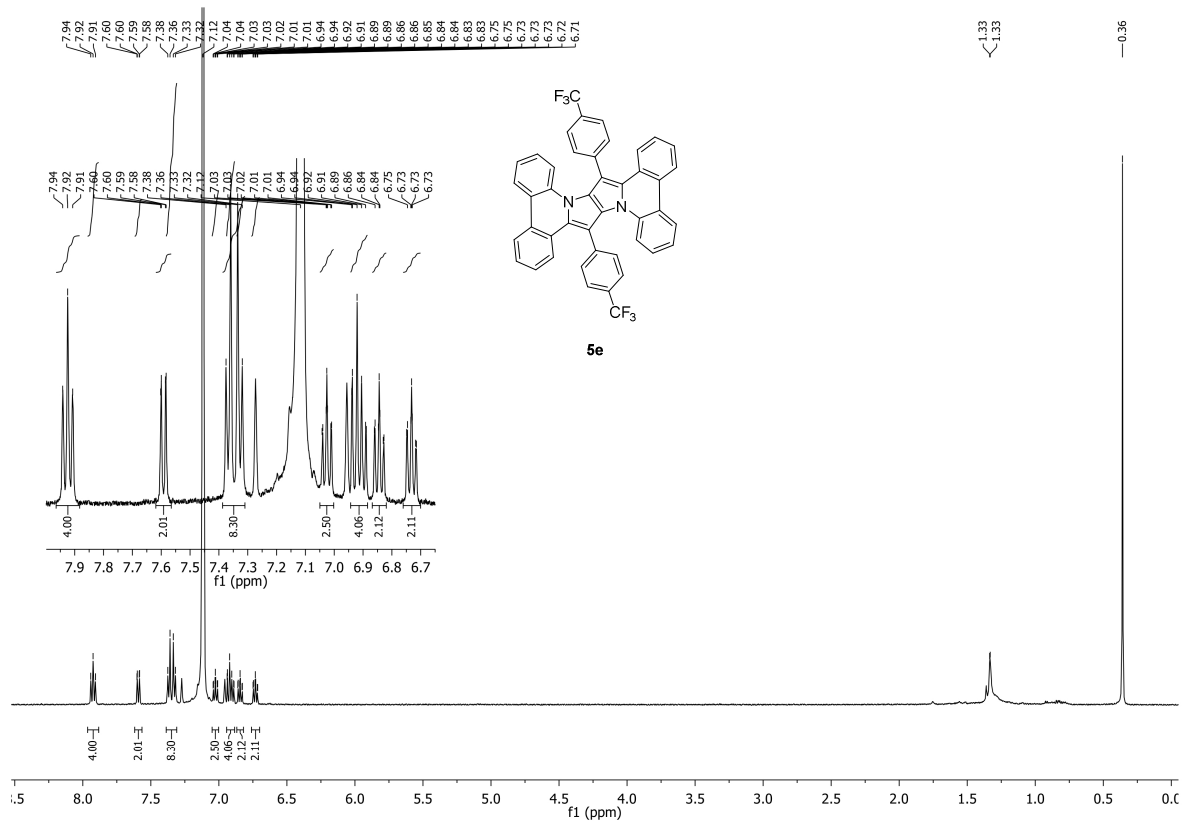


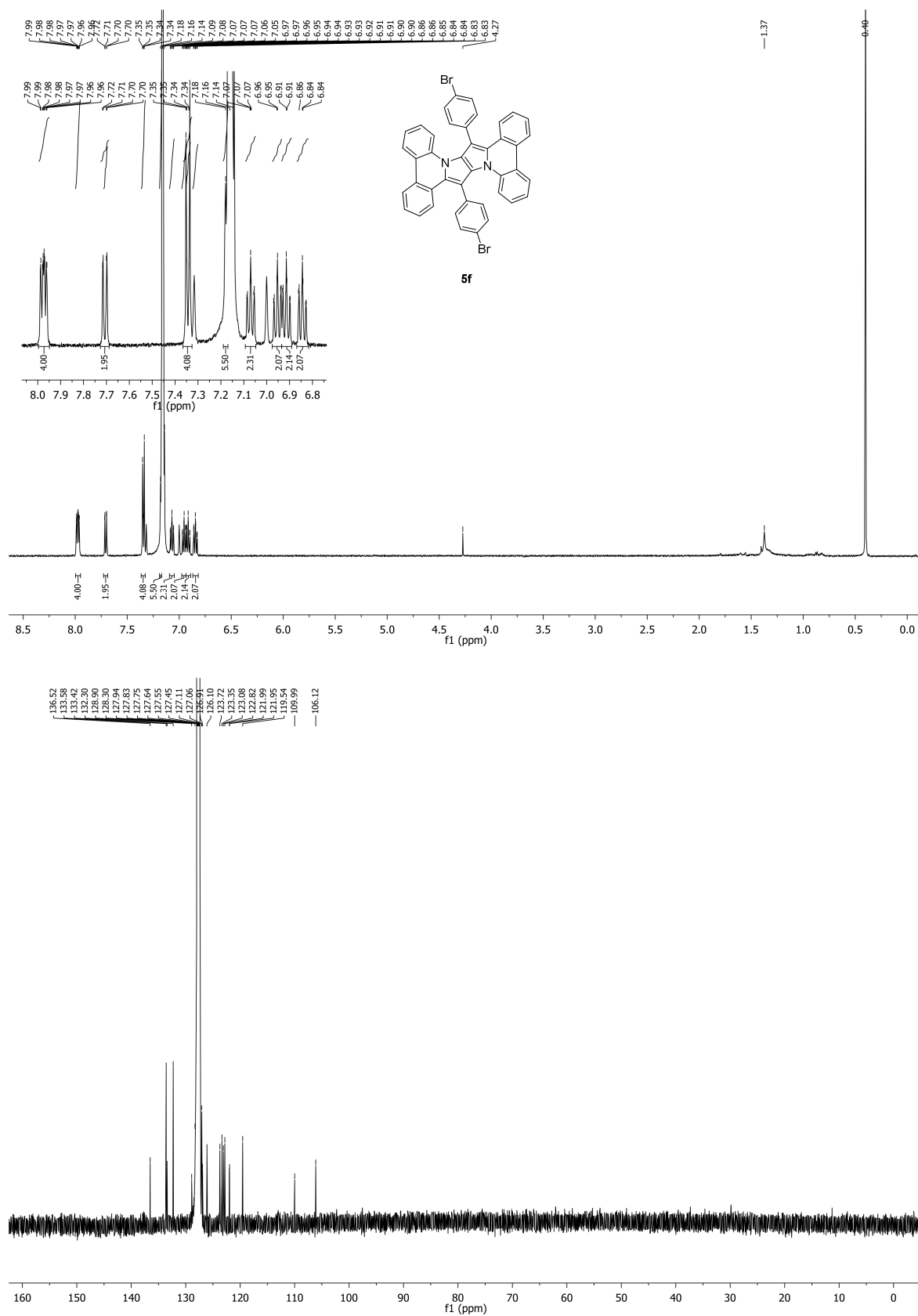












6. Computational investigation

We employed M06-2X density functional theory (DFT) for geometry optimizations and energy calculations. Vibrational frequency calculations were performed on stationary points to ensure the characteristics of minima (no imaginary frequency) and TSs (one imaginary frequency). ZPE correction were applied to the minima and TSs. All quantum mechanical calculations were performed with the Gaussian 09 package (C.01). (Frisch, M. J.; et al. Gaussian 09, rev C.01; Gaussian, Inc.: Wallingford, CT, **2009**.)

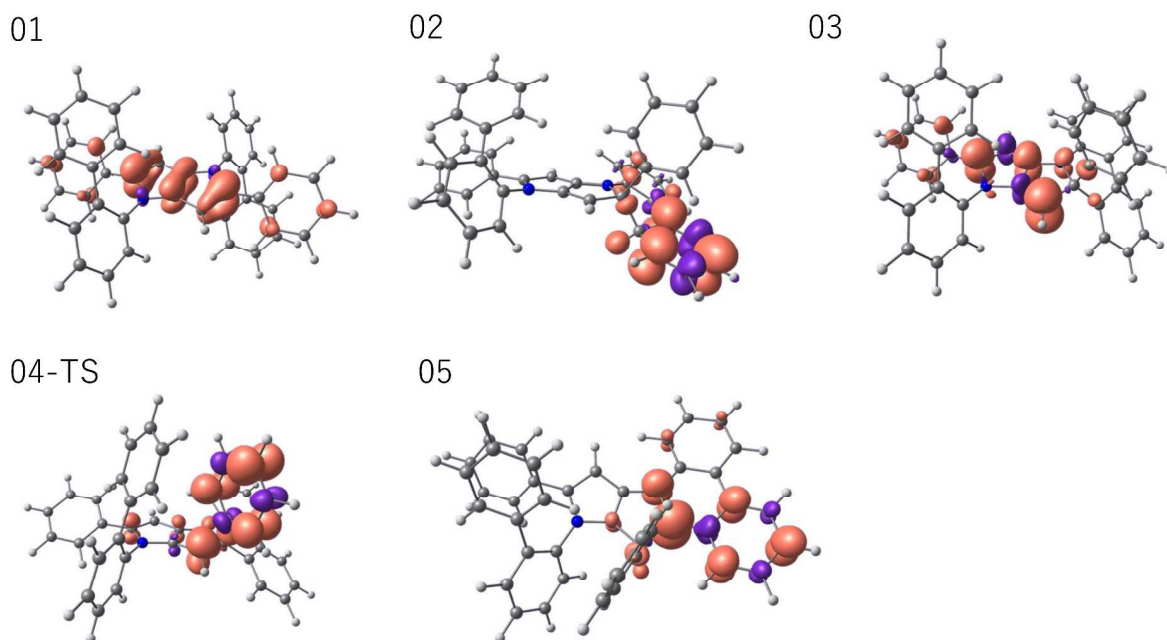


Figure S3. Spin density map.

Cartesian coordinates of the converged geometries and the corresponding absolute energies (in Hartrees).

4b: M062X/6-31G(d,p) , -1726.785089 a.u.

7	-1.543097000	0.695827000	0.333678000
6	-1.895220000	-0.583455000	0.772970000
6	-0.814770000	-1.436483000	0.634087000
6	0.228406000	-0.648680000	0.083967000
6	-0.228145000	0.648233000	-0.085447000
7	1.543451000	-0.696187000	-0.334877000
6	1.895613000	0.583124000	-0.774035000
6	0.815124000	1.436121000	-0.635242000
6	-2.379684000	1.824605000	0.116332000
6	-3.227166000	-0.907537000	1.297441000
6	2.380125000	-1.824856000	-0.117296000
6	3.227782000	0.907499000	-1.297772000
6	-3.811368000	-2.133947000	0.960069000
6	-5.080110000	-2.463392000	1.420532000
6	-5.791678000	-1.566664000	2.213747000
6	-5.216465000	-0.345311000	2.557888000
6	-3.940715000	-0.018574000	2.111346000
6	-3.565675000	1.742504000	-0.634424000
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6	-3.923517000	4.117373000	-0.218837000
6	-2.728767000	4.187405000	0.491692000
6	-1.966880000	3.038944000	0.664985000
6	3.565635000	-1.742614000	0.634197000
6	4.329534000	-2.907249000	0.769065000

6	3.924312000	-4.117295000	0.218308000
6	2.729993000	-4.187482000	-0.492934000
6	1.967920000	-3.039171000	-0.666433000
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6	5.080569000	2.463699000	-1.419125000
6	5.792737000	1.567413000	-2.212297000
6	5.217908000	0.346122000	-2.557292000
6	3.941947000	0.018982000	-2.111628000
6	4.026212000	-0.485266000	1.277848000
6	-4.027060000	0.485158000	-1.277498000
6	3.150016000	0.314804000	2.020247000
6	3.603760000	1.489470000	2.609466000
6	4.932681000	1.882671000	2.462898000
6	5.809482000	1.091351000	1.726548000
6	5.358486000	-0.085910000	1.139698000
6	-3.151680000	-0.315262000	-2.020481000
6	-3.606231000	-1.489886000	-2.609168000
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1	-0.794586000	-2.469700000	0.947814000
1	0.794999000	2.469390000	-0.948800000
1	-3.277172000	-2.804540000	0.293759000
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1	-5.760926000	0.354370000	3.184495000
1	-3.492166000	0.929439000	2.392967000
1	-5.243908000	2.857924000	-1.352614000
1	-4.532019000	5.005074000	-0.356819000
1	-2.396175000	5.127176000	0.919912000
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1	5.243710000	-2.857785000	1.353173000
1	4.532955000	-5.004875000	0.356455000
1	2.397889000	-5.127249000	-0.921540000
1	1.048346000	-3.057217000	-1.243551000
1	3.276931000	2.804081000	-0.293262000
1	5.524384000	3.413426000	-1.136592000
1	5.762855000	-0.353202000	-3.183875000
1	3.493721000	-0.928988000	-2.393915000
1	2.110708000	0.015207000	2.130069000
1	2.916119000	2.100967000	3.185372000
1	5.281426000	2.804561000	2.917878000
1	6.842003000	1.398604000	1.593187000
1	6.030033000	-0.682310000	0.528384000
1	-2.112369000	-0.015985000	-2.131150000
1	-2.919228000	-2.101669000	-3.185531000
1	-5.284517000	-2.804552000	-2.916044000
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1	-6.030222000	0.682890000	-0.526477000
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4b radical cation: UM062X/6-31G(d,p) , -1726.564653 a.u.

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6	-0.230035000	-0.669302000	0.074650000
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6	1.887094000	-0.550893000	0.766322000
6	0.783311000	-1.439336000	0.601145000
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6	-4.950049000	2.552794000	-1.494291000
6	-5.707081000	1.650985000	-2.239506000

6	-5.206578000	0.380033000	-2.524784000
6	-3.957404000	0.000016000	-2.056160000
6	-3.525868000	-1.742661000	0.698274000
6	-4.311749000	-2.889243000	0.851683000
6	-3.970005000	-4.093366000	0.245279000
6	-2.826859000	-4.179663000	-0.544548000
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6	3.526085000	1.742922000	-0.697882000
6	4.311592000	2.889978000	-0.849708000
6	3.968275000	4.093740000	-0.243477000
6	2.823830000	4.179200000	0.544567000
6	2.038369000	3.048286000	0.735016000
6	3.694261000	-2.186411000	1.030168000
6	4.949094000	-2.552909000	1.495165000
6	5.704929000	-1.650959000	2.241416000
6	5.203687000	-0.380185000	2.526220000
6	3.954976000	-0.000511000	2.056114000
6	3.915811000	0.471717000	-1.360212000
6	-3.913877000	-0.471063000	1.360875000
6	2.993844000	-0.271723000	-2.105043000
6	3.368790000	-1.478747000	-2.685401000
6	4.669032000	-1.955484000	-2.530082000
6	5.595420000	-1.214655000	-1.800417000
6	5.221727000	-0.007191000	-1.219568000
6	-2.990336000	0.272046000	2.104084000
6	-3.363640000	1.479480000	2.684641000
6	-4.663827000	1.956969000	2.531178000
6	-5.591791000	1.216444000	1.803211000
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1	0.778667000	-2.478530000	0.893943000
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1	-5.341866000	3.538738000	-1.269174000
1	-5.791336000	-0.312874000	-3.119999000
1	-3.564615000	-0.984290000	-2.289142000
1	-5.190843000	-2.830878000	1.486018000
1	-4.593598000	-4.967734000	0.397496000
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1	-1.163476000	-3.077974000	-1.375742000
1	5.191705000	2.832279000	-1.482687000
1	4.591654000	4.968482000	-0.394416000
1	2.549586000	5.115146000	1.018427000
1	1.159833000	3.076368000	1.372942000
1	3.118502000	-2.870777000	0.414884000
1	5.341488000	-3.538713000	1.270436000
1	5.787514000	0.312837000	3.122218000
1	3.561587000	0.983642000	2.288733000
1	1.983747000	0.107373000	-2.242918000
1	2.649440000	-2.042007000	-3.271216000
1	4.961358000	-2.896599000	-2.984288000
1	6.609200000	-1.581214000	-1.676608000
1	5.934170000	0.556400000	-0.623468000
1	-1.980269000	-0.107625000	2.240596000
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6: UM062X/6-31G(d,p) , -1726.524894 a.u.

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6	-0.709825000	1.589706000	-0.858521000
6	0.375377000	0.756293000	-0.579270000
6	-0.105357000	-0.613568000	-0.549027000
7	1.683807000	0.752315000	-0.350781000

6	2.163176000	-0.639926000	-0.144567000
6	0.904915000	-1.461362000	-0.303573000
6	-2.312610000	-1.731927000	-0.634972000
6	-3.189522000	1.159807000	-1.253030000
6	2.612573000	1.813846000	-0.431436000
6	2.721071000	-0.782796000	1.275943000
6	-3.646842000	2.355707000	-0.685635000
6	-4.951987000	2.773364000	-0.909627000
6	-5.799615000	2.009136000	-1.708691000
6	-5.342030000	0.825966000	-2.288393000
6	-4.042570000	0.394639000	-2.060318000
6	-3.313943000	-1.759503000	0.346780000
6	-4.105580000	-2.910535000	0.418259000
6	-3.888029000	-3.996808000	-0.422586000
6	-2.870445000	-3.954582000	-1.371772000
6	-2.086494000	-2.812378000	-1.483874000
6	3.928578000	1.512549000	-0.845890000
6	4.820457000	2.595453000	-0.928520000
6	4.429832000	3.886556000	-0.610170000
6	3.125570000	4.147469000	-0.188198000
6	2.214967000	3.104542000	-0.094287000
6	1.959914000	-0.275663000	2.334381000
6	2.399799000	-0.401663000	3.644502000
6	3.607726000	-1.043465000	3.913817000
6	4.366488000	-1.548544000	2.865745000
6	3.929164000	-1.420237000	1.547549000
6	4.301215000	0.140839000	-1.188252000
6	-3.564244000	-0.613173000	1.256675000
6	3.176040000	-0.863133000	-1.316528000
6	3.623499000	-2.278689000	-1.525161000
6	4.921769000	-2.589500000	-1.754987000
6	5.935602000	-1.588836000	-1.702127000
6	5.604400000	-0.264106000	-1.401922000
6	-2.520961000	-0.016379000	1.973132000
6	-2.766361000	1.083295000	2.788365000
6	-4.057618000	1.595980000	2.899579000
6	-5.103480000	0.996879000	2.201834000
6	-4.859189000	-0.102670000	1.385682000
1	-0.734753000	2.654330000	-1.025488000
1	0.884146000	-2.536884000	-0.186720000
1	-2.994008000	2.925428000	-0.031464000
1	-5.310420000	3.690951000	-0.455877000
1	-5.998851000	0.240497000	-2.922434000
1	-3.684900000	-0.522144000	-2.517640000
1	-4.886016000	-2.953875000	1.171830000
1	-4.510687000	-4.880343000	-0.332504000
1	-2.695790000	-4.797650000	-2.030899000
1	-1.312673000	-2.736570000	-2.242348000
1	5.834000000	2.425685000	-1.272695000
1	5.145625000	4.696901000	-0.692407000
1	2.824090000	5.154960000	0.074872000
1	1.207986000	3.277158000	0.271422000
1	1.021052000	0.234826000	2.130070000
1	1.802512000	0.000918000	4.455709000
1	5.310882000	-2.043302000	3.065776000
1	4.540523000	-1.815440000	0.745751000
1	2.575148000	-0.586623000	-2.205458000
1	2.856955000	-3.046787000	-1.569875000
1	5.200651000	-3.617199000	-1.964071000
1	6.970751000	-1.860158000	-1.869195000
1	6.410254000	0.455907000	-1.307528000
1	-1.517942000	-0.432800000	1.905122000
1	-1.952518000	1.533848000	3.347935000
1	-4.249517000	2.453369000	3.536306000
1	-6.110612000	1.391684000	2.286853000
1	-5.667392000	-0.549909000	0.813460000
1	-6.818612000	2.337588000	-1.885110000
1	3.954838000	-1.144158000	4.936551000

7a: M062X/6-31G(d,p) , -1725.991687 a.u.

7	1.416014000	0.723272000	-0.919403000
6	1.789297000	-0.587143000	-1.250837000
6	0.648317000	-1.404470000	-1.242284000
6	-0.421904000	-0.589772000	-0.877090000
6	0.059089000	0.731732000	-0.667725000
7	-1.772039000	-0.592407000	-0.629507000
6	-2.176511000	0.713753000	-0.055168000
6	-0.933514000	1.573947000	-0.245409000
6	2.266585000	1.792132000	-0.516698000
6	3.161708000	-0.983862000	-1.526457000
6	-2.696386000	-1.621279000	-0.682286000
6	-2.427488000	0.554074000	1.462597000
6	3.578554000	-2.278299000	-1.174768000
6	4.886591000	-2.686168000	-1.394408000
6	5.811732000	-1.808786000	-1.957909000
6	5.408286000	-0.523488000	-2.314692000
6	4.096806000	-0.113183000	-2.109723000
6	3.194928000	1.628145000	0.524787000
6	4.035869000	2.704072000	0.823830000
6	3.931160000	3.915943000	0.149596000
6	2.973793000	4.075410000	-0.848462000
6	2.148880000	3.008293000	-1.186314000
6	-4.055446000	-1.262191000	-0.818999000
6	-5.009690000	-2.281460000	-0.796951000
6	-4.639547000	-3.616778000	-0.695485000
6	-3.289266000	-3.954990000	-0.612934000
6	-2.317400000	-2.964265000	-0.597532000
6	-1.686628000	-0.380925000	2.192540000
6	-1.838395000	-0.480239000	3.570427000
6	-2.731382000	0.353429000	4.240567000
6	-3.471344000	1.283485000	3.519376000
6	-3.322178000	1.382591000	2.137034000
6	-4.384668000	0.154675000	-1.078023000
6	3.295388000	0.361129000	1.293044000
6	-3.439055000	1.151318000	-0.775446000
6	-3.692404000	2.481614000	-1.093359000
6	-4.894703000	2.847644000	-1.691279000
6	-5.838169000	1.869399000	-1.993281000
6	-5.577318000	0.535782000	-1.703366000
6	2.154523000	-0.227317000	1.850236000
6	2.256390000	-1.420874000	2.554946000
6	3.495668000	-2.039481000	2.713256000
6	4.635013000	-1.454775000	2.167263000
6	4.535496000	-0.260081000	1.461382000
1	0.645854000	-2.444483000	-1.531343000
1	-0.860629000	2.595680000	0.095961000
1	2.876326000	-2.943461000	-0.681267000
1	5.191805000	-3.686935000	-1.105021000
1	6.117926000	0.163386000	-2.765363000
1	3.791018000	0.883217000	-2.411348000
1	4.760532000	2.586082000	1.624001000
1	4.587623000	4.738832000	0.412516000
1	2.878540000	5.020520000	-1.372582000
1	1.417659000	3.091893000	-1.984603000
1	-6.062524000	-2.023647000	-0.856285000
1	-5.399245000	-4.390596000	-0.679261000
1	-2.992317000	-4.995958000	-0.534564000
1	-1.268646000	-3.215496000	-0.481349000
1	-0.989026000	-1.035831000	1.675806000
1	-1.262280000	-1.215776000	4.123710000
1	-4.175450000	1.933177000	4.029946000
1	-3.914690000	2.102737000	1.580982000
1	-2.941678000	3.234002000	-0.871141000
1	-5.088668000	3.888313000	-1.929766000
1	-6.771038000	2.142368000	-2.476022000
1	-6.297643000	-0.222090000	-1.994232000

1	1.186717000	0.256334000	1.734078000
1	1.364409000	-1.866634000	2.985506000
1	3.571582000	-2.973947000	3.260332000
1	5.601569000	-1.936308000	2.276900000
1	5.415054000	0.177321000	0.996433000
1	6.837270000	-2.124539000	-2.119763000
1	-2.851937000	0.273338000	5.316129000

7b: M062X/6-31G(d,p) , -1725.954789 a.u.

7	-1.563961000	0.320964000	-0.962096000
6	-1.853995000	1.608348000	-0.525985000
6	-0.664829000	2.228006000	-0.140609000
6	0.361567000	1.289867000	-0.370292000
6	-0.212211000	0.136002000	-0.863534000
7	1.740242000	1.107196000	-0.282449000
6	2.052564000	-0.261798000	-0.647454000
6	0.759049000	-0.913189000	-1.024398000
6	-2.431092000	-0.713094000	-1.436101000
6	-3.202471000	2.182891000	-0.441594000
6	2.698096000	1.850803000	0.382346000
6	1.649932000	-1.319258000	0.416609000
6	-3.491840000	3.033424000	0.638199000
6	-4.738310000	3.633273000	0.761789000
6	-5.732534000	3.383771000	-0.181320000
6	-5.461783000	2.535256000	-1.250556000
6	-4.209976000	1.943893000	-1.386224000
6	-2.894561000	-1.711348000	-0.568209000
6	-3.660607000	-2.745757000	-1.122941000
6	-3.946395000	-2.793260000	-2.481338000
6	-3.456000000	-1.805167000	-3.331752000
6	-2.688884000	-0.774291000	-2.805235000
6	4.054527000	1.531454000	0.139497000
6	5.031524000	2.237596000	0.844642000
6	4.696595000	3.255024000	1.729357000
6	3.355668000	3.582873000	1.924536000
6	2.357012000	2.883309000	1.262464000
6	1.137565000	-0.908082000	1.702171000
6	1.179953000	-1.763216000	2.776999000
6	1.711227000	-3.058453000	2.670684000
6	2.230007000	-3.474409000	1.435290000
6	2.225013000	-2.640004000	0.341951000
6	4.372869000	0.526371000	-0.896092000
6	-2.579939000	-1.740790000	0.884739000
6	3.366526000	-0.353301000	-1.339230000
6	3.621443000	-1.258741000	-2.365219000
6	4.882016000	-1.327378000	-2.948132000
6	5.886468000	-0.466108000	-2.514705000
6	5.628063000	0.459765000	-1.511493000
6	-2.074097000	-2.917862000	1.447147000
6	-1.843061000	-3.006283000	2.814715000
6	-2.110217000	-1.916103000	3.638179000
6	-2.599838000	-0.736207000	3.084878000
6	-2.835611000	-0.646141000	1.716729000
1	-0.592862000	3.251625000	0.193509000
1	0.683437000	-1.750892000	-1.705092000
1	-2.729419000	3.200011000	1.393284000
1	-4.938883000	4.286304000	1.605315000
1	-6.226776000	2.339055000	-1.995167000
1	-4.011988000	1.308892000	-2.240840000
1	-4.041352000	-3.516060000	-0.459309000
1	-4.549007000	-3.604269000	-2.877255000
1	-3.661426000	-1.841050000	-4.396229000
1	-2.271581000	-0.001035000	-3.443785000
1	6.076255000	1.978610000	0.704772000
1	5.475269000	3.786739000	2.264750000
1	3.083248000	4.375029000	2.614755000
1	1.311569000	3.102883000	1.446983000

1	0.712338000	0.083338000	1.815866000
1	0.784435000	-1.421317000	3.728860000
1	2.664918000	-4.464972000	1.337471000
1	2.664620000	-2.972364000	-0.593176000
1	2.823003000	-1.905999000	-2.717116000
1	5.074351000	-2.039169000	-3.744056000
1	6.869295000	-0.501570000	-2.973515000
1	6.406134000	1.158088000	-1.221554000
1	-1.844463000	-3.760594000	0.801155000
1	-1.434260000	-3.920557000	3.232626000
1	-1.930689000	-1.983855000	4.706825000
1	-2.815418000	0.116503000	3.721222000
1	-3.255641000	0.262955000	1.299101000
1	-6.709848000	3.844442000	-0.081454000
1	1.734183000	-3.718009000	3.530805000

7c: M062X/6-31G(d,p) , -1726.011322 a.u.

7	-1.060958000	0.170020000	-1.020147000
6	-1.369124000	1.485552000	-0.703739000
6	-0.195996000	2.160740000	-0.402910000
6	0.851178000	1.217606000	-0.564289000
6	0.296794000	0.022909000	-0.933765000
7	2.234675000	1.033168000	-0.372488000
6	2.527364000	-0.322587000	-0.566053000
6	1.266249000	-1.120974000	-0.839879000
6	-1.943018000	-0.892007000	-1.374415000
6	-2.741374000	2.010409000	-0.694741000
6	3.217262000	1.977752000	-0.130606000
6	0.862066000	-2.078341000	0.287018000
6	-3.148846000	2.808922000	0.379580000
6	-4.445745000	3.304945000	0.438025000
6	-5.356815000	2.999882000	-0.569823000
6	-4.958069000	2.207189000	-1.644359000
6	-3.657246000	1.719955000	-1.712858000
6	-2.978300000	-1.305843000	-0.522052000
6	-3.779635000	-2.370189000	-0.948016000
6	-3.549818000	-3.020869000	-2.155435000
6	-2.511157000	-2.602451000	-2.982483000
6	-1.716142000	-1.530524000	-2.592957000
6	4.560628000	1.547817000	0.006170000
6	5.526042000	2.529435000	0.263100000
6	5.200943000	3.873379000	0.379749000
6	3.875552000	4.275009000	0.228147000
6	2.889683000	3.336146000	-0.028155000
6	1.252482000	-1.833248000	1.605422000
6	0.782322000	-2.636446000	2.640053000
6	-0.087641000	-3.690461000	2.370039000
6	-0.470806000	-3.947236000	1.056840000
6	0.008143000	-3.150136000	0.020290000
6	4.892964000	0.119895000	-0.134825000
6	-3.244687000	-0.657770000	0.787115000
6	3.837137000	-0.796762000	-0.433926000
6	4.139870000	-2.177293000	-0.576191000
6	5.434835000	-2.628794000	-0.434955000
6	6.470814000	-1.732139000	-0.144597000
6	6.189224000	-0.378671000	0.002869000
6	-2.219056000	-0.466988000	1.718548000
6	-2.488518000	0.153078000	2.933405000
6	-3.778809000	0.588858000	3.230167000
6	-4.804338000	0.393684000	2.309035000
6	-4.538824000	-0.230008000	1.094575000
1	-0.159942000	3.206337000	-0.140932000
1	1.356235000	-1.700644000	-1.771970000
1	-2.450097000	2.995686000	1.189677000
1	-4.751154000	3.912125000	1.284458000
1	-5.660754000	1.974938000	-2.438599000
1	-3.347115000	1.113662000	-2.558642000

1	-4.577951000	-2.705613000	-0.292677000
1	-4.179176000	-3.854829000	-2.448044000
1	-2.326305000	-3.097867000	-3.929730000
1	-0.914915000	-1.165474000	-3.228691000
1	6.563810000	2.235393000	0.369946000
1	5.977713000	4.603486000	0.578620000
1	3.607277000	5.323742000	0.303510000
1	1.864487000	3.649994000	-0.167218000
1	1.926146000	-1.007452000	1.817041000
1	1.094615000	-2.436641000	3.660385000
1	-1.146328000	-4.767469000	0.834900000
1	-0.302692000	-3.349046000	-1.002786000
1	3.334532000	-2.875811000	-0.782439000
1	5.648913000	-3.687446000	-0.545126000
1	7.488269000	-2.089357000	-0.031095000
1	7.005765000	0.296962000	0.232308000
1	-1.213523000	-0.810140000	1.490110000
1	-1.686554000	0.291884000	3.651777000
1	-3.982988000	1.078767000	4.177139000
1	-5.809149000	0.741400000	2.527698000
1	-5.326809000	-0.347227000	0.355485000
1	-6.372842000	3.378351000	-0.519920000
1	-0.461026000	-4.310580000	3.178534000

7d: UM062X/6-31G(d,p) , -1726.165490 a.u.

7	-1.351584000	0.101773000	1.219967000
6	-1.820420000	-1.080541000	0.627228000
6	-0.729393000	-1.811598000	0.136086000
6	0.410119000	-1.057294000	0.410706000
6	0.023414000	0.132541000	1.084591000
7	1.774544000	-1.040277000	0.267928000
6	2.308617000	0.271949000	0.706680000
6	1.098319000	0.937480000	1.351265000
6	-2.107227000	1.267984000	1.531865000
6	-3.229180000	-1.432713000	0.547052000
6	2.627735000	-1.952354000	-0.326754000
6	2.722237000	1.103524000	-0.527896000
6	-3.688874000	-2.164030000	-0.559789000
6	-5.029190000	-2.494751000	-0.684996000
6	-5.964584000	-2.103203000	0.277648000
6	-5.505916000	-1.373314000	1.377022000
6	-4.163469000	-1.046576000	1.520128000
6	-2.948506000	1.867015000	0.578910000
6	-3.698861000	2.977196000	0.978229000
6	-3.587095000	3.507463000	2.258866000
6	-2.714158000	2.928784000	3.175745000
6	-1.983437000	1.802793000	2.812804000
6	3.983212000	-1.919396000	0.067282000
6	4.875821000	-2.777909000	-0.577767000
6	4.443165000	-3.678056000	-1.543891000
6	3.091226000	-3.732218000	-1.882091000
6	2.183485000	-2.868965000	-1.284601000
6	2.039829000	0.947165000	-1.738580000
6	2.344818000	1.749975000	-2.829186000
6	3.337168000	2.732251000	-2.750258000
6	4.011098000	2.882888000	-1.540467000
6	3.712428000	2.078448000	-0.442148000
6	4.359434000	-1.059849000	1.208074000
6	-3.054053000	1.359076000	-0.812937000
6	3.507247000	-0.009504000	1.596903000
6	3.798639000	0.750206000	2.725143000
6	4.948974000	0.498570000	3.467837000
6	5.799586000	-0.536753000	3.089802000
6	5.497508000	-1.316631000	1.980385000
6	-1.905547000	1.118307000	-1.575048000
6	-2.015497000	0.626030000	-2.870442000
6	-3.270561000	0.372174000	-3.421255000

6	-4.417044000	0.618948000	-2.671338000
6	-4.309222000	1.110749000	-1.374374000
1	-0.806137000	-2.793774000	-0.305112000
1	1.117432000	1.941324000	1.748533000
1	-2.989677000	-2.423175000	-1.349410000
1	-5.363312000	-3.049436000	-1.558432000
1	-6.213581000	-1.061359000	2.141095000
1	-3.835684000	-0.492300000	2.393840000
1	-4.354972000	3.444984000	0.249953000
1	-4.171066000	4.379177000	2.535087000
1	-2.612065000	3.341638000	4.173796000
1	-1.321951000	1.308785000	3.518149000
1	5.929777000	-2.738399000	-0.320780000
1	5.155654000	-4.335250000	-2.030192000
1	2.744992000	-4.434331000	-2.633824000
1	1.138900000	-2.869009000	-1.577466000
1	1.266482000	0.187892000	-1.826915000
1	1.807266000	1.611545000	-3.764457000
1	4.788386000	3.637687000	-1.452744000
1	4.263125000	2.210541000	0.484432000
1	3.118846000	1.543434000	3.021585000
1	5.174097000	1.100248000	4.342366000
1	6.689444000	-0.752267000	3.672403000
1	6.138699000	-2.155283000	1.729102000
1	-0.924439000	1.320695000	-1.150336000
1	-1.116868000	0.441708000	-3.451955000
1	-3.353635000	-0.017236000	-4.431072000
1	-5.397442000	0.413823000	-3.089761000
1	-5.199955000	1.263184000	-0.770505000
1	-7.009233661	-2.357122927	0.174537591
1	3.573616475	3.354568558	-3.600677294

7e: UM062X/6-31G(d,p) , -1726.116536 a.u.

7	-1.554231000	0.248378000	-1.028715000
6	-1.859875000	1.566540000	-0.656180000
6	-0.666534000	2.206346000	-0.300023000
6	0.368972000	1.253504000	-0.464623000
6	-0.199132000	0.064021000	-0.894558000
7	1.750414000	1.074884000	-0.323251000
6	2.075313000	-0.316599000	-0.630256000
6	0.773200000	-0.999375000	-0.997170000
6	-2.425657000	-0.817185000	-1.433360000
6	-3.215976000	2.116131000	-0.572890000
6	2.716136000	1.892975000	0.238144000
6	1.595921000	-1.331697000	0.479274000
6	-3.479502000	3.085636000	0.414083000
6	-4.746143000	3.646490000	0.542775000
6	-5.783969000	3.239396000	-0.298399000
6	-5.538184000	2.269127000	-1.269959000
6	-4.267540000	1.711833000	-1.412251000
6	-2.904496000	-1.731509000	-0.487136000
6	-3.690056000	-2.803027000	-0.938952000
6	-3.984173000	-2.956650000	-2.291384000
6	-3.483555000	-2.045750000	-3.225633000
6	-2.694518000	-0.983129000	-2.793512000
6	4.078545000	1.550881000	0.041685000
6	5.057572000	2.329987000	0.667676000
6	4.719882000	3.442223000	1.434188000
6	3.375678000	3.792846000	1.584997000
6	2.379494000	3.022319000	0.998710000
6	1.037575000	-0.831583000	1.716942000
6	1.104956000	-1.585439000	2.865194000
6	1.689518000	-2.866887000	2.876445000
6	2.235789000	-3.375305000	1.682637000
6	2.213848000	-2.639225000	0.518709000
6	4.410103000	0.439585000	-0.883126000
6	-2.578411000	-1.611299000	0.960096000

6	3.402941000	-0.471625000	-1.268412000
6	3.673161000	-1.473542000	-2.200952000
6	4.952051000	-1.612914000	-2.736629000
6	5.958302000	-0.723814000	-2.357099000
6	5.683826000	0.301101000	-1.455076000
6	-2.014666000	-2.704523000	1.629617000
6	-1.783550000	-2.643869000	3.001872000
6	-2.105019000	-1.487286000	3.713624000
6	-2.641498000	-0.385628000	3.045268000
6	-2.881394000	-0.444265000	1.672565000
1	-0.589994000	3.241534000	-0.018556000
1	0.706307000	-1.850606000	-1.658446000
1	-2.685393000	3.373013000	1.093086000
1	-4.927297000	4.391432000	1.308659000
1	-6.336697000	1.945774000	-1.926774000
1	-4.095002000	0.967475000	-2.177185000
1	-4.076111000	-3.505150000	-0.208819000
1	-4.599580000	-3.786199000	-2.617884000
1	-3.697426000	-2.168980000	-4.279838000
1	-2.274786000	-0.272648000	-3.496811000
1	6.100293000	2.057084000	0.561326000
1	5.494895000	4.027154000	1.912324000
1	3.102254000	4.656299000	2.180005000
1	1.336754000	3.266141000	1.151215000
1	0.549246000	0.135057000	1.722018000
1	0.683485000	-1.183241000	3.778920000
1	2.705767000	-4.352539000	1.680902000
1	2.685491000	-3.024419000	-0.377661000
1	2.875751000	-2.134926000	-2.521444000
1	5.156388000	-2.396491000	-3.455708000
1	6.951336000	-0.815233000	-2.780452000
1	6.461509000	1.014304000	-1.212680000
1	-1.738995000	-3.589682000	1.066776000
1	-1.324957000	-3.485183000	3.507009000
1	-1.928424000	-1.441743000	4.781904000
1	-2.890949000	0.514924000	3.593740000
1	-3.328912000	0.397368000	1.158599000
1	-6.772770000	3.669124000	-0.192716000
1	1.730922000	-3.445383000	3.790720000

7f: UM062X/6-31G(d,p) , -1726.178881 a.u.

7	0.849977000	-0.316637000	-1.074330000
6	1.232973000	-1.546399000	-0.556647000
6	0.098215000	-2.237841000	-0.160238000
6	-1.001535000	-1.398734000	-0.475678000
6	-0.516301000	-0.243957000	-1.024794000
7	-2.392499000	-1.265036000	-0.298829000
6	-2.759883000	0.033572000	-0.672344000
6	-1.546272000	0.850477000	-1.075061000
6	1.668696000	0.714976000	-1.619470000
6	2.636002000	-1.970446000	-0.457207000
6	-3.321966000	-2.220494000	0.073903000
6	-1.173750000	1.964245000	-0.091376000
6	3.086858000	-2.541950000	0.738762000
6	4.413782000	-2.918695000	0.884795000
6	5.335424000	-2.727919000	-0.148977000
6	4.879345000	-2.165857000	-1.342186000
6	3.547459000	-1.797260000	-1.502592000
6	2.685728000	1.330697000	-0.872887000
6	3.417495000	2.347673000	-1.495010000
6	3.138473000	2.762745000	-2.792718000
6	2.118457000	2.147205000	-3.512982000
6	1.393591000	1.116809000	-2.926240000
6	-4.682440000	-1.840903000	0.190741000
6	-5.592225000	-2.828295000	0.588188000
6	-5.198417000	-4.132076000	0.853882000
6	-3.858868000	-4.488128000	0.711472000

6	-2.925706000	-3.541485000	0.321180000
6	-1.540317000	1.886237000	1.253819000
6	-1.062157000	2.817046000	2.169878000
6	-0.199135000	3.842630000	1.774905000
6	0.136991000	3.933620000	0.423504000
6	-0.349308000	3.012702000	-0.500416000
6	-5.089508000	-0.460147000	-0.119300000
6	3.003895000	0.945836000	0.526051000
6	-4.089611000	0.456358000	-0.571718000
6	-4.466785000	1.788428000	-0.890419000
6	-5.778781000	2.193609000	-0.766995000
6	-6.759334000	1.297743000	-0.321893000
6	-6.405045000	-0.008779000	-0.004596000
6	2.002240000	0.882688000	1.499726000
6	2.320593000	0.524229000	2.805127000
6	3.636478000	0.221201000	3.150561000
6	4.637092000	0.285100000	2.184592000
6	4.323360000	0.651276000	0.879890000
1	0.118696000	-3.228038000	0.267011000
1	-1.675129000	1.294342000	-2.074504000
1	2.393177000	-2.641285000	1.568332000
1	4.750403000	-3.343693000	1.827458000
1	5.577548000	-2.019266000	-2.162170000
1	3.213341000	-1.370042000	-2.443531000
1	4.200738000	2.837851000	-0.924406000
1	3.714646000	3.566743000	-3.238817000
1	1.894202000	2.457162000	-4.528164000
1	0.608844000	0.600994000	-3.471558000
1	-6.641201000	-2.573023000	0.684855000
1	-5.933507000	-4.868068000	1.160692000
1	-3.538864000	-5.507992000	0.898730000
1	-1.890133000	-3.821665000	0.183410000
1	-2.198819000	1.086297000	1.581591000
1	-1.356302000	2.741157000	3.213845000
1	0.797054000	4.729575000	0.088234000
1	-0.058890000	3.094722000	-1.545454000
1	-3.704748000	2.488726000	-1.219232000
1	-6.049640000	3.215962000	-1.012424000
1	-7.790058000	1.619119000	-0.221725000
1	-7.178805000	-0.684855000	0.342372000
1	0.976089000	1.117792000	1.232748000
1	1.534677000	0.483339000	3.553369000
1	3.880082000	-0.064980000	4.169055000
1	5.662466000	0.038063000	2.442789000
1	5.095454000	0.668274000	0.115250000
1	6.371465984	-3.007703517	-0.027578357
1	0.196191110	4.544344165	2.494428799

8: M062X/6-31G(d,p) , -1725.631612 a.u.

7	0.931122000	0.029578000	-0.693557000
6	1.451721000	-1.258119000	-0.805245000
6	0.427876000	-2.182662000	-0.710154000
6	-0.766103000	-1.431667000	-0.515567000
6	-0.427460000	-0.087118000	-0.492007000
7	-2.132779000	-1.504151000	-0.321223000
6	-2.625258000	-0.197901000	-0.149134000
6	-1.576617000	0.712649000	-0.251988000
6	1.633692000	1.261865000	-0.553243000
6	2.886630000	-1.521554000	-0.959890000
6	-2.945635000	-2.637908000	-0.315858000
6	-1.544787000	2.190100000	-0.151566000
6	3.462697000	-2.590763000	-0.263877000
6	4.822907000	-2.847990000	-0.362200000
6	5.655032000	-2.041258000	-1.142893000
6	5.076787000	-0.973801000	-1.833170000
6	3.712775000	-0.718088000	-1.753946000
6	2.555987000	1.465483000	0.485630000

6	3.157484000	2.725756000	0.581980000
6	2.839328000	3.754292000	-0.297056000
6	1.919891000	3.534259000	-1.319543000
6	1.332774000	2.282800000	-1.453405000
6	-4.327446000	-2.492218000	-0.085289000
6	-5.111476000	-3.656271000	-0.098062000
6	-4.563524000	-4.907303000	-0.321991000
6	-3.192028000	-5.027924000	-0.546926000
6	-2.388804000	-3.901239000	-0.546123000
6	-2.049016000	3.000528000	-1.171308000
6	-1.869160000	4.380953000	-1.135085000
6	-1.175771000	4.988630000	-0.087539000
6	-0.689625000	4.177102000	0.941708000
6	-0.873819000	2.801655000	0.914537000
6	-4.887661000	-1.156346000	0.164773000
6	2.921635000	0.396770000	1.451326000
6	-4.037949000	-0.027295000	0.139554000
6	-4.575426000	1.243278000	0.415777000
6	-5.920905000	1.402602000	0.687774000
6	-6.767757000	0.291396000	0.698000000
6	-6.250476000	-0.965495000	0.444585000
6	4.271726000	0.132347000	1.700981000
6	4.644674000	-0.874955000	2.584131000
6	3.670780000	-1.628823000	3.232826000
6	2.322644000	-1.370169000	2.992158000
6	1.948244000	-0.366454000	2.105590000
1	0.578759000	-3.245623000	-0.812894000
1	2.839126000	-3.187284000	0.395284000
1	5.254479000	-3.673697000	0.198390000
1	5.704689000	-0.335680000	-2.449767000
1	3.284989000	0.111971000	-2.307911000
1	3.865573000	2.898245000	1.387175000
1	3.305999000	4.727240000	-0.180493000
1	1.657471000	4.330197000	-2.008784000
1	0.612860000	2.083732000	-2.240918000
1	-6.179219000	-3.582304000	0.069545000
1	-5.199990000	-5.785306000	-0.323962000
1	-2.747888000	-6.001373000	-0.726873000
1	-1.328330000	-3.991588000	-0.732961000
1	-2.569336000	2.536122000	-2.004636000
1	-2.260565000	4.994846000	-1.942303000
1	-0.146591000	4.630563000	1.767372000
1	-0.470018000	2.181769000	1.710553000
1	-3.923701000	2.107418000	0.422881000
1	-6.313760000	2.392207000	0.897581000
1	-7.825222000	0.408640000	0.910628000
1	-6.921101000	-1.816027000	0.471092000
1	5.030071000	0.694049000	1.162532000
1	5.697089000	-1.080790000	2.753166000
1	3.959641000	-2.418479000	3.919391000
1	1.557361000	-1.953621000	3.494281000
1	0.894913000	-0.178692000	1.910634000
1	6.714875048	-2.237630438	-1.210499062
1	-1.018948828	6.057076182	-0.072387672

8 radical cation: UM062X/6-31G(d,p), -1725.410102 a.u.

7	-1.567385000	0.068282000	-0.717782000
6	-2.154481000	1.219595000	-0.784313000
6	-1.236268000	2.180554000	-0.547395000
6	-0.075245000	1.576963000	-0.295025000
6	-0.319355000	0.282217000	-0.494836000
7	1.115822000	1.806934000	0.089737000
6	1.677229000	0.654192000	0.137009000
6	0.909210000	-0.279507000	-0.493514000
6	-2.125370000	-1.084153000	-0.845657000
6	-3.465304000	1.582342000	-0.799125000
6	1.707053000	2.894309000	0.423509000

6	-3.863880000	2.820265000	-1.169686000
6	-5.150868000	3.203643000	-1.173936000
6	-6.109455000	2.357225000	-0.777390000
6	-5.751539000	1.134613000	-0.365894000
6	-4.459026000	0.771527000	-0.373348000
6	-1.748627000	-2.214546000	-0.178983000
6	-2.339663000	-3.382362000	-0.522339000
6	-3.304290000	-3.468397000	-1.447707000
6	-3.709274000	-2.356383000	-2.066315000
6	-3.113597000	-1.195842000	-1.763959000
6	1.134851000	4.109872000	0.299562000
6	1.749985000	5.254424000	0.624692000
6	2.998041000	5.204600000	1.095369000
6	3.585433000	4.009188000	1.234707000
6	2.971347000	2.848950000	0.914306000
6	-0.906655000	-2.246000000	0.889186000
6	-0.141428000	-3.318981000	1.188776000
6	0.681107000	-3.347296000	2.249659000
6	0.754220000	-2.296305000	3.076585000
6	-0.015674000	-1.228912000	2.829613000
6	-0.830384000	-1.218272000	1.762797000
6	1.333017000	-1.412084000	-1.124587000
6	3.550001000	1.643400000	1.125668000
6	0.543038000	-2.202876000	-1.882261000
6	0.939345000	-3.312355000	-2.526307000
6	2.230296000	-3.660004000	-2.529849000
6	3.089344000	-2.813297000	-1.952765000
6	2.637600000	-1.716592000	-1.322491000
6	2.868679000	0.534603000	0.761473000
6	3.335035000	-0.662504000	1.175174000
6	4.519479000	-0.812054000	1.780887000
6	5.256275000	0.276081000	2.020869000
6	4.756519000	1.481119000	1.712256000
1	-1.441260000	3.245866000	-0.435861000
1	-3.155393000	3.576133000	-1.545753000
1	-5.427211000	4.217445000	-1.510875000
1	-7.167270000	2.667319000	-0.769744000
1	-6.522271000	0.438743000	0.007308000
1	-4.254302000	-0.216635000	0.067416000
1	-2.126102000	-4.332824000	-0.006529000
1	-3.778803000	-4.435922000	-1.683082000
1	-4.491514000	-2.406093000	-2.842179000
1	-3.422164000	-0.344052000	-2.394538000
1	0.130555000	4.258844000	-0.104493000
1	1.245763000	6.227307000	0.496543000
1	3.526685000	6.134252000	1.365891000
1	4.605848000	4.067148000	1.639220000
1	-0.107402000	-4.209905000	0.540119000
1	1.311919000	-4.232531000	2.438494000
1	1.427434000	-2.313415000	3.949287000
1	0.008929000	-0.366960000	3.517683000
1	-1.481253000	-0.333298000	1.671028000
1	-0.498092000	-1.948883000	-2.083834000
1	0.216462000	-3.911127000	-3.106949000
1	2.583022000	-4.545075000	-3.083460000
1	4.173461000	-2.994735000	-2.053159000
1	3.448634000	-1.035434000	-1.032186000
1	2.735095000	-1.581832000	1.076898000
1	4.871008000	-1.807483000	2.099569000
1	6.231805000	0.180325000	2.527084000
1	5.401260000	2.316650000	2.019732000

9: UM062X/6-31G(d,p) , -1725.355942 a.u.

7	-0.614667000	-0.956602000	-1.533129000
6	-0.523974000	0.225200000	-2.040662000
6	0.097328000	1.104062000	-1.205929000
6	0.766975000	0.349888000	-0.093377000

6	0.025163000	-0.937483000	-0.423722000
7	0.432463000	0.319397000	1.357941000
6	0.930027000	-1.010261000	1.729025000
6	0.217544000	-1.759354000	0.630779000
6	-1.279717000	-1.902056000	-2.096654000
6	-0.273237000	1.066751000	2.120926000
6	2.440585000	-1.087804000	1.478573000
6	-1.379375000	-3.152314000	-1.595997000
6	-2.091873000	-4.140497000	-2.152402000
6	-2.752206000	-3.896442000	-3.284678000
6	-2.646706000	-2.677633000	-3.827098000
6	-1.919834000	-1.680810000	-3.273440000
6	-0.724968000	0.643996000	3.341261000
6	-1.499156000	1.432448000	4.127628000
6	-1.931825000	2.668784000	3.852161000
6	-1.535729000	3.260002000	2.491823000
6	-0.663273000	2.280573000	1.686540000
6	3.236652000	-0.053440000	1.811249000
6	4.562837000	-0.098619000	1.612053000
6	5.123636000	-1.194730000	1.081000000
6	4.349298000	-2.241107000	0.758917000
6	3.023596000	-2.185795000	0.961254000
6	-0.464250000	-0.615317000	3.786072000
6	0.676558000	-1.383100000	3.176649000
6	0.683972000	-2.852793000	3.474647000
6	-0.083819000	-3.353527000	4.448174000
6	-0.944833000	-2.552662000	5.089544000
6	-1.142178000	-1.264361000	4.759798000
6	-1.012351000	0.455239000	-3.282451000
6	0.307177000	2.434773000	-1.312648000
6	-0.685682000	1.539582000	-4.016559000
6	-1.206624000	1.811382000	-5.219513000
6	-2.070072000	0.943651000	-5.750755000
6	1.426810000	2.977282000	-0.788288000
6	1.661691000	4.298065000	-0.837135000
6	0.760473000	5.121775000	-1.390183000
6	-0.380978000	4.612423000	-1.874016000
6	-0.603072000	3.289468000	-1.823289000
6	-2.317626000	-0.195826000	-5.091467000
6	-1.773468000	-0.484345000	-3.887664000
1	-0.155455000	-2.761075000	0.848690000
1	-0.873216000	-3.482808000	-0.689669000
1	-2.135812000	-5.143085000	-1.693580000
1	-3.346282000	-4.690971000	-3.766810000
1	-3.200067000	-2.585225000	-4.771804000
1	-1.828935000	1.121731000	5.130374000
1	-2.544714000	3.256738000	4.553871000
1	-1.247987000	4.325676000	2.471231000
1	-0.369672000	2.666591000	0.719473000
1	2.802327000	0.856338000	2.257992000
1	5.192861000	0.763425000	1.888494000
1	6.213280000	-1.238114000	0.917686000
1	4.804955000	-3.149550000	0.330230000
1	2.420115000	-3.067556000	0.692215000
1	1.541629000	-0.984342000	3.770753000
1	1.404600000	-3.502897000	2.953651000
1	-0.017212000	-4.422979000	4.708696000
1	-1.577388000	-3.005496000	5.874593000
1	-1.982639000	-0.811496000	5.306836000
1	0.094655000	2.245888000	-3.704640000
1	-0.907740000	2.713076000	-5.780073000
1	-2.507530000	1.134760000	-6.745256000
1	2.198760000	2.343996000	-0.317935000
1	2.593722000	4.709830000	-0.414551000
1	0.943040000	6.208688000	-1.420036000
1	-1.149951000	5.286758000	-2.287167000
1	-1.591250000	2.931452000	-2.159529000
1	-2.975388000	-0.877214000	-5.648688000

10a: M062X/6-31G(d,p) , -1724.834647 a.u.

6	-0.663400000	1.343062000	0.288410000
6	2.591320000	-2.312691000	0.326076000
6	2.550611000	-3.654920000	0.414492000
6	3.671902000	-4.377075000	0.520965000
6	4.843276000	-3.731910000	0.521221000
6	4.871922000	-2.393096000	0.427702000
6	3.755092000	-1.636817000	0.330138000
6	0.100502000	-2.795567000	-1.748412000
6	-0.187175000	-3.027491000	-3.038729000
6	0.401628000	-2.302541000	-4.000307000
6	1.282060000	-1.351849000	-3.657199000
6	1.561680000	-1.129869000	-2.363612000
6	3.726051000	-0.279951000	0.302185000
6	4.887134000	0.415277000	0.287258000
6	4.960040000	1.745393000	0.423924000
6	3.830983000	2.421273000	0.640135000
6	2.676303000	1.745705000	0.623600000
6	-4.094039000	-0.490477000	1.283022000
6	-5.135772000	-1.253181000	1.682637000
6	-5.009262000	-2.548294000	2.002078000
6	-3.806071000	-3.121577000	1.919855000
6	-2.762206000	-2.378243000	1.530862000
6	-3.317231000	2.718300000	-0.017319000
6	-4.503526000	3.339211000	-0.028722000
6	-5.565011000	2.703145000	0.471672000
6	-5.412617000	1.448440000	0.915364000
6	-4.222597000	0.807335000	0.915072000
6	0.971475000	-1.835366000	-1.379024000
6	2.562507000	0.426667000	0.364208000
6	-3.125210000	1.488382000	0.501948000
6	-2.872302000	-1.070453000	1.215416000
6	0.151216000	-2.011570000	0.941915000
6	1.310401000	-1.569685000	0.099069000
7	1.387364000	-0.080862000	0.334437000
6	-0.655189000	-0.717567000	0.723672000
6	0.158848000	0.280516000	0.369741000
6	-1.917037000	0.880639000	0.554036000
7	-1.867304000	-0.363317000	0.861783000
6	-0.268800000	2.589468000	-0.032400000
6	-0.653116000	3.663705000	0.684780000
6	-0.235300000	4.898607000	0.364539000
6	0.580965000	5.081970000	-0.683527000
6	0.981976000	4.023117000	-1.401992000
6	0.565197000	2.790284000	-1.072743000
1	1.587901000	-4.190547000	0.382493000
1	3.632953000	-5.476470000	0.592077000
1	5.780685000	-4.307971000	0.606942000
1	5.888636000	-1.977004000	0.465565000
1	-0.402693000	-3.423098000	-0.995259000
1	-0.906637000	-3.818033000	-3.311207000
1	0.169817000	-2.490816000	-5.061689000
1	1.778799000	-0.754931000	-4.440600000
1	2.297064000	-0.344991000	-2.128411000
1	5.876710000	-0.052959000	0.189692000
1	5.930957000	2.268843000	0.430235000
1	3.856921000	3.504727000	0.844651000
1	1.806358000	2.354826000	0.885969000
1	-6.166609000	-0.881791000	1.768930000
1	-5.882811000	-3.142026000	2.320777000
1	-3.680989000	-4.188079000	2.172395000
1	-1.812501000	-2.926197000	1.496055000
1	-2.523371000	3.278727000	-0.523374000
1	-4.614644000	4.345952000	-0.465674000
1	-6.555363000	3.189096000	0.466496000
1	-6.352851000	0.990655000	1.253467000
1	0.539946000	-1.845145000	1.986975000

1	-1.291804000	3.543861000	1.577356000
1	-0.552998000	5.763098000	0.971321000
1	0.927510000	6.094994000	-0.947056000
1	1.656120000	4.166015000	-2.263115000
1	0.905609000	1.943133000	-1.693234000

10b: M062X/6-31G(d,p) , -1724.798369 a.u.

6	1.133818000	1.163612000	-0.175344000
6	-1.170711000	-1.222871000	2.126715000
6	-1.528084000	-1.633353000	3.406480000
6	-2.423283000	-2.694601000	3.581578000
6	-2.971264000	-3.339872000	2.471631000
6	-2.636215000	-2.922977000	1.183940000
6	-1.737470000	-1.866857000	1.024615000
6	-3.191848000	-1.096172000	-1.159218000
6	-3.527190000	-2.246705000	-1.886360000
6	-4.780484000	-2.354657000	-2.473181000
6	-5.694753000	-1.300605000	-2.352715000
6	-5.353049000	-0.146789000	-1.659719000
6	-4.097200000	-0.023028000	-1.040697000
6	-3.686273000	1.192621000	-0.312824000
6	-4.608722000	2.175093000	0.077536000
6	-4.196978000	3.329769000	0.729752000
6	-2.843527000	3.518786000	1.022247000
6	-1.909765000	2.553121000	0.669454000
6	4.019501000	-1.949566000	-0.313666000
6	4.851062000	-3.085613000	-0.284083000
6	4.325004000	-4.366802000	-0.245155000
6	2.937998000	-4.552716000	-0.215253000
6	2.095209000	-3.453328000	-0.239833000
6	4.177325000	1.840885000	-0.325997000
6	5.540840000	2.059941000	-0.413565000
6	6.422889000	0.972658000	-0.465796000
6	5.931902000	-0.322269000	-0.435748000
6	4.551225000	-0.576258000	-0.341848000
6	-2.322288000	1.401117000	-0.005571000
6	3.664039000	0.528733000	-0.279596000
6	2.627605000	-2.159986000	-0.305385000
6	-0.732757000	-1.843206000	-0.552983000
6	-1.880372000	-0.937549000	-0.532989000
7	-1.405261000	0.372820000	-0.340669000
6	0.399931000	-1.005679000	-0.425740000
6	-0.009717000	0.340317000	-0.307533000
6	2.234659000	0.281663000	-0.228402000
7	1.776916000	-1.037326000	-0.328100000
6	1.157504000	2.636193000	-0.048065000
6	0.709111000	3.436221000	-1.104202000
6	0.627371000	4.820736000	-0.946237000
6	0.993284000	5.409730000	0.264741000
6	1.450475000	4.613878000	1.319637000
6	1.530703000	3.230678000	1.165945000
1	-2.798230000	-3.038030000	-2.021746000
1	-5.039716000	-3.237491000	-3.043601000
1	-6.666985000	-1.375751000	-2.823747000
1	-6.057285000	0.673284000	-1.618762000
1	-5.662378000	2.022814000	-0.115498000
1	-4.926554000	4.073617000	1.022739000
1	-2.512577000	4.409262000	1.541336000
1	-0.870586000	2.695848000	0.918704000
1	5.924823000	-2.962906000	-0.282699000
1	4.987571000	-5.222182000	-0.224103000
1	2.521841000	-5.550301000	-0.158712000
1	1.027229000	-3.597374000	-0.171106000
1	3.499100000	2.680335000	-0.304388000
1	5.921828000	3.072263000	-0.450969000
1	7.489724000	1.141606000	-0.539636000
1	6.630486000	-1.144846000	-0.496883000

1	-0.781947000	-2.850696000	-0.931424000
1	0.418774000	2.969414000	-2.038388000
1	0.278182000	5.436866000	-1.765462000
1	0.928913000	6.484192000	0.386449000
1	1.739198000	5.071038000	2.258330000
1	1.876732000	2.602918000	1.980072000
1	-3.103396000	-3.390901000	0.325508000
1	-3.669681000	-4.156054000	2.603863000
1	-2.689354000	-3.016675000	4.580342000
1	-1.098249000	-1.136030000	4.266432000
1	-0.446079000	-0.428431000	1.985342000

10c: M062X/6-31G(d,p) , -1724.845259 a.u.

6	-0.527798000	1.444041000	-0.562168000
6	0.212434000	-3.866634000	1.581291000
6	0.115608000	-4.401615000	2.808120000
6	-0.100874000	-3.610286000	3.869173000
6	-0.215454000	-2.285405000	3.694283000
6	-0.117572000	-1.758261000	2.463929000
6	0.089815000	-2.540585000	1.388672000
6	2.855797000	-1.957685000	-0.652689000
6	2.907138000	-3.218505000	-1.108170000
6	4.078796000	-3.735511000	-1.498751000
6	5.175258000	-2.970364000	-1.424007000
6	5.097387000	-1.710713000	-0.963783000
6	3.934188000	-1.152759000	-0.562021000
6	3.790676000	0.106590000	-0.062786000
6	4.877962000	0.845644000	0.255050000
6	4.806074000	2.068663000	0.799565000
6	3.608623000	2.593341000	1.073251000
6	2.516045000	1.891510000	0.750035000
6	-4.053237000	-0.441780000	-0.458268000
6	-5.159551000	-1.210165000	-0.342293000
6	-5.114026000	-2.524139000	-0.087981000
6	-3.921801000	-3.107229000	0.049373000
6	-2.820877000	-2.352800000	-0.058429000
6	-3.035987000	2.825409000	-1.369234000
6	-4.192580000	3.458921000	-1.601145000
6	-5.335594000	2.807423000	-1.375957000
6	-5.279489000	1.527960000	-0.983018000
6	-4.115765000	0.875748000	-0.764218000
6	2.575443000	0.690697000	0.141062000
6	-2.958936000	1.567864000	-0.887277000
6	-2.839220000	-1.024808000	-0.298495000
6	0.209598000	-1.960325000	-0.004314000
6	1.553117000	-1.348337000	-0.109692000
7	1.489604000	0.092147000	-0.164958000
6	-0.552570000	-0.683503000	-0.256331000
6	0.260489000	0.378562000	-0.351387000
6	-1.790940000	0.946300000	-0.606266000
7	-1.771705000	-0.317770000	-0.373727000
6	-0.067508000	2.705591000	-0.671117000
6	-0.642001000	3.727551000	-0.005482000
6	-0.159485000	4.977357000	-0.090170000
6	0.920371000	5.231754000	-0.843006000
6	1.516341000	4.226293000	-1.499731000
6	1.029960000	2.978744000	-1.404868000
1	0.392632000	-4.532289000	0.721200000
1	0.215110000	-5.491473000	2.944838000
1	-0.179957000	-4.045651000	4.879191000
1	-0.387865000	-1.628920000	4.563690000
1	-0.209542000	-0.665890000	2.350235000
1	2.000606000	-3.840033000	-1.167758000
1	4.139163000	-4.769393000	-1.876792000
1	6.145942000	-3.383542000	-1.748279000
1	6.055247000	-1.170007000	-0.958469000
1	5.908689000	0.483271000	0.128903000

1	5.721898000	2.623844000	1.064808000
1	3.525820000	3.574317000	1.570007000
1	1.555920000	2.337745000	1.047251000
1	-6.184371000	-0.829863000	-0.455231000
1	-6.037174000	-3.122144000	-0.003755000
1	-3.853320000	-4.189939000	0.249705000
1	-1.898428000	-2.923602000	0.069645000
1	-2.151426000	3.401672000	-1.664288000
1	-4.208498000	4.488565000	-1.996521000
1	-6.302528000	3.302933000	-1.567060000
1	-6.270354000	1.062976000	-0.884500000
1	0.045184000	-2.681131000	-0.834716000
1	-1.500816000	3.550370000	0.665343000
1	-0.640386000	5.794295000	0.473616000
1	1.322111000	6.256239000	-0.911658000
1	2.407982000	4.425774000	-2.117568000
1	1.540609000	2.182948000	-1.973904000

10d: UM062X/6-31G(d,p) , -1725.008675 a.u.

6	-0.663400000	1.343062000	0.288410000
6	2.591320000	-2.312691000	0.326076000
6	2.550611000	-3.654920000	0.414492000
6	3.671902000	-4.377075000	0.520965000
6	4.843276000	-3.731910000	0.521221000
6	4.871922000	-2.393096000	0.427702000
6	3.755092000	-1.636817000	0.330138000
6	0.100502000	-2.795567000	-1.748412000
6	-0.187175000	-3.027491000	-3.038729000
6	0.401628000	-2.302541000	-4.000307000
6	1.282060000	-1.351849000	-3.657199000
6	1.561680000	-1.129869000	-2.363612000
6	3.726051000	-0.279951000	0.302185000
6	4.887134000	0.415277000	0.287258000
6	4.960040000	1.745393000	0.423924000
6	3.830983000	2.421273000	0.640135000
6	2.676303000	1.745705000	0.623600000
6	-4.094039000	-0.490477000	1.283022000
6	-5.135772000	-1.253181000	1.682637000
6	-5.009262000	-2.548294000	2.002078000
6	-3.806071000	-3.121577000	1.919855000
6	-2.762206000	-2.378243000	1.530862000
6	-3.317231000	2.718300000	-0.017319000
6	-4.503526000	3.339211000	-0.028722000
6	-5.565011000	2.703145000	0.471672000
6	-5.412617000	1.448440000	0.915364000
6	-4.222597000	0.807335000	0.915072000
6	0.971475000	-1.835366000	-1.379024000
6	2.562507000	0.426667000	0.364208000
6	-3.125210000	1.488382000	0.501948000
6	-2.872302000	-1.070453000	1.215416000
6	0.151216000	-2.011570000	0.941915000
6	1.310401000	-1.569685000	0.099069000
7	1.387364000	-0.080862000	0.334437000
6	-0.655189000	-0.717567000	0.723672000
6	0.158848000	0.280516000	0.369741000
6	-1.917037000	0.880639000	0.554036000
7	-1.867304000	-0.363317000	0.861783000
6	-0.268800000	2.589468000	-0.032400000
6	-0.653116000	3.663705000	0.684780000
6	-0.235300000	4.898607000	0.364539000
6	0.580965000	5.081970000	-0.683527000
6	0.981976000	4.023117000	-1.401992000
6	0.565197000	2.790284000	-1.072743000
1	1.587901000	-4.190547000	0.382493000
1	3.632953000	-5.476470000	0.592077000
1	5.780685000	-4.307971000	0.606942000
1	5.888636000	-1.977004000	0.465565000

1	-0.402693000	-3.423098000	-0.995259000
1	-0.906637000	-3.818033000	-3.311207000
1	0.169817000	-2.490816000	-5.061689000
1	1.778799000	-0.754931000	-4.440600000
1	2.297064000	-0.344991000	-2.128411000
1	5.876710000	-0.052959000	0.189692000
1	5.930957000	2.268843000	0.430235000
1	3.856921000	3.504727000	0.844651000
1	1.806358000	2.354826000	0.885969000
1	-6.166609000	-0.881791000	1.768930000
1	-5.882811000	-3.142026000	2.320777000
1	-3.680989000	-4.188079000	2.172395000
1	-1.812501000	-2.926197000	1.496055000
1	-2.523371000	3.278727000	-0.523374000
1	-4.614644000	4.345952000	-0.465674000
1	-6.555363000	3.189096000	0.466496000
1	-6.352851000	0.990655000	1.253467000
1	0.539946000	-1.845145000	1.986975000
1	-1.291804000	3.543861000	1.577356000
1	-0.552998000	5.763098000	0.971321000
1	0.927510000	6.094994000	-0.947056000
1	1.656120000	4.166015000	-2.263115000
1	0.905609000	1.943133000	-1.693234000

10e: UM062X/6-31G(d,p) , -1724.965832 a.u.

6	1.104603000	1.194350000	-0.108985000
6	-1.276557000	-1.369850000	2.160620000
6	-1.565737000	-1.982716000	3.356022000
6	-2.331349000	-3.166805000	3.412733000
6	-2.830562000	-3.715285000	2.214186000
6	-2.566763000	-3.130331000	0.997741000
6	-1.735506000	-1.942751000	0.907750000
6	-3.124016000	-1.088102000	-1.202746000
6	-3.387750000	-2.151004000	-2.066693000
6	-4.562320000	-2.174618000	-2.816751000
6	-5.463195000	-1.113044000	-2.720688000
6	-5.188813000	-0.035072000	-1.882869000
6	-4.025752000	-0.007762000	-1.099745000
6	-3.690891000	1.140415000	-0.224098000
6	-4.651381000	2.073450000	0.182456000
6	-4.299225000	3.195288000	0.927050000
6	-2.963990000	3.389844000	1.288437000
6	-1.993534000	2.462158000	0.929392000
6	4.064992000	-1.829923000	-0.327713000
6	4.922799000	-2.945357000	-0.290080000
6	4.430848000	-4.236289000	-0.176201000
6	3.051080000	-4.449838000	-0.074456000
6	2.181357000	-3.371994000	-0.104612000
6	4.135939000	1.958072000	-0.434652000
6	5.486493000	2.205660000	-0.607251000
6	6.391582000	1.139107000	-0.692804000
6	5.929378000	-0.163689000	-0.606279000
6	4.562696000	-0.446148000	-0.422821000
6	-2.343406000	1.335338000	0.172208000
6	3.650644000	0.637284000	-0.331036000
6	2.677474000	-2.068508000	-0.249721000
6	-0.693605000	-1.916710000	-0.407992000
6	-1.907362000	-1.016269000	-0.360603000
7	-1.421207000	0.349617000	-0.182263000
6	0.421525000	-0.984200000	-0.296669000
6	-0.020616000	0.326139000	-0.179147000
6	2.234018000	0.362412000	-0.198590000
7	1.799003000	-0.975402000	-0.274064000
6	1.057061000	2.663837000	0.022630000
6	0.396205000	3.435078000	-0.940367000
6	0.247216000	4.810625000	-0.759948000
6	0.759580000	5.427083000	0.381994000

6	1.426021000	4.663798000	1.344903000
6	1.570378000	3.288681000	1.168954000
1	-2.664180000	-2.952438000	-2.168246000
1	-4.763756000	-3.003586000	-3.483657000
1	-6.368794000	-1.114695000	-3.315208000
1	-5.871748000	0.804591000	-1.857578000
1	-5.690669000	1.909528000	-0.075244000
1	-5.058300000	3.903677000	1.233175000
1	-2.675950000	4.255391000	1.873167000
1	-0.968755000	2.601817000	1.240417000
1	5.992804000	-2.796638000	-0.335709000
1	5.114791000	-5.074686000	-0.147548000
1	2.659254000	-5.452056000	0.045306000
1	1.119469000	-3.526426000	0.025574000
1	3.437657000	2.780964000	-0.388384000
1	5.839718000	3.226169000	-0.687605000
1	7.447685000	1.329743000	-0.836935000
1	6.638838000	-0.975206000	-0.695643000
1	-0.678191000	-2.823006000	-0.997787000
1	-0.015206000	2.945279000	-1.815257000
1	-0.275596000	5.396823000	-1.505699000
1	0.638830000	6.494358000	0.524367000
1	1.821897000	5.138185000	2.234752000
1	2.071688000	2.684075000	1.916959000
1	-2.993033000	-3.538865000	0.088517000
1	-3.448627000	-4.605805000	2.249404000
1	-2.546098000	-3.636558000	4.363577000
1	-1.200398000	-1.541708000	4.276929000
1	-0.685237000	-0.462548000	2.131287000

10f: UM062X/6-31G(d,p) , -1725.013695 a.u.

6	-1.043779000	1.348970000	-0.027638000
6	1.468225000	-4.040604000	0.381464000
6	1.715762000	-4.952569000	1.405601000
6	1.654987000	-4.539792000	2.731951000
6	1.344730000	-3.213139000	3.029397000
6	1.097971000	-2.305795000	2.006220000
6	1.158091000	-2.712978000	0.672300000
6	3.342353000	-0.804375000	-0.899974000
6	3.836691000	-2.034625000	-1.408293000
6	5.121872000	-2.125391000	-1.899363000
6	5.962040000	-1.004620000	-1.902905000
6	5.505582000	0.197827000	-1.375424000
6	4.219398000	0.323327000	-0.848868000
6	3.738942000	1.542777000	-0.181226000
6	4.591069000	2.605297000	0.147015000
6	4.142171000	3.721314000	0.837305000
6	2.817069000	3.777841000	1.263711000
6	1.948202000	2.737616000	0.973018000
6	-3.870643000	-1.767406000	-0.415103000
6	-4.676977000	-2.916171000	-0.483019000
6	-4.137228000	-4.186992000	-0.553819000
6	-2.751190000	-4.346492000	-0.560157000
6	-1.927554000	-3.238696000	-0.485266000
6	-4.100505000	1.996812000	-0.351421000
6	-5.463502000	2.195888000	-0.456875000
6	-6.329000000	1.100913000	-0.514671000
6	-5.810101000	-0.179077000	-0.488690000
6	-4.428274000	-0.410111000	-0.384559000
6	2.384223000	1.644794000	0.216775000
6	-3.557583000	0.698851000	-0.289828000
6	-2.475995000	-1.953831000	-0.404688000
6	0.912067000	-1.699225000	-0.447408000
6	2.011893000	-0.651383000	-0.492787000
7	1.518890000	0.604602000	-0.121704000
6	-0.268757000	-0.784873000	-0.250314000
6	0.112016000	0.521867000	-0.074529000

6	-2.124662000	0.472971000	-0.175225000
7	-1.639483000	-0.831023000	-0.299869000
6	-1.085569000	2.821869000	0.113358000
6	-1.596723000	3.414999000	1.274164000
6	-1.560449000	4.795774000	1.436573000
6	-1.009269000	5.601807000	0.441468000
6	-0.503606000	5.020594000	-0.717817000
6	-0.543062000	3.638657000	-0.881794000
1	1.504941000	-4.367157000	-0.656560000
1	1.954462000	-5.983719000	1.164789000
1	1.846172000	-5.247435000	3.532073000
1	1.294178000	-2.886308000	4.063187000
1	0.853253000	-1.270961000	2.233933000
1	3.188023000	-2.903395000	-1.418239000
1	5.479903000	-3.071490000	-2.293595000
1	6.965844000	-1.074070000	-2.306970000
1	6.169949000	1.055246000	-1.380749000
1	5.638400000	2.545206000	-0.126213000
1	4.829699000	4.527901000	1.068102000
1	2.456969000	4.623646000	1.840386000
1	0.934372000	2.760885000	1.346557000
1	-5.754886000	-2.812591000	-0.476983000
1	-4.790807000	-5.051096000	-0.601812000
1	-2.309106000	-5.335734000	-0.613628000
1	-0.857685000	-3.376459000	-0.463453000
1	-3.444080000	2.855252000	-0.332461000
1	-5.855074000	3.206733000	-0.504097000
1	-7.400475000	1.249961000	-0.597049000
1	-6.494153000	-1.015402000	-0.564952000
1	0.861707000	-2.242634000	-1.404063000
1	-2.017358000	2.778915000	2.048080000
1	-1.956130000	5.242662000	2.343166000
1	-0.974081000	6.678736000	0.571158000
1	-0.070826000	5.643100000	-1.494352000
1	-0.134627000	3.179425000	-1.777174000

5b: M062X/6-31G(d,p) , -1724.465963 a.u.

6	-2.211561315	1.176404286	0.018055278
6	2.522238685	-1.112895714	1.355455278
6	3.891038685	-1.333895714	1.483355278
6	4.614638685	-1.871995714	0.420555278
6	3.969038685	-2.195095714	-0.772444722
6	2.600538685	-1.978695714	-0.906544722
6	1.874638685	-1.432295714	0.158055278
6	-0.584961315	-3.541295714	0.329755278
6	0.604538685	-4.228595714	0.614755278
6	0.588138685	-5.577395714	0.932855278
6	-0.626561315	-6.265795714	0.985555278
6	-1.810161315	-5.601095714	0.703755278
6	-1.810161315	-4.240395714	0.358555278
6	-3.042861315	-3.551795714	0.006055278
6	-4.264561315	-4.229795714	-0.124244722
6	-5.412261315	-3.576395714	-0.545444722
6	-5.358061315	-2.221395714	-0.886844722
6	-4.170261315	-1.522595714	-0.762744722
6	1.284438685	3.552604286	0.002055278
6	2.505638685	4.231504286	-0.131244722
6	3.653538685	3.577704286	-0.550644722
6	3.600638685	2.221304286	-0.886644722
6	2.413538685	1.522104286	-0.760044722
6	-2.362661315	4.228004286	0.613855278
6	-2.346761315	5.576904286	0.931455278
6	-1.132361315	6.266404286	0.981655278
6	0.051138685	5.602204286	0.698055278
6	0.051638685	4.241204286	0.354255278
6	-3.023961315	-2.164895714	-0.265644722
6	-1.173161315	3.541504286	0.327155278

6	1.266438685	2.165004286	-0.265644722
6	0.454138685	-1.176395714	0.021355278
6	-0.583361315	-2.121195714	0.067055278
7	-1.831261315	-1.461295714	-0.075644722
6	-0.163261315	0.096904286	-0.108944722
6	-1.593961315	-0.097095714	-0.110044722
6	-1.174261315	2.121204286	0.065155278
7	0.073938685	1.461304286	-0.075044722
6	-3.632561315	1.432304286	0.149855278
6	-4.353361315	1.982204286	-0.916344722
6	-5.722561315	2.198404286	-0.787844722
6	-6.373961315	1.871204286	0.400755278
6	-5.655261315	1.329204286	1.465155278
6	-4.285861315	1.108804286	1.343055278
1	1.951138685	-0.689295714	2.181155278
1	4.395538685	-1.082495714	2.413755278
1	5.683638685	-2.038995714	0.521855278
1	4.535538685	-2.614995714	-1.600344722
1	2.089838685	-2.228395714	-1.835544722
1	1.558938685	-3.700995714	0.598855278
1	1.518638685	-6.098095714	1.147855278
1	-0.640861315	-7.321195714	1.248555278
1	-2.749961315	-6.148895714	0.755055278
1	-4.315561315	-5.295695714	0.100855278
1	-6.351761315	-4.117695714	-0.627544722
1	-6.249561315	-1.716795714	-1.256844722
1	-4.119861315	-0.478995714	-1.072044722
1	2.555538685	5.298104286	0.090455278
1	4.592438685	4.119804286	-0.635444722
1	4.492538685	1.715904286	-1.254844722
1	2.364238685	0.477304286	-1.065444722
1	-3.316661315	3.699604286	0.599955278
1	-3.277361315	6.096804286	1.148155278
1	-1.118361315	7.321904286	1.244155278
1	0.990638685	6.150804286	0.747455278
1	-3.838461315	2.234704286	-1.842244722
1	-6.285161315	2.621104286	-1.616944722
1	-7.443361315	2.037704286	0.497555278
1	-6.164261315	1.074504286	2.392055278
1	-3.718761315	0.682204286	2.169955278

11: UM062X/6-31G(d,p) , -1726.504964 a.u.

7	-1.510860000	-0.772371000	-0.364625000
6	-1.974254000	0.514615000	-0.548700000
6	-0.922972000	1.449032000	-0.315582000
6	0.177183000	0.688647000	0.015872000
6	-0.177571000	-0.688016000	-0.018879000
7	1.510444000	0.772963000	0.361747000
6	1.973666000	-0.514008000	0.546247000
6	0.922549000	-1.448437000	0.312676000
6	-2.267739000	-1.986970000	-0.248621000
6	-3.332858000	0.841315000	-0.932190000
6	2.267380000	1.987603000	0.246599000
6	3.331842000	-0.840670000	0.931381000
6	-3.895836000	2.035213000	-0.455019000
6	-5.202854000	2.368282000	-0.773508000
6	-5.980141000	1.534838000	-1.584149000
6	-5.407197000	0.350151000	-2.067636000
6	-4.106697000	-0.001393000	-1.749009000
6	-3.326369000	-2.087433000	0.667384000
6	-4.027160000	-3.297082000	0.703050000
6	-3.671320000	-4.368708000	-0.109028000
6	-2.600968000	-4.252327000	-0.991385000
6	-1.902327000	-3.052407000	-1.066799000
6	1.879715081	2.991417796	-0.654475246
6	2.682869845	4.134265864	-0.721298026
6	3.799665810	4.287805303	0.093359877

6	4.148694105	3.288332147	0.997217309
6	3.383190864	2.129559238	1.066916807
6	4.193428089	-1.378954621	-0.038170120
6	5.507627772	-1.675928865	0.282691506
6	5.998783951	-1.462048494	1.575651228
6	5.130200775	-0.936239828	2.540947700
6	3.816591072	-0.623482040	2.232038924
6	0.693946694	2.854851351	-1.538450820
6	-3.730590000	-0.959714000	1.545425000
6	-0.023216934	1.656201569	-1.612543302
6	-1.107127609	1.538360712	-2.476326615
6	-1.486718022	2.615779291	-3.274567137
6	-0.784174825	3.815628605	-3.197359550
6	0.299207197	3.935282162	-2.333009437
6	-2.794615000	-0.277801000	2.329974000
6	-3.188665000	0.800726000	3.115055000
6	-4.520964000	1.209357000	3.125589000
6	-5.460052000	0.527632000	2.355815000
6	-5.067579000	-0.551985000	1.571269000
1	-1.249674962	2.219294450	0.363282991
1	1.007527000	-2.517435000	0.436961000
1	-3.321729000	2.671792000	0.211190000
1	-5.633475000	3.284113000	-0.379973000
1	-5.995553000	-0.300756000	-2.707957000
1	-3.682181000	-0.917794000	-2.145309000
1	-4.847659000	-3.396391000	1.406963000
1	-4.226535000	-5.298417000	-0.047291000
1	-2.317954000	-5.084728000	-1.625974000
1	-1.086424000	-2.922249000	-1.771642000
1	2.398523395	4.924020014	-1.409780798
1	4.393987915	5.192682212	0.026968668
1	5.017407060	3.402889433	1.635891470
1	3.653361768	1.318839461	1.737133691
1	3.841293013	-1.510157492	-1.056733458
1	6.170035631	-2.070894347	-0.481901440
1	5.494501248	-0.775354660	3.551343547
1	3.160585960	-0.228129333	3.000436122
1	0.566165209	0.858138549	-1.970641402
1	-1.664374318	0.607964853	-2.517915123
1	-2.332227673	2.521744604	-3.947978261
1	-1.074623114	4.658290379	-3.816416826
1	0.869199155	4.859558339	-2.295643189
1	-1.757002000	-0.604213000	2.334828000
1	-2.457072000	1.315906000	3.729262000
1	-4.826271000	2.051170000	3.738244000
1	-6.499004000	0.841021000	2.359446000
1	-5.792295000	-1.064266000	0.944426000
1	-6.997943527	1.797700746	-1.831901279
1	7.023410070	-1.696850726	1.823460081

12: UM062X/6-31G(d,p) , -1725.603379 a.u.

7	-1.477300000	-0.930700000	-0.391300000
6	-1.883400000	0.308100000	-0.920800000
6	-0.771500000	1.169600000	-1.019600000
6	0.306300000	0.454700000	-0.451100000
6	-0.125200000	-0.858100000	-0.097700000
7	1.662300000	0.601100000	-0.180600000
6	2.082300000	-0.660600000	0.341800000
6	1.016400000	-1.560900000	0.374600000
6	-2.302300000	-2.025800000	-0.026000000
6	-3.266700000	0.580700000	-1.267600000
6	2.100500000	1.892400000	0.210800000
6	3.469900000	-0.969600000	0.639000000
6	-3.836000000	1.793800000	-0.861100000
6	-5.167700000	2.067700000	-1.155100000
6	-5.935800000	1.134100000	-1.850200000
6	-5.366300000	-0.067500000	-2.267300000

6	-4.031600000	-0.344300000	-1.983300000
6	-3.281500000	-1.910300000	0.974700000
6	-4.056400000	-3.032700000	1.283900000
6	-3.857100000	-4.239300000	0.621000000
6	-2.873200000	-4.345400000	-0.361700000
6	-2.092300000	-3.243000000	-0.687700000
6	1.538800000	3.048900000	-0.376100000
6	1.884400000	4.289000000	0.183300000
6	2.810500000	4.405900000	1.213200000
6	3.407300000	3.260900000	1.731300000
6	3.036600000	2.012600000	1.249200000
6	4.495700000	-0.535600000	-0.208100000
6	5.818200000	-0.860800000	0.079800000
6	6.122300000	-1.623000000	1.207000000
6	5.100800000	-2.062400000	2.047700000
6	3.776700000	-1.737600000	1.767600000
6	0.645500000	3.131900000	-1.550000000
6	-3.517400000	-0.657300000	1.700200000
6	-0.529900000	2.383400000	-1.757700000
6	-1.385500000	2.723300000	-2.814900000
6	-1.061400000	3.743000000	-3.701000000
6	0.149500000	4.416800000	-3.561500000
6	0.989900000	4.107700000	-2.498000000
6	-2.468700000	-0.006100000	2.354800000
6	-2.703300000	1.197900000	3.013600000
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6	-5.034500000	1.089900000	2.393900000
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1	1.058900000	-2.586800000	0.669100000
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1	-5.610300000	3.008800000	-0.836700000
1	-5.963700000	-0.791800000	-2.815500000
1	-3.583900000	-1.279800000	-2.316000000
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1	4.254100000	0.056500000	-1.091500000
1	6.616100000	-0.519400000	-0.576700000
1	5.338700000	-2.660000000	2.924800000
1	2.977600000	-2.075900000	2.425700000
1	-2.307400000	2.159900000	-2.960800000
1	-1.739000000	3.996800000	-4.512400000
1	0.436900000	5.181500000	-4.277500000
1	1.939100000	4.635500000	-2.403800000
1	-1.465000000	-0.432900000	2.336400000
1	-1.880800000	1.713000000	3.506700000
1	-4.164200000	2.691200000	3.541600000
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1	-5.619400000	-0.614700000	1.213100000
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1	7.155900000	-1.876100000	1.430200000

15: M062X/6-31G(d,p) , -1724.420213 a.u.

7	0.000000000	0.000000000	0.000000000
6	1.424800000	0.000000000	0.000000000
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7	0.379300000	3.484200000	-0.140400000
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6	-1.525800000	2.173800000	0.064300000
6	-0.902300000	-0.941500000	-0.555000000

6	2.194300000	-1.227800000	0.097700000
6	1.248000000	4.380700000	-0.811400000
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6	3.231000000	-1.465600000	-0.811600000
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6	2.672500000	-3.322600000	1.197200000
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6	-2.634000000	-2.642600000	-1.940700000
6	-1.262200000	-2.872200000	-1.978900000
6	-0.401200000	-2.013100000	-1.308300000
6	2.647900000	4.192600000	-0.748900000
6	3.439500000	4.979900000	-1.600100000
6	2.897800000	5.974000000	-2.406800000
6	1.524500000	6.198100000	-2.393000000
6	0.703100000	5.391500000	-1.616500000
6	-1.474100000	5.720600000	0.910200000
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6	-3.309500000	7.064700000	0.101700000
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6	3.411100000	3.289500000	0.139400000
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6	3.179900000	1.913600000	0.343000000
6	4.121800000	1.153700000	1.049400000
6	5.247000000	1.744500000	1.611100000
6	5.425700000	3.121300000	1.504400000
6	4.514100000	3.878600000	0.777000000
6	-2.773100000	1.608300000	0.518000000
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6	-4.770700000	1.873700000	1.877800000
6	-4.953500000	0.493300000	1.878900000
6	-4.080600000	-0.316800000	1.161000000
1	3.446000000	-0.733600000	-1.590900000
1	4.789900000	-2.819600000	-1.417300000
1	4.292000000	-4.472700000	0.364200000
1	2.457600000	-4.047700000	1.979300000
1	1.110400000	-1.963900000	1.813700000
1	-4.210100000	-1.410800000	-1.175200000
1	-3.313500000	-3.281200000	-2.499200000
1	-0.859600000	-3.707300000	-2.549500000
1	0.673500000	-2.170400000	-1.400500000
1	4.517300000	4.804700000	-1.634800000
1	3.544300000	6.570600000	-3.045500000
1	1.089400000	6.986400000	-3.004700000
1	-0.375800000	5.539700000	-1.663800000
1	-0.627700000	5.577600000	1.582900000
1	-1.968000000	7.670300000	1.675600000
1	-3.895200000	7.979900000	0.144400000
1	-4.492000000	6.203200000	-1.480500000
1	-3.155500000	4.107500000	-1.580700000
1	3.956700000	0.084600000	1.186400000
1	5.970100000	1.137100000	2.150200000
1	6.273100000	3.602900000	1.985000000
1	4.661500000	4.956900000	0.706300000
1	-3.504000000	3.494700000	1.270800000
1	-5.464800000	2.520100000	2.409300000
1	-5.774700000	0.049600000	2.435600000
1	-4.230800000	-1.396900000	1.175900000

7. Cyclic voltammetry

The CV characteristics on compounds **4a-g** and **5a-g** are show in Figures S4a-g and summarized in Table S1.

Table S1. Summary of electrochemical properties^a of compounds **4a-g** and **5a-g**.

Compd	$E_{\text{red}}^{1/2}$, [V]	$E_{\text{ox1}}^{1/2}$, [V]	$E_{\text{ox2}}^{1/2}$, [V]	$E_{\text{red}}^{\text{onset}}$, [V]	$E_{\text{ox1}}^{\text{onset}}$, [V]	<i>Ionic potential</i> , [eV]	<i>Electron affinity</i> , [eV]
4a	-	0.54	$E_{\text{pa}} 1.25$ $E_{\text{pc}} 1.14$	-	0.47	-4.8	-
4b	-	0.62	$E_{\text{pa}} 1.31$ $E_{\text{pc}} -$	-	0.55	-4.9	-
4c	-	0.90	$E_{\text{pa}} 1.48$ $E_{\text{pc}} -$	-	0.82	-5.2	-
4d	-1.10	0.97	$E_{\text{pa}} 1.51$ $E_{\text{pc}} -$	-1.00	0.87	-5.2	-3.3
4e	-	0.83	$E_{\text{pa}} 1.45$ $E_{\text{pc}} -$	-	0.76	-5.1	-
4f	-	0.73	$E_{\text{pa}} 1.37$ $E_{\text{pc}} -$	-	0.64	-5.0	-
4g	-	0.60	$E_{\text{pa}} 1.32$ $E_{\text{pc}} -$	-	0.52	-4.9	-
5a	-	0.52	0.90	-	0.45	-4.8	-
5b	-	0.55	0.91	-	0.48	-4.8	-
5c	-	0.70	0.96	-	0.63	-5.0	-
5d	-1.06	0.72	0.97	-0.90	0.64	-5.0	-3.4
5e	-	0.66	0.94	-	0.58	-4.9	-
5f	-	0.62	0.93	-	0.55	-4.9	-
5g	-	0.56	0.91	-	0.49	-4.8	-

a: Measurements conditions: compound ($c = 0.1\text{-}0.2$ M); electrolyte (NBu_4ClO_4 , $c = 0.1$ M); solvent: dry, degassed dichloromethane; potential sweep rate: 100 mV/s; working electrode: GC; auxiliary electrode: Pt wire; reference electrode: Ag/AgCl/NaCl_{sat}; all measurements were carried out at room temperature and under Ar atmosphere; b: calculated according to the equations: $IP(\text{eV}) = -[E_{\text{ox}}^{\text{onset}} - E^{1/2}(\text{Fc/Fc}^+) + 4.8]$; $EA(\text{eV}) = -[E_{\text{red}}^{\text{onset}} - E^{1/2}(\text{Fc/Fc}^+) + 4.8]$.

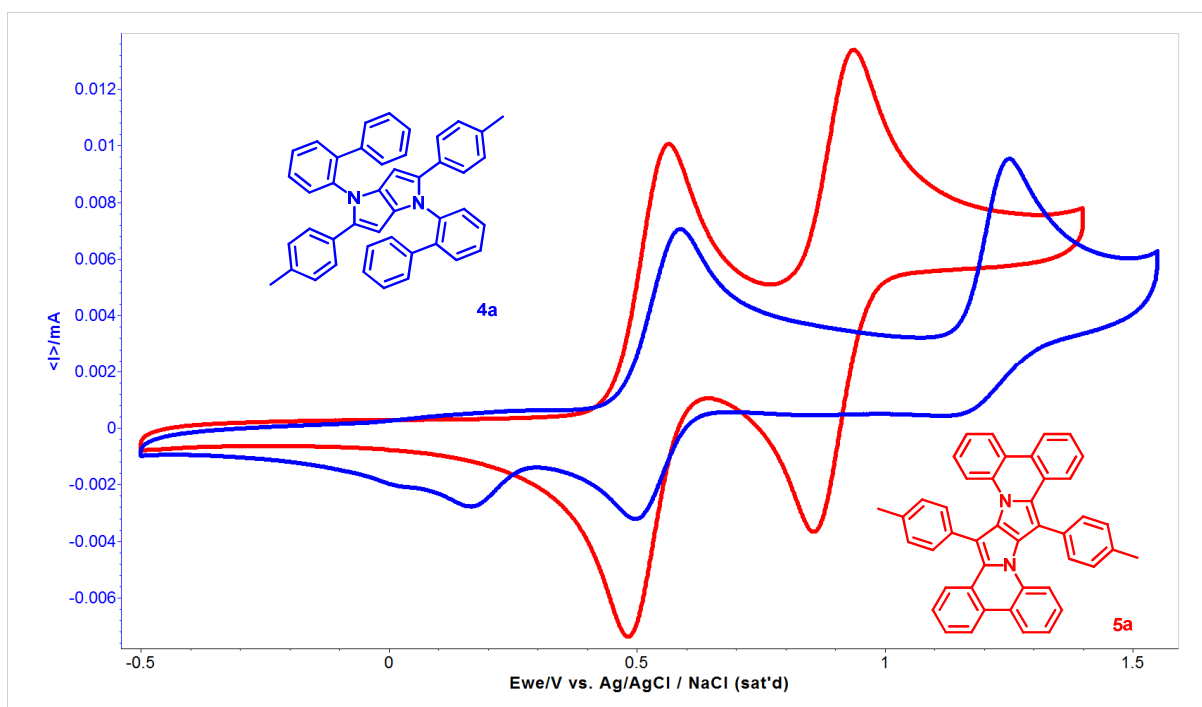


Figure S4a. Cyclic voltammograms of **4a** and **5a**.

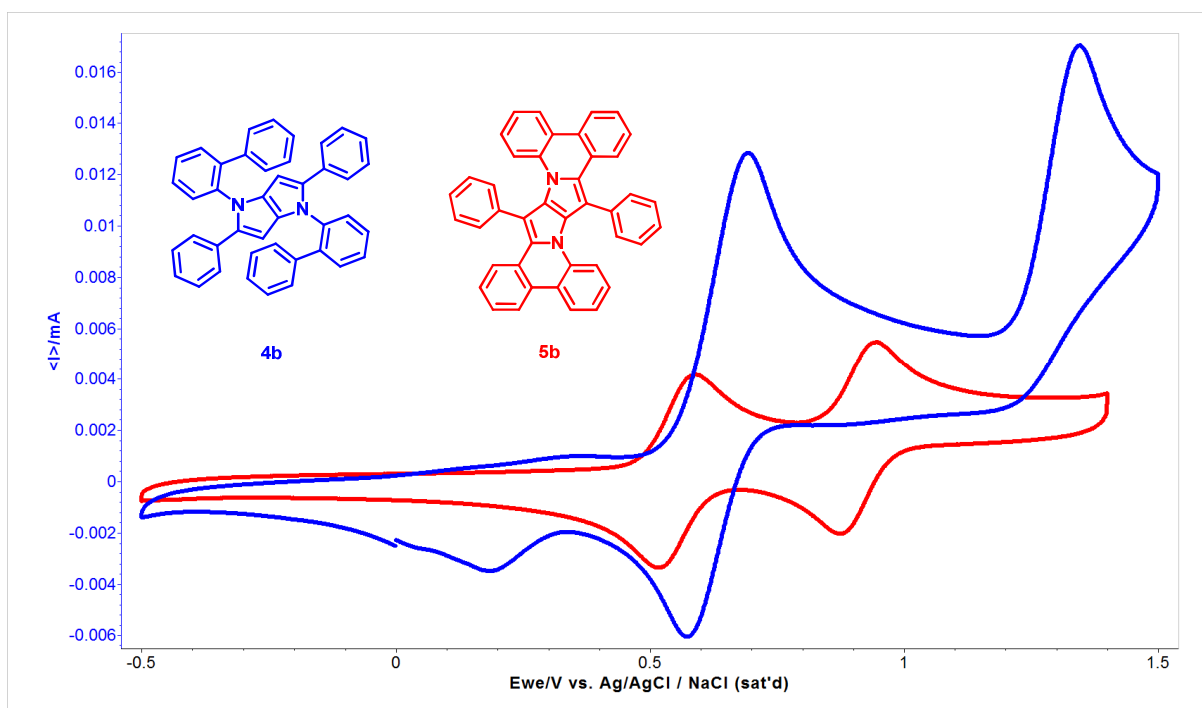


Figure S4b. Cyclic voltammograms of **4b** and **5b**.

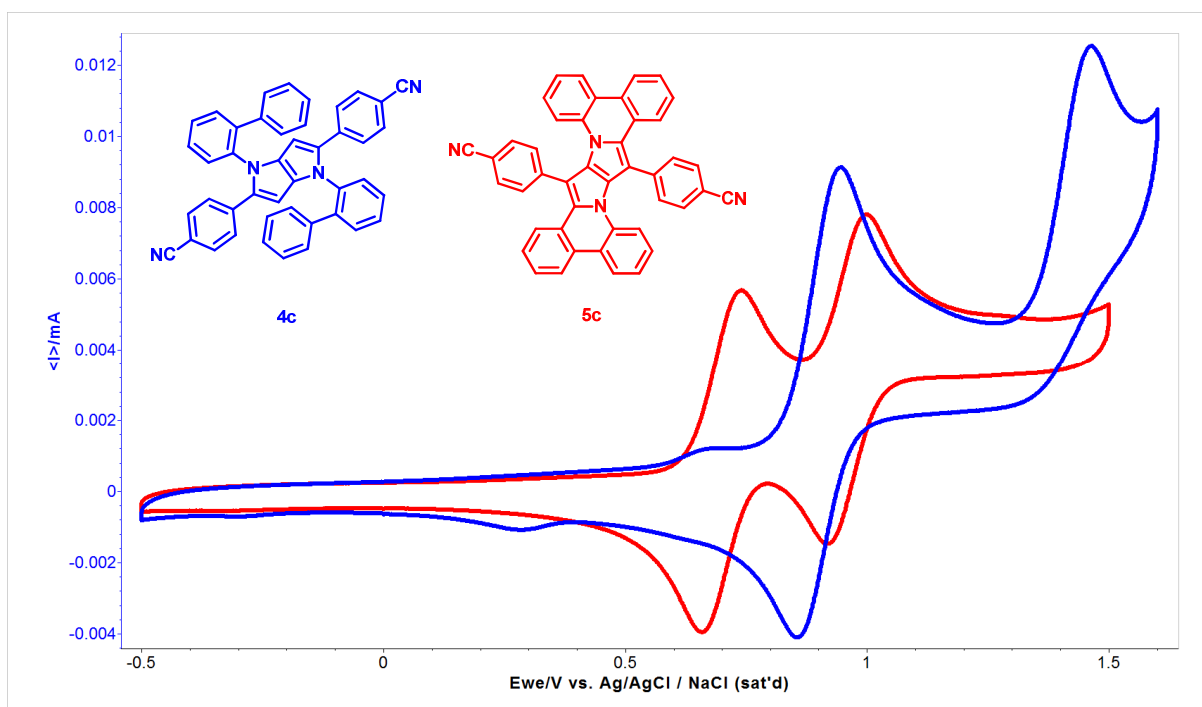


Figure S4c. Cyclic voltammograms of **4c** and **5c**.

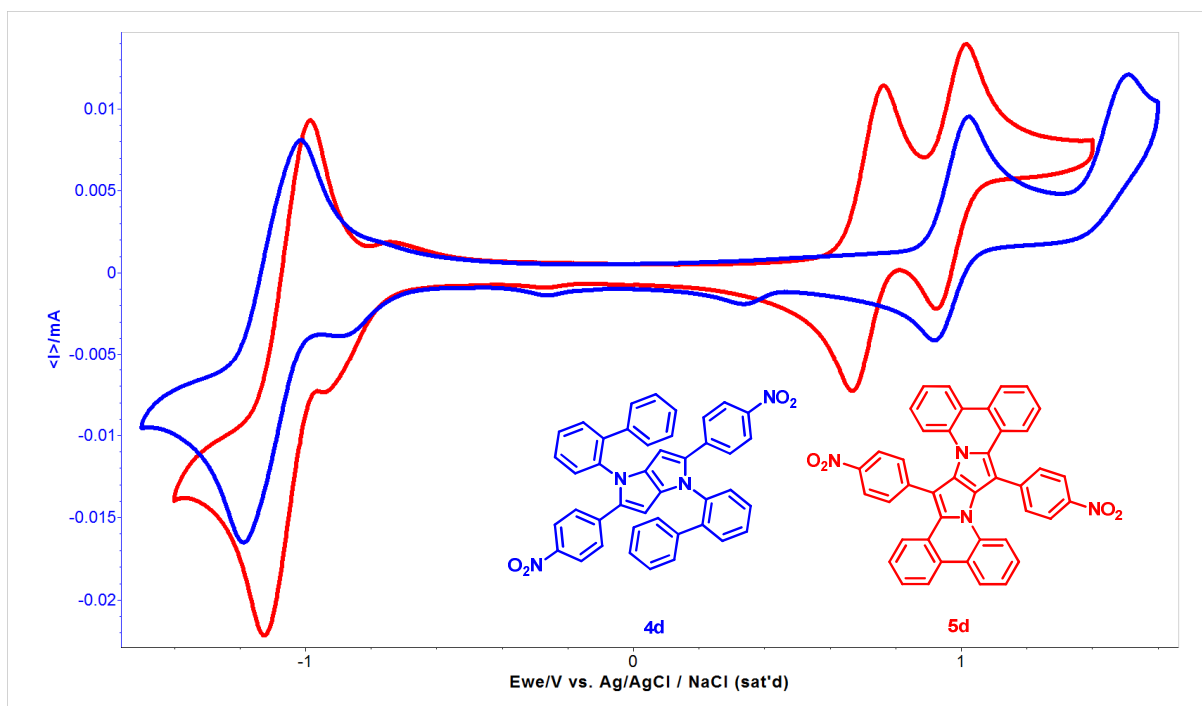


Figure S4d. Cyclic voltammograms of **4d** and **5d**.

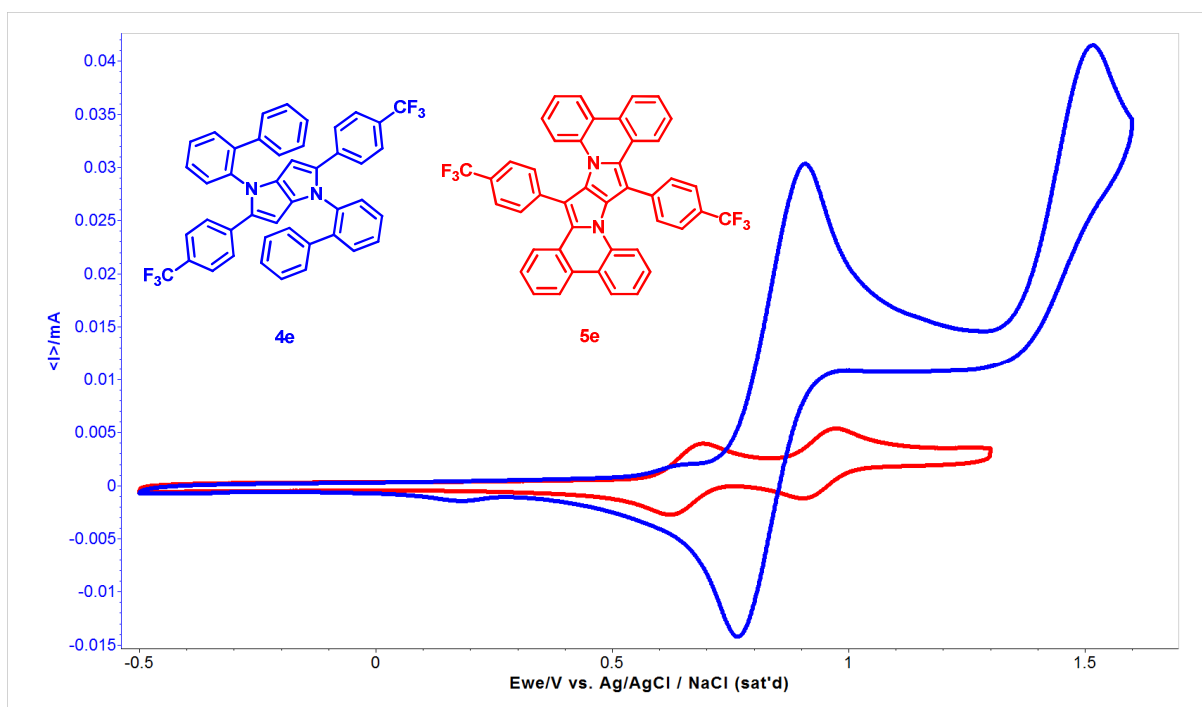


Figure S4e. Cyclic voltammograms of **4e** and **5e**.

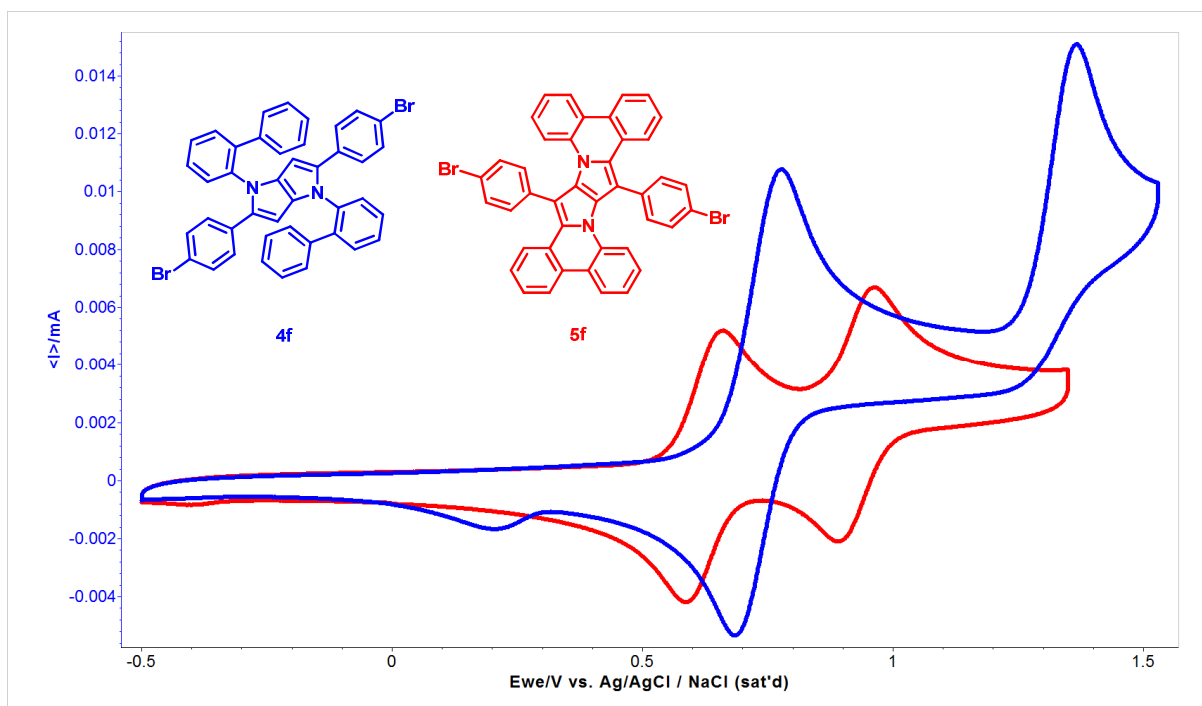


Figure S4f. Cyclic voltammograms of **4f** and **5f**.

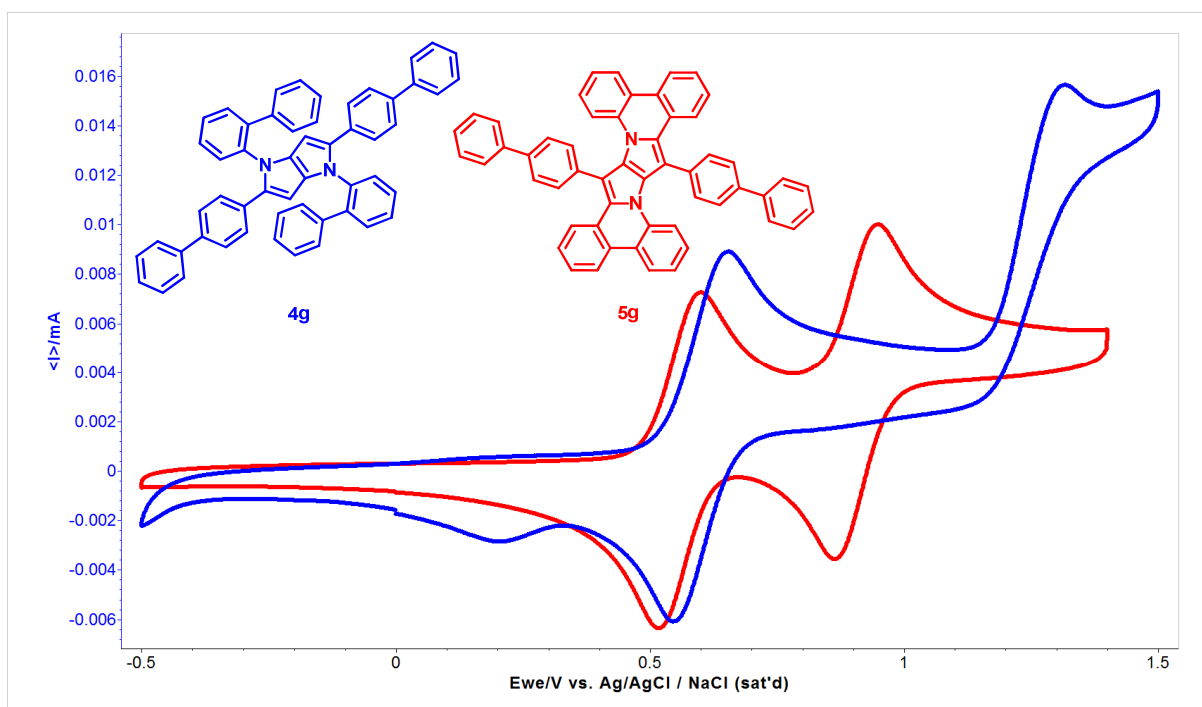


Figure S4g. Cyclic voltammograms of **4g** and **5g**.