Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting Information for

Exceptionally Flexible Quinodimethanes with Multiple Conformations: Polymorph-Dependent Colour Tone and Emission of Crystals

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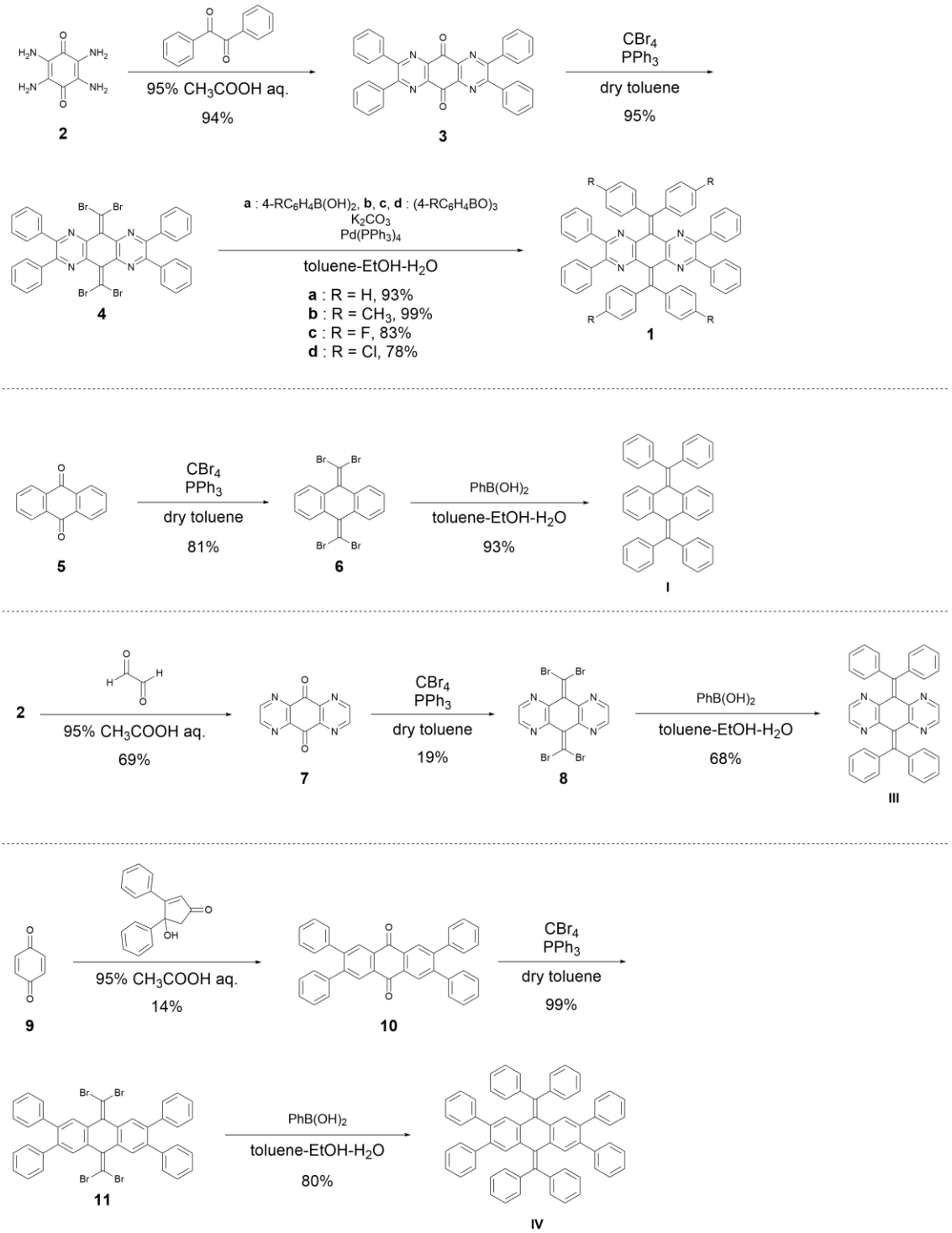
General

All reactions were carried out under an argon atmosphere. All commercially available compounds were used without further purification unless otherwise indicated. Dry toluene was obtained by distillation from CaH_2 prior to use. Column chromatography was performed on silica gel 60N (KANTO KAGAKU, spherical neutral) of particle size 40-50 μm or Wakogel® 60N (neutral) of particle size 38-100 μm. ^{1}H and ^{13}C NMR spectra were recorded on a BRUKER Ascend^{TM} 400 (^{1}H/400 MHz and ^{13}C/100 MHz) spectrometer. IR spectra were measured on a Shimadzu IRAffinity-1S spectrophotometer using the attenuated total reflection (ATR) mode. Mass spectra were recorded on a JMS-T100GCV spectrometer in FD mode by Dr. Eri Fukushi and Mr. Yusuke Takata (GC-MS & NMR Laboratory, Research Faculty of Agriculture, Hokkaido University). Melting points were measured on a Stanford Research Systems OptiMelt MPA100 and are uncorrected. UV-vis-NIR spectra were recorded on a Hitachi U-2910 spectrophotometer. UV/Vis diffuse reflectance measurements were recorded using a JASCO V-770 spectrometer (JASCO) with an integration sphere. A JASCO FP-8500 fluorescence spectrometer was used to collect excitation and emission spectra at room temperature. The absolute photoluminescence quantum yields (Φ_F) were calculated using the C9920-02 absolute photoluminescence quantum yields measurement system (Hamamatsu photonics). Time-resolved photoluminescence lifetimes were measured using a time-correlated single-photon counting lifetime spectroscopy system, Quantaurus-Tau C11367-02 (Hamamatsu photonics). PXRD data were collected at room temperature using a Rigaku SmartLab system (Rigaku) diffractometer with a copper K-alpha source. Redox potentials (E^{ox} and E^{red}) were measured on a BAS ALS-600A by cyclic voltammetry in dry DMF containing 0.1 M Bu_4NBF_4 as a supporting electrolyte. All of the values shown in the text are in E/V vs. SCE measured at the scan rate of 0.1 V s^{-1}. Pt electrodes were used as the working (disk) and counter electrodes. The working electrode was polished using a water suspension of aluminum oxide (0.05 μm) before use. DFT calculations were performed with the Gaussian 16W program package.[1] The geometries of the compounds were optimised by using the B3LYP method in combination with the 6-31G* basis set unless otherwise indicated.

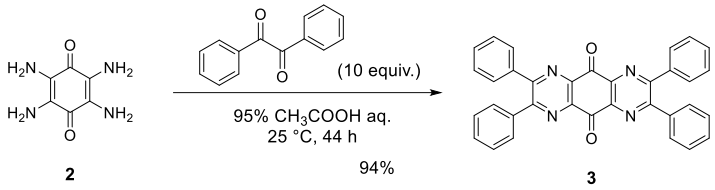
Experimental Section

Synthetic procedures



Scheme S1. Preparation of **1**, **I**, **III**, and **IV**.

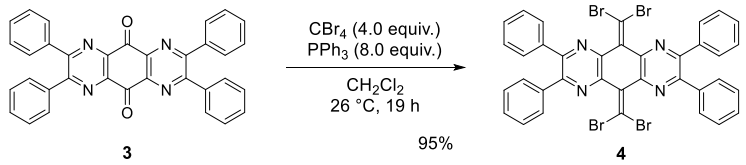
2,3,6,7-Tetraphenyl-1,4,5,8-tetraaza-9,10-anthraquinone (3)



A mixture of 2,3,5,6-tetraamino-1,4-benzoquinone **2**[2] (1.26 g, 7.50 mmol) and benzil (15.8 g, 75.0 mmol) in 95% CH_3COOH aq. (263 mL) was stirred at 25 ℃ for 44 h. Then, the precipitates were collected by filtration, washed with water and EtOH, and dried *in vacuo* to give a **3** (3.63 g) as a yellow powder in 94% yield.

^{1}H NMR data were identical to those in literature.[3]

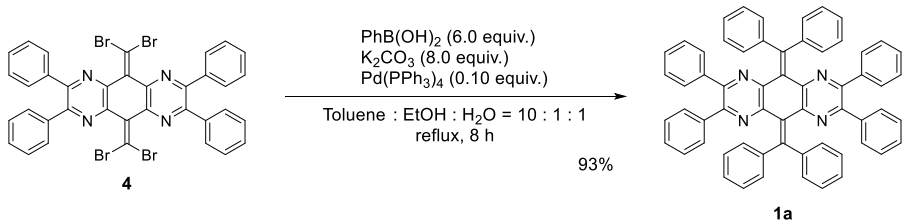
11,11,12,12-Tetrabromo-2,3,6,7-tetraphenyl-1,4,5,8-tetraaza-9,10-anthraquinodimethane (4)



A mixture of CBr_4 (82.65 g, 8.00 mmol) and PPh_3 (4.20 g, 16.0 mmol) in dry CH_2Cl_2 (20 mL) was stirred at 26 ℃ for 1 h, and then 2,3,6,7-tetraphenyl-1,4,5,8-tetraaza-9,10-anthraquinone **3** (1.03 g, 2.00 mmol) was added to the mixture at 0 ℃. After warming to 26 ℃, the mixture was stirred at 26 ℃ for 19 h. After diluting with water, the reaction mixture was extracted with CH_2Cl_2 three times. The combined organic layers were washed with water and brine, and dried over anhydrous $MgSO_4$. After filtration, the solvent was concentrated under reduced pressure. The crude product was washed with CH_2Cl_2 until the filtrate becomes colourless, and the residue was dried *in vacuo* to give **4** (1.48 g) as a white powder in 89 %. The resulting filtrate was concentrated under reduced pressure, and purified by column chromatography on silica gel (CH_2Cl_2) to give **4** (101 mg) as a white powder in 6% yield (total 1.58 g, 95%).

^{1}H NMR data were identical to those in literature.[4]

2,3,6,7,11,11,12,12-Octaphenyl-1,4,5,8-tetraaza-9,10-anthraquinodimethane (1a)

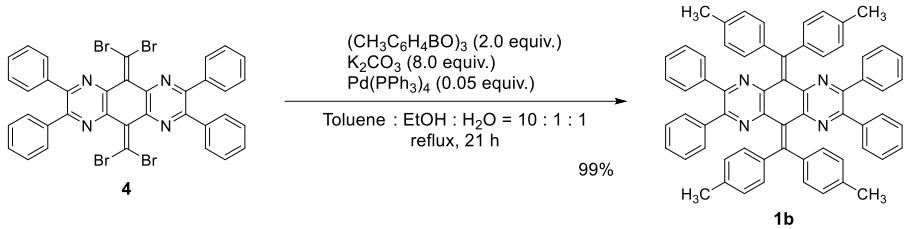


A mixture of 11,11,12,12-tetrabromo-2,3,6,7-tetraphenyl-1,4,5,8-tetraaza-9,10-

anthraquinodimethane **4** (108 mg, 130 μmol), phenylboronic acid (95.7 mg, 785 μmol), K_2CO_3 (144 mg, 1.04 mmol) and $Pd(PPh_3)_4$ (15.6 mg, 13.5 μmol) in a mixture of toluene (6 mL), EtOH (0.6 mL) and water (0.6 mL) was stirred at 120 ℃ for 8 h. After cooling to 26 ℃, the reaction mixture was extracted with EtOAc three times. The combined organic layers were washed with water and brine, and dried over anhydrous $MgSO_4$. After filtration, the solvent was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane/EtOAc = 10) to give **1a** (99.0 mg) as a red solid in 93% yield.

^{1}H NMR data were identical to those in literature.[4]

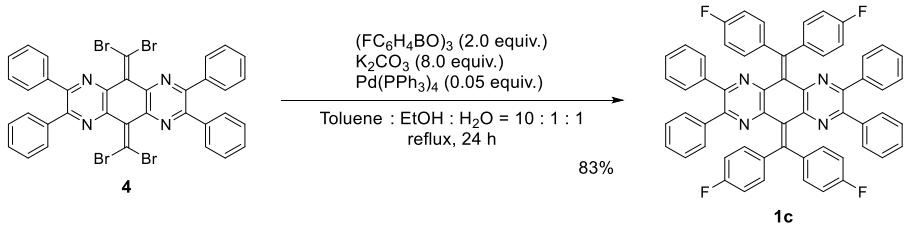
11,11,12,12-Tetrakis(4-methylphenyl)-2,3,6,7-tetraphenyl-1,4,5,8-tetraaza-9,10-anthraquinodimethane (1b)



A mixture of 11,11,12,12-tetrabromo-2,3,6,7-tetraphenyl-1,4,5,8-tetraaza-9,10-anthraquinodimethane **4** (828 mg, 1.00 mmol), tris(4-methylphenyl)boroxine (708 mg, 2.00 mmol), K_2CO_3 (1.11 g, 8.00 mmol) and $Pd(PPh_3)_4$ (57.8 mg, 50.0 μmol) in a mixture of toluene (10 mL), EtOH (1 mL) and water (1 mL) was stirred at 120 ℃ for 21 h. After cooling to 25 ℃, the reaction mixture was extracted with CH_2Cl_2 three times. The combined organic layers were washed with water and brine, and dried over anhydrous Na_2SO_4. After filtration, the solvent was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane/CH_2Cl_2 = 1) to give **4** (863 mg) as a wine red solid in 99% yield.

Mp: 254.3-260.1 ℃ (decomp); ^{1}H NMR (400 MHz, $CDCl_3$): δ/ppm 7.19-7.10 (20H, m), 7.04 (8H, t, J = 7.6 Hz), 6.71 (8H, d, J = 7.6 Hz), 2.45 (12H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm 151.64, 146.06, 144.01, 141.39, 137.83, 137.68, 131.30, 129.82, 128.70, 128.30, 127.61, 127.56, 21.43; IR (ATR): ν/cm^{-1} 3056, 3021, 2917, 2862, 1603, 1572, 1517, 1503, 1478, 1450, 1400, 1372, 1310, 1266, 1205, 1180, 1115, 1090, 1075, 1032, 1005, 922, 881, 845, 818, 808, 791, 783, 773, 761, 735, 693, 952, 639, 617, 601, 581, 544, 502, 487, 479; LR-MS(FD) m/z (%): 873.34 (28), 873.33 (73), 872.33 (M^+, bp); HR-MS (FD) Calcd. for $C_{64}H_{48}N_4$: 872.38790; Found: 872.38885.

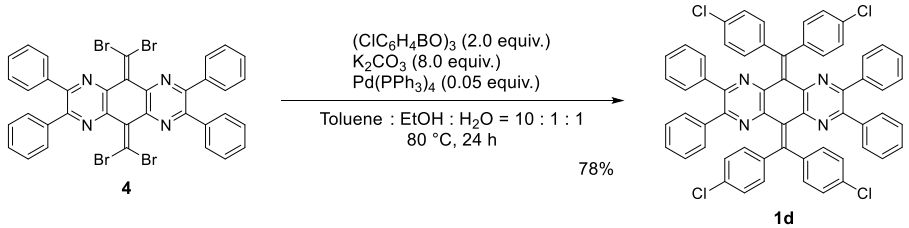
11,11,12,12-Tetrakis(4-fluorophenyl)-2,3,6,7-tetraphenyl-1,4,5,8-tetraaza-9,10-anthraquinodimethane (1c)



A mixture of 11,11,12,12-tetrabromo-2,3,6,7-tetraphenyl-1,4,5,8-tetraaza-9,10-anthraquinodimethane **4** (828 mg, 1.00 mmol), tris(4-fluorophenyl)boroxine (732 mg, 2.00 mmol), K_2CO_3 (1.11 g, 8.00 mmol) and $Pd(PPh_3)_4$ (57.8 mg, 50.0 μmol) in a mixture of toluene (10 mL), EtOH (1 mL) and water (1 mL) was stirred at 120 ℃ for 24 h. After cooling to 24 ℃, the reaction mixture was extracted with CH_2Cl_2 three times. The combined organic layers were washed with water and brine, and dried over anhydrous Na_2SO_4. After filtration, the solvent was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane/CH_2Cl_2 = 1) to give **1c** (742 mg) as a yellow solid in 83% yield.

Mp: 274.4-280.0 ℃ (decomp); ^{1}H NMR (400 MHz, $CDCl_3$): δ/ppm 7.25-7.18 (12H, m), 7.12 (8H, t, J = 7.8 Hz), 7.04 (8H, t, J = 8.7 Hz), 6.82 (8H, d, J = 7.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm 162.68 (d, $J_{C\text{-}F}$ = 247 Hz), 149.11, 147.24, 141.86, 141.26 (d, $J_{C\text{-}F}$ = 4.0 Hz), 137.54, 132.81 (d, $J_{C\text{-}F}$ = 8.0 Hz), 129.55, 128.75, 128.54, 127.86, 115.04 (d, $J_{C\text{-}F}$ = 21 Hz); IR (ATR): ν/cm^{-1} 3052, 3041, 3000, 2982, 1731, 1596, 1500, 1452, 1398, 1368, 1314, 1296, 1221, 1174, 1153, 1116, 1101, 1074, 1049, 1030, 1015, 940, 920, 882, 830, 810, 797, 788, 772, 762, 756, 741, 695, 638, 633, 619, 611, 594, 587, 573, 543, 525, 508, 501, 471; LR-MS(FD) m/z (%): 890.24 (25), 889.24 (69), 888.24 (M^+, bp); HR-MS (FD) Calcd. for $C_{60}H_{36}F_4N_4$: 888.28761; Found: 888.28895.

11,11,12,12-Tetrakis(4-chlorophenyl)-2,3,6,7-tetraphenyl-1,4,5,8-tetraaza-9,10-anthraquinodimethane (1d)

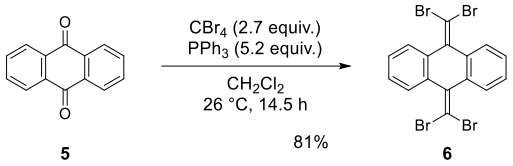


A mixture of 11,11,12,12-tetrabromo-2,3,6,7-tetraphenyl-1,4,5,8-tetraaza-9,10-anthraquinodimethane **4** (828 mg, 1.00 mmol), tris(4-chlorophenyl)boroxine (830 mg, 2.00 mmol), K_2CO_3 (1.11 g, 8.00 mmol) and $Pd(PPh_3)_4$ (57.8 mg, 50.0 μmol) in a mixture of toluene (10 mL), EtOH (1 mL) and water (1 mL) was stirred at 80 ℃ for 24 h. After cooling to 24 ℃, the reaction mixture was extracted with CH_2Cl_2 three times. The combined organic layers were

washed with water and brine, and dried over anhydrous Na_2SO_4. After filtration, the solvent was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane/CH_2Cl_2 = 1) to give **1d** (740 mg) as an orange solid in 78% yield.

Mp: 300.1-303.2 ℃ (decomp); ^{1}H NMR (400 MHz, $CDCl_3$): δ/ppm 7.33 (8H, d, *J* = 8.4 Hz), 7.22 (4H, d, *J* = 7.4 Hz), 7.16 (8H, d, *J* = 8.4 Hz), 7.13 (8H, t, *J* = 7.4 Hz), 6.75 (8H, d, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm 148.65, 147.47, 144.43, 141.20, 137.29, 133.92, 132.21, 129.54, 128.86, 128.64, 128.44, 127.92; IR (ATR): *ν*/cm^{-1} 3058, 3046, 2986, 2955, 2926, 1583, 1520, 1484, 1451, 1396, 1374, 1269, 1205, 1179, 1118, 1085, 1030, 1012, 1004, 920, 880, 843, 827, 810, 804, 791, 785, 766, 734, 692, 665, 642, 631, 617, 598, 545, 530, 521, 507, 490, 454; LR-MS(FD) *m*/*z* (%): 959.12 (10), 958.12(23), 957.12 (37), 956.12 (66), 955.12 (67), 954.12 (bp), 953.13 (49), 952.12 (M^+, 70); HR-MS (FD) Calcd. for $C_{60}H_{36}Cl_4N_4$: 952.16941; Found: 952.16801.

11,11,12,12-Tetrabromo-9,10-anthraquinodimethane (6)

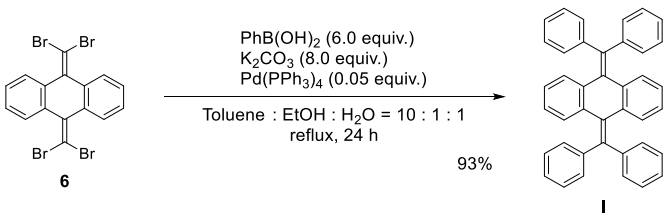


5 **6**

To a solution of 9,10-anthraquinone **5** (4.18 g, 20.1 mmol) and CBr_4 (17.7 g, 53.4 mmol) in dry CH_2Cl_2 (300 mL) was added PPh_3 (27.4 g, 104 mmol) at 26 ℃. After stirring at 26 ℃ for 14.5 h, the precipitates were filtered and washed with CH_2Cl_2. The resulting filtrate was extracted with CH_2Cl_2 three times. The combined organic layers were washed with water and brine, and dried over anhydrous $MgSO_4$. After filtration, the solvent was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane) to give **6** (8.44 g) as a colourless crystal in 81% yield.

^{1}H NMR data were identical to those in literature.[5]

11,11,12,12-Tetraphenyl-9,10-anthraquinodimethane (I)



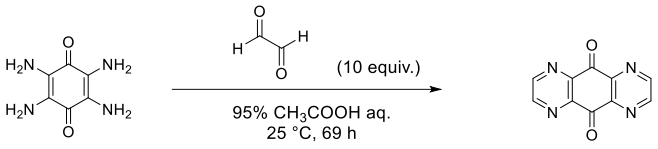
6 **I**

A mixture of 11,11,12,12-tetrabromo-9,10-anthraquinodimethane **6** (130 mg, 250 μmol), phenylboronic acid (183 mg, 1.50 mmol), K_2CO_3 (277 mg, 2.00 mmol) and $Pd(PPh_3)_4$ (14.5 mg, 12.5 μmol) in a mixture of toluene (3 mL), EtOH (0.3 mL) and water (0.3 mL) was stirred at

120 ℃ for 24 h. After cooling to 25 ℃, the reaction mixture was extracted with EtOAc three times. The combined organic layers were washed with water and brine, and dried over anhydrous $MgSO_4$. After filtration, the solvent was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane/EtOAc = 30) to give **I** (118 mg) as an orange solid in 93% yield.

^{1}H NMR data were identical to those in literature.[6]

1,4,5,8-Tetraaza-9,10-anthraquinone (7)

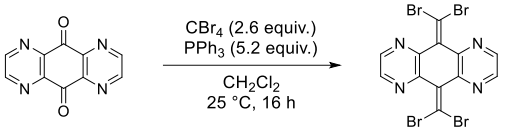


2 **7**

A mixture of 2,3,5,6-tetraamino-1,4-benzoquinone **2** (1.01 g, 6.00 mmol) and glyoxal (40% in water, 13.7 mL, 120 mmol) in 95% CH_3COOH aq. (210 mL) was stirred at 25 ℃ for 69 h. After stirring, the precipitates were collected by filtration and washed with water. The residue was redissolved in EtOH (50 mL) and stirred at 80 ℃ for 1 h, and the solution was filtered to give a **7** (882 mg) as a gray solid in 69% yield.

^{1}H NMR data were identical to those in literature.[7]

11,11,12,12-Tetrabromo-1,4,5,8-tetraaza-9,10-anthraquinodimethane (8)

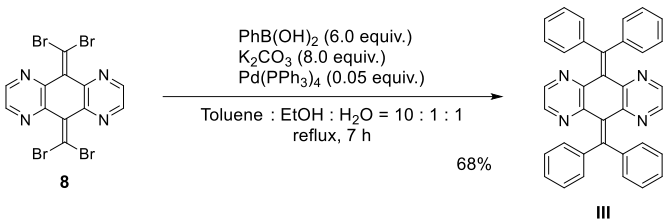


7 **8**

A mixture of CBr_4 (4.07 g, 12.3 mmol) and PPh_3 (6.44 g, 24.6 mmol) in dry CH_2Cl_2 (50 mL) was stirred at 25 ℃ for 1 h, and then 1,4,5,8-tetraaza-9,10-anthraquinone **7** (1.00 g, 4.72 mmol) was added to the mixture at 0 ℃. After warming to 25 ℃, the mixture was stirred at 25 ℃ for 16 h. After diluting with water, the precipitates were filtered and washed with $CHCl_3$. The resulting filtrate was extracted with $CHCl_3$ three times. The combined organic layers were washed with water and brine, and dried over anhydrous $MgSO_4$. After filtration, the solvent was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane/EtOAc/$CHCl_3$ = 4/1/4) to give **8** (467 mg) as a white solid in 19% yield.

^{1}H NMR data were identical to those in literature.[8]

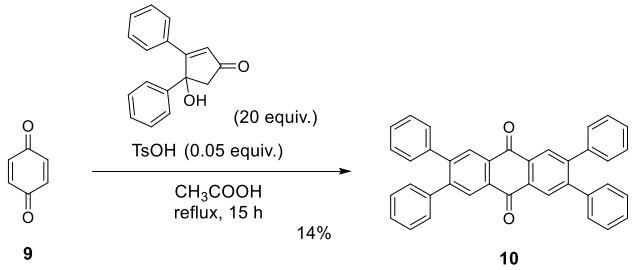
11,11,12,12-Tetraphenyl-1,4,5,8-tetraaza-9,10-anthraquinodimethane (III)



A mixture of 11,11,12,12-tetrabromo-1,4,5,8-tetraaza-9,10-anthraquinodimethane **8** (81.4 mg, 155 μmol), phenylboronic acid (114 mg, 933 μmol), K_2CO_3 (172 mg, 1.24 mmol) and $Pd(PPh_3)_4$ (9.1 mg, 7.9 μmol) in a mixture of toluene (3 mL), EtOH (0.3 mL) and water (0.3 mL) was stirred at 120 ℃ for 7 h. After cooling to 24 ℃, the reaction mixture was extracted with CH_2Cl_2 three times. The combined organic layers were washed with water and brine, and dried over anhydrous $MgSO_4$. After filtration, the solvent was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane/EtOAc = 3) to give **III** (54.3 mg) as an orange solid in 68% yield.

^{1}H NMR data were identical to those in literature.[8]

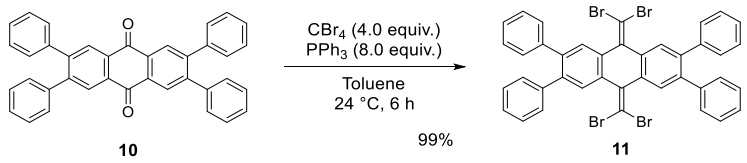
2,3,6,7-Tetraphenyl-9,10-anthraquinone (10)



A mixture of 1,4-benzoquinone **9** (216 mg, 2.00 mmol), 4-hydroxy-3,4-diphenylcyclopent-2-en-1-one (1.00 g, 4.00 mmol) and *p*-toluenesulfonic acid monohydrate (19.0 mg, 100 μmol) in CH_3COOH (55 mL) was stirred at reflux for 15 h. After cooling to 26 ℃, the mixture was diluted with water and extracted with CH_2Cl_2 three times. The combined organic layers were washed with water, saturated $NaHCO_3$ aq. and brine, and dried over anhydrous $MgSO_4$. After filtration, the solvent was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane/CH_2Cl_2 = 1) to give **10** (143 mg) as a yellow powder in 14% yield.

^{1}H NMR data were identical to those in literature.[9]

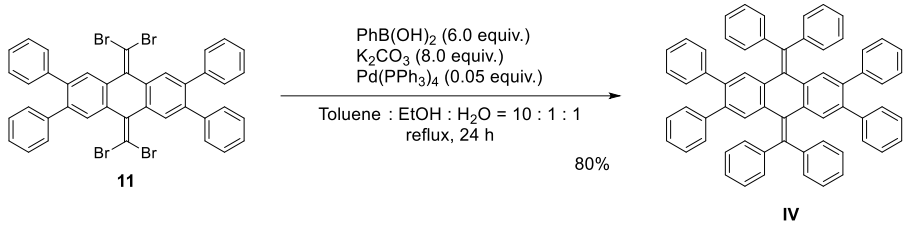
11,11,12,12-Tetrabromo-2,3,6,7-tetraphenyl -9,10-anthraquinodimethane (11)



A mixture of CBr_4 (265 mg, 799 μmol) and PPh_3 (412 mg, 1.60 mmol) in dry toluene (2 mL) was stirred at 24 ℃ for 1 h. To the suspension was added 2,3,6,7-tetraphenyl-9,10-anthraquinone **10** (102 mg, 200 μmol), and the mixture was heated at reflux for 6 h. After cooling to 24 ℃, the reaction mixture was diluted with water, and extracted with CH_2Cl_2 three times. The combined organic layers were washed with water and brine, and dried over anhydrous $MgSO_4$. After filtration, the solvent was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane/CH_2Cl_2 = 1) to give **11** (164 mg) as a white powder in 99% yield.

Mp: >400 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ/ppm 7.96 (4H, s), 7.25-7.18 (12H, m), 7.17-7.09 (8H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm 140.57, 139.43, 138.75, 134.90, 129.85, 129.81, 128.05, 126.94, 90.67; IR (ATR): ν/cm^{-1} 3077, 3050, 3021, 2959, 2926, 2862, 1726, 1600, 1576, 1539, 1494, 1467, 1381, 1279, 1262, 1182, 1122, 1074, 1026, 1000, 960, 909, 783, 769, 746, 697, 650, 622, 614, 585, 564, 536, 521, 503; LR-MS(FD) *m*/*z* (%): 827.76 (24), 826.77 (32), 824.77 (44), 823.76 (bp), 822.77 (30), 821.77 (66), 819.77 (M^+, 17); HR-MS (FD) Calcd. for $C_{40}H_{24}Br_4$: 819.86115; Found: 819.86086.

2,3,6,7,11,11,12,12-Octaphenyl-9,10-anthraquinodimethane (IV)



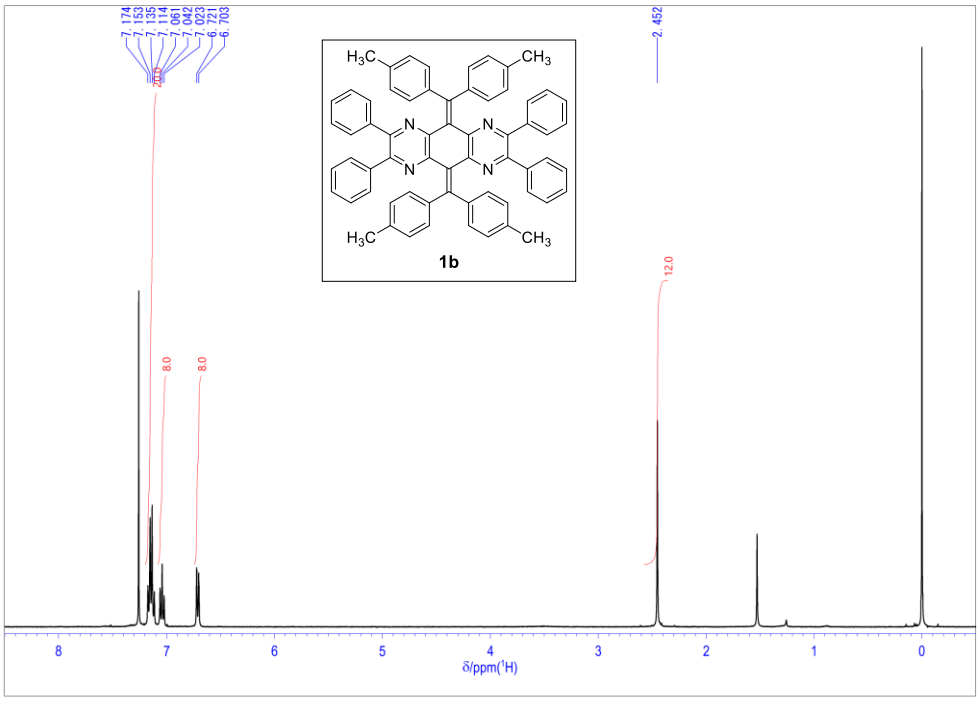
A mixture of 11,11,12,12-tetrabromo-2,3,6,7-tetraphenyl-9,10-anthraquinodimethane **11** (124 mg, 150 μmol), phenylboronic acid (110 mg, 901 μmol), K_2CO_3 (166 mg, 1.20 mmol) and $Pd(PPh_3)_4$ (8.70 mg, 7.50 μmol) in a mixture of toluene (3 mL), EtOH (0.3 mL) and water (0.3 mL) was stirred at 120 ℃ for 24 h. After cooling to 25 ℃, the reaction mixture was extracted with EtOAc three times. The combined organic layers were washed with water and brine, and dried over anhydrous $MgSO_4$. After filtration, the solvent was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane/EtOAc = 20) to give **IV** (98.0 mg) as a pale-yellow powder in 80% yield.

Mp: 297.6-298.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ/ppm 7.47 (8H, dd, J = 1.3, 7.4 Hz), 7.30

(8H, t, J = 7.4 Hz), 7.20 (4H, tt, J = 1.3, 7.4 Hz), 7.10-6.99 (12H, m), 7.07 (4H, s), 6.65 (8H, dd, J = 1.4, 7.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm 142.51, 141.17, 140.58, 137.56, 136.61, 134.63, 130.41, 129.77, 129.66, 128.33, 127.39, 126.72, 126.05; IR (ATR): $\tilde{\nu}$/cm^{-1} 3077, 3055, 3020, 1599, 1576, 1490, 1472, 1464, 1442, 1383, 1243, 1179, 1155, 1073, 1030, 1001, 980, 964, 925, 917, 905, 777, 769, 754, 747, 719, 697, 644, 624, 616, 596, 576, 537, 506, 475; LR-MS(FD) m/z (%): 814.32 (27), 813.31 (73), 812.31 (M^+, bp), 406.66 (11), 406.16 (M^{2+}, 16); HR-MS (FD) Calcd. for $C_{64}H_{44}$: 812.34430; Found: 812.34621.

NMR spectra of new compounds

(a)



(b)

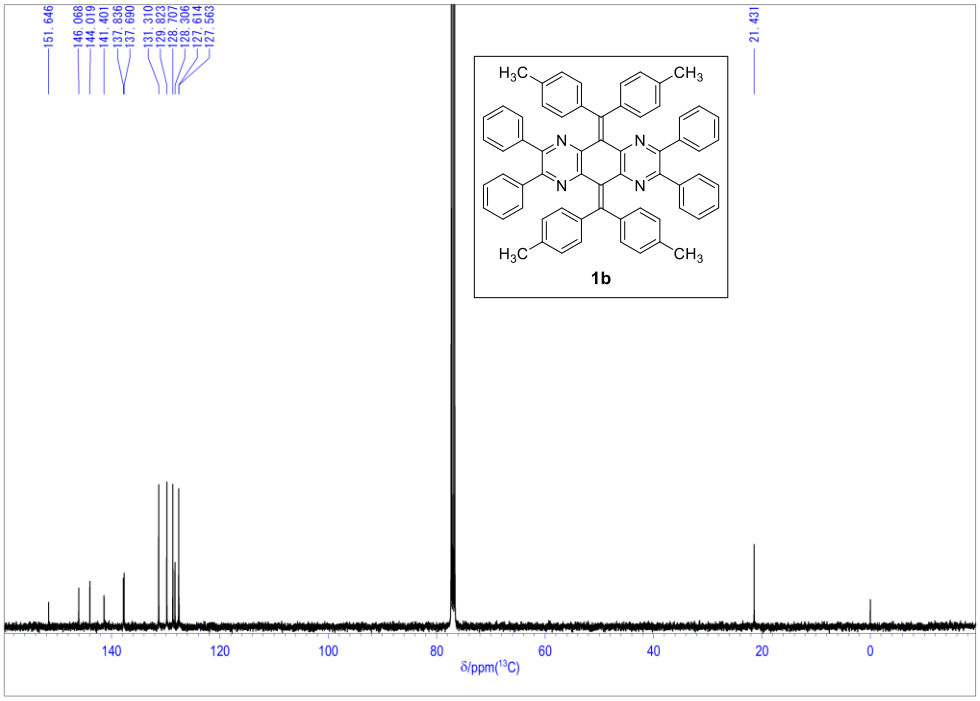
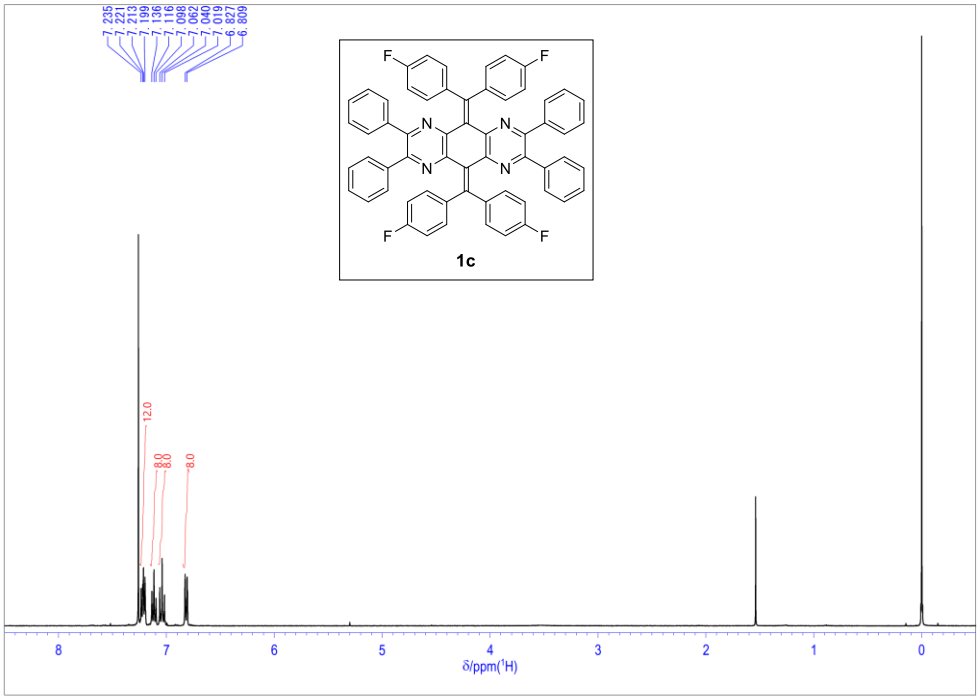


Figure S1. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **1b** in $CDCl_3$.

(a)



(b)

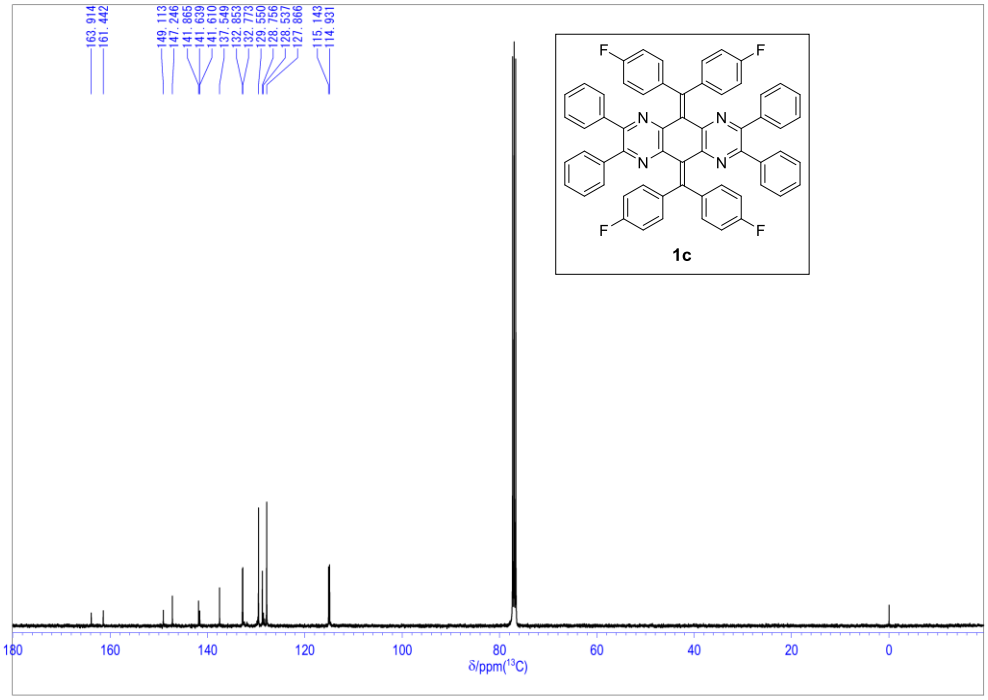
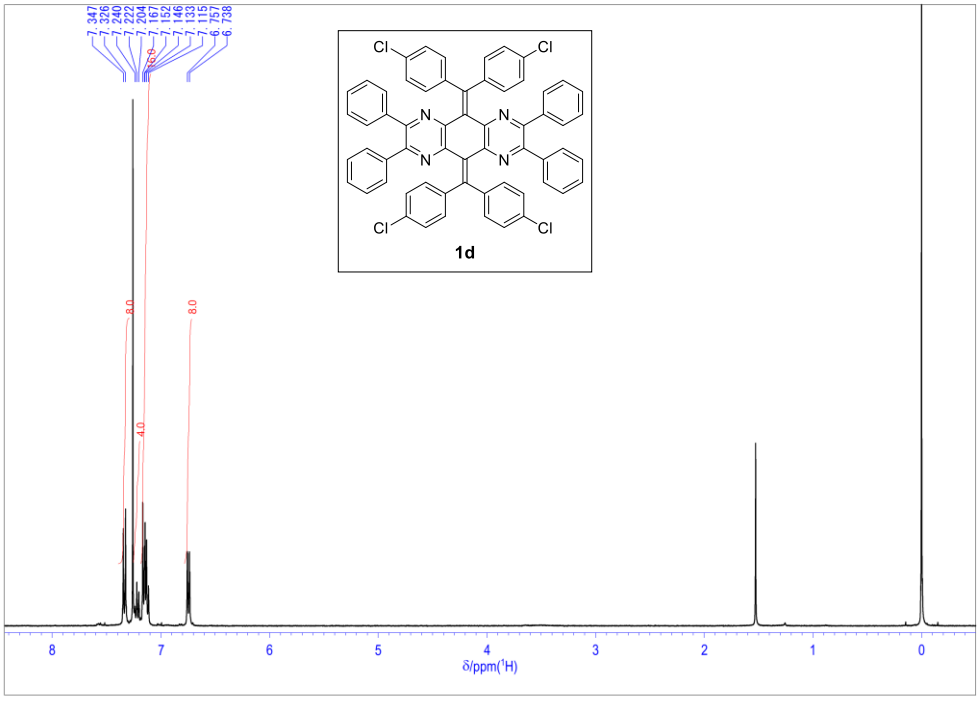


Figure S2. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **1c** in $CDCl_3$.

(a)



(b)

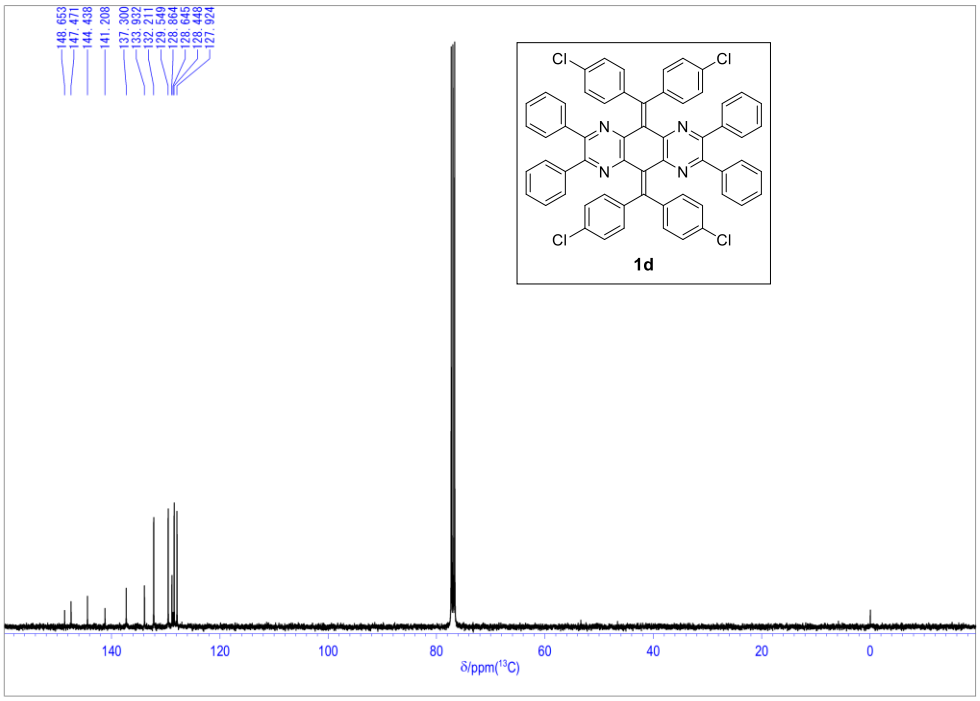
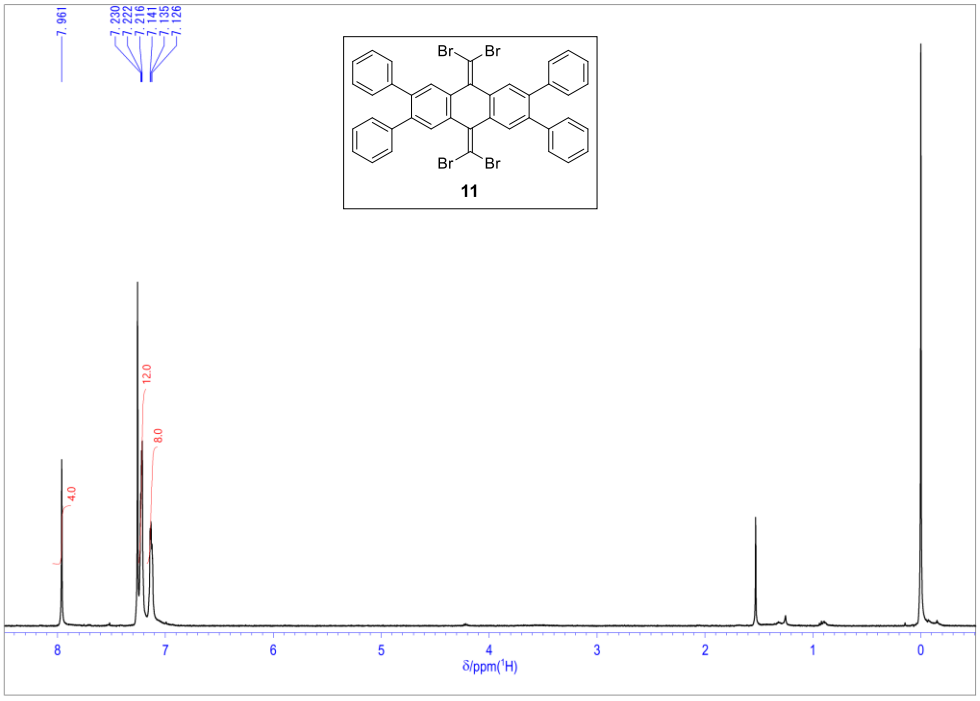


Figure S3. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **1d** in $CDCl_3$.

(a)



(b)

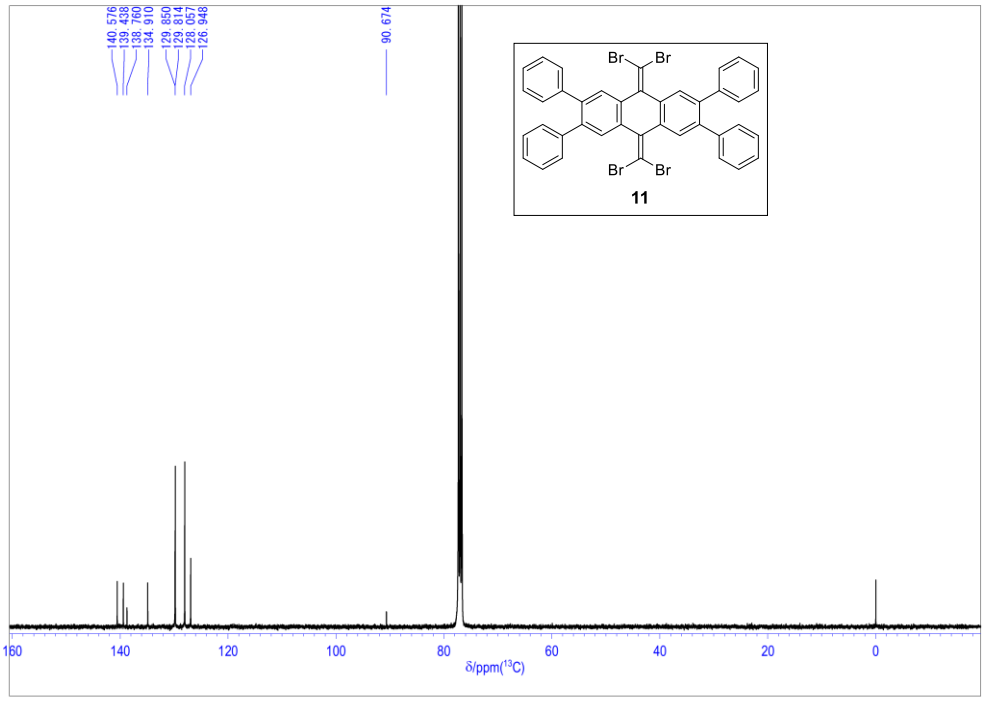
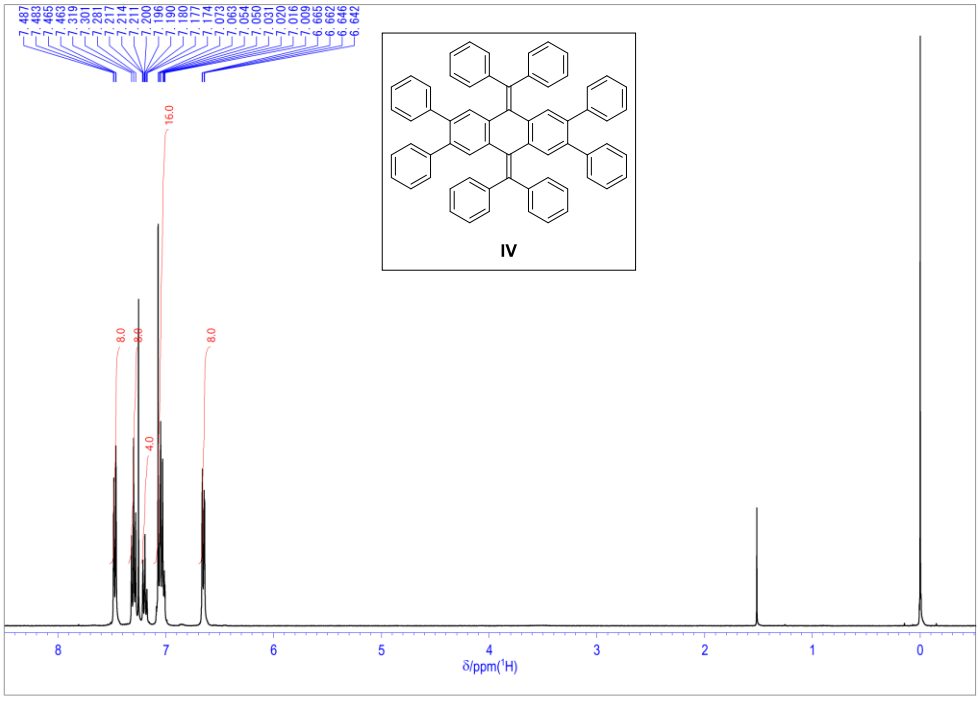


Figure S4. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **11** in $CDCl_3$.

(a)



(b)

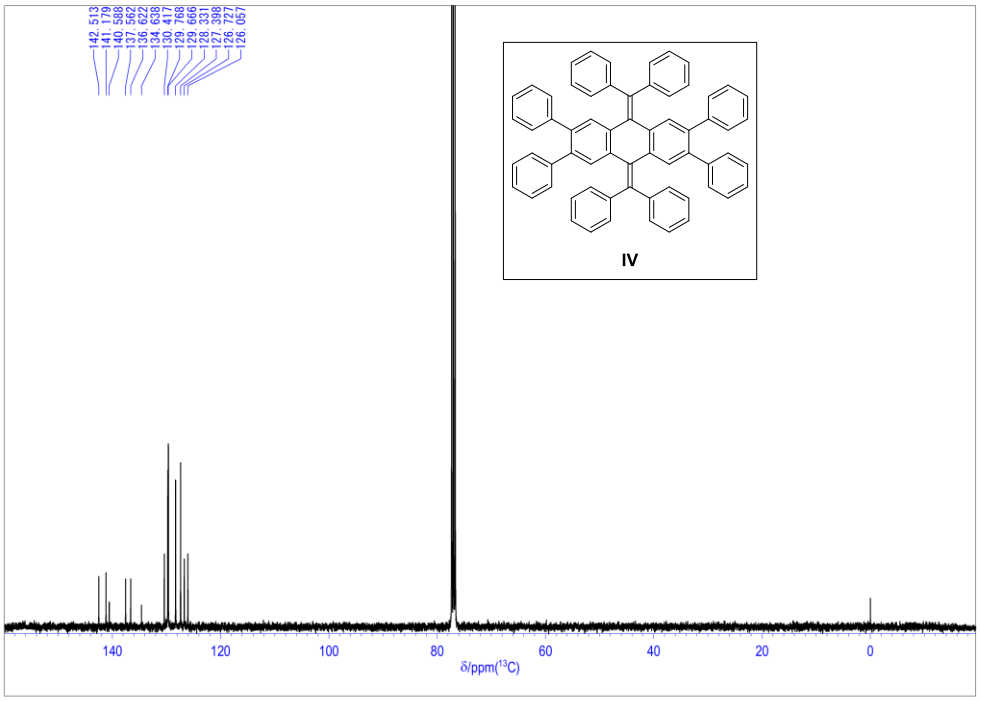


Figure S5. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **IV** in $CDCl_3$.

X-ray Analyses

Crystal structures

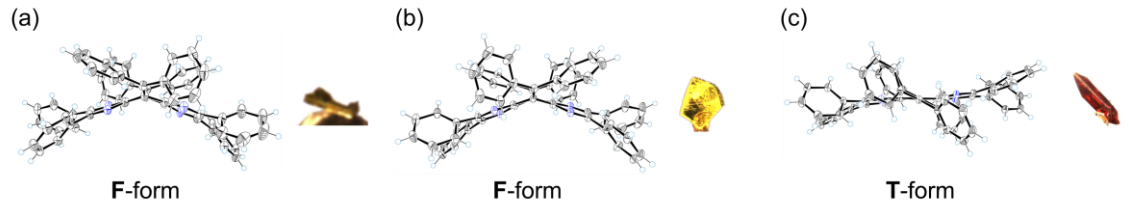


Figure S6. ORTEP drawings of **1a** [(a) **F**-form in CH_2Cl_2 solvate (recrystallised from CH_2Cl_2/hexane), (b) **F**-form in $CHCl_3$ solvate (recrystallised from $CHCl_3$/EtOH), and (c) **T**-form without crystallisation solvent (recrystallised from CH_2Cl_2/EtOH)]. The solvent molecules are omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

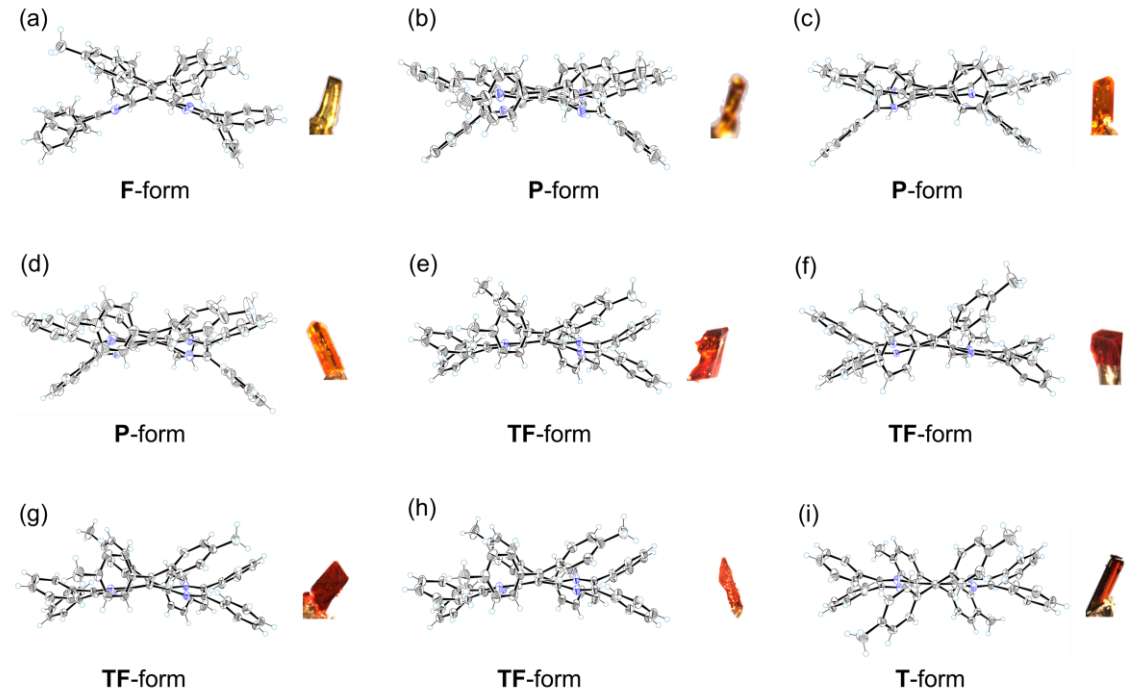


Figure S7. ORTEP drawings of **1b** [(a) **F**-form in 2EtOH solvate (recrystallised from EtOAc/EtOH), (b) **P**-form in H_2O solvate (recrystallised from EtOAc/EtOH), (c) **P**-form in CH_2Cl_2 solvate (recrystallised from CH_2Cl_2/hexane), (d) **P**-form in $0.5CHCl_3$ solvate (recrystallised from $CHCl_3$/EtOH), (e) **TF**-form in $0.5CH_2Cl_2$ solvate (recrystallised from CH_2Cl_2/hexane), (f) **TF**-form in 0.5hexane solvate (recrystallised from EtOAc/hexane), (g) **TF**-form in 0.5EtOAc solvate (recrystallised from EtOAc/EtOH), (h) **TF**-form in CH_2Cl_2 solvate (recrystallised from CH_2Cl_2/EtOH), and (i) **T**-form without crystallisation solvent (recrystallised from EtOAc/hexane)]. The solvent molecules are omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

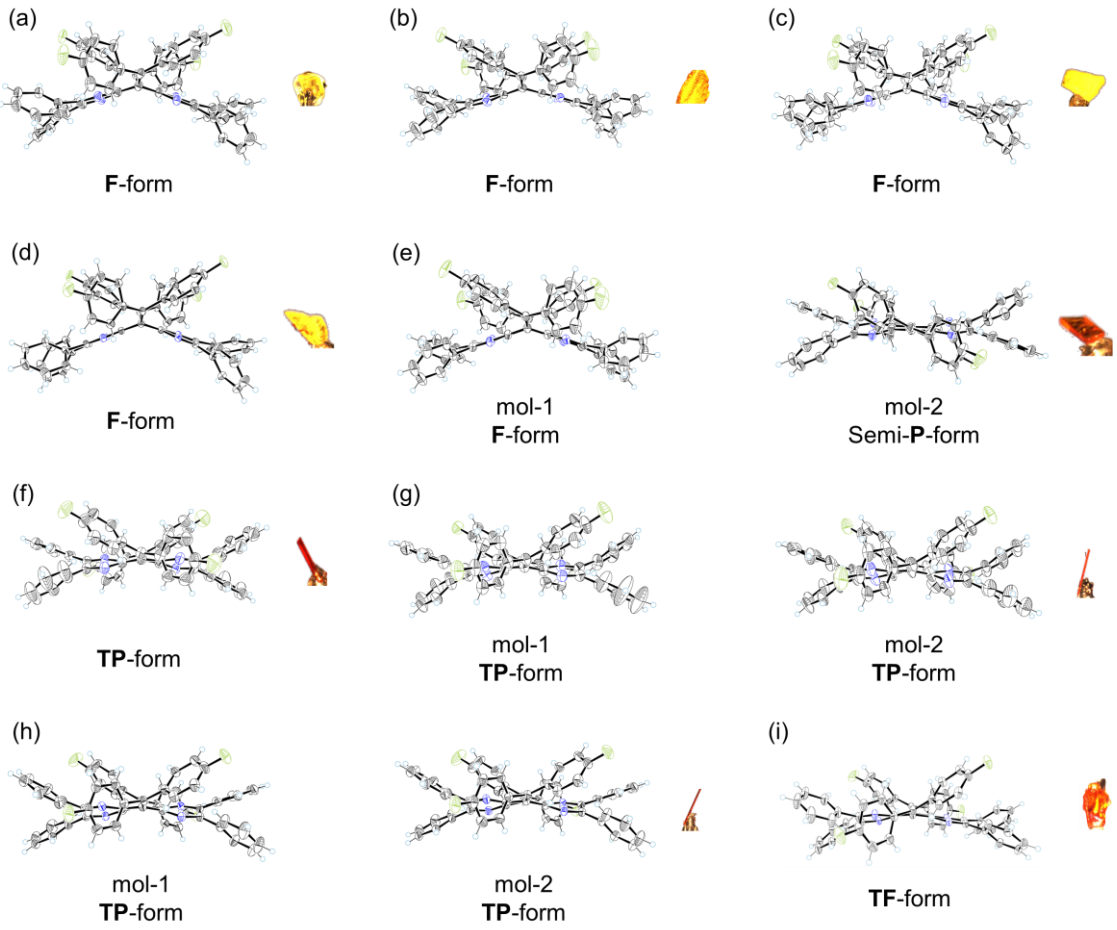


Figure S8. ORTEP drawings of **1c** [(a) **F**-form in EtOAc solvate (recrystallised from EtOAc), (b) **F**-form in $0.25CH_2Cl_2$ solvate (recrystallised from CH_2Cl_2/hexane) (c) **F**-form in $1.25CH_2Cl_2$ solvate (recrystallised from CH_2Cl_2/EtOH), (d) **F**-form in $2CHCl_3$ solvate (recrystallised from $CHCl_3$/EtOH), (e) **F**-form (mol-1) and semi-**P**-form (mol-2) in H_2O solvate (recrystallised from $CHCl_3$/hexane), (f) **TP**-form in $CHCl_3$ solvate (recrystallised from $CHCl_3$/hexane), (g) **TP**-form (mol-1 and mol-2) in CH_2Cl_2 solvate (recrystallised from CH_2Cl_2/hexane), (h) **TP**-form (mol-1 and mol-2) in EtOH solvate (recrystallised from EtOAc/EtOH), and (i) **TF**-form in $CHCl_3$ solvate (recrystallised from $CHCl_3$/hexane)]. The solvent molecules are omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

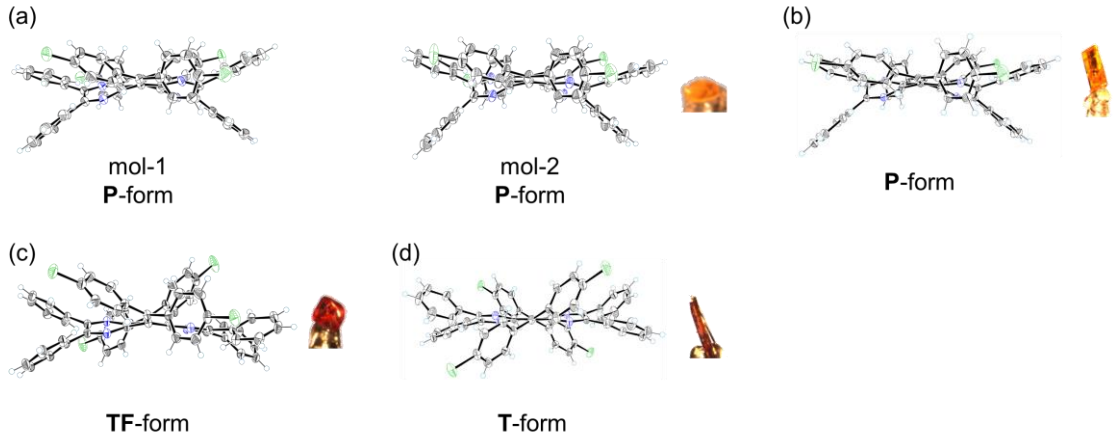


Figure S9. ORTEP drawings of **1d** [(a) **P**-form (mol-1 and mol-2) $CHCl_3$ in solvate (recrystallised from $CHCl_3$/EtOH), (b) **P**-form in CH_2Cl_2 solvate (recrystallised from CH_2Cl_2/hexane), (c) **TF**-form in $CHCl_3$ solvate (recrystallised from $CHCl_3$/hexane), and (d) **T**-form without crystallisation solvent (recrystallised from $CHCl_3$/hexane)]. The solvent molecules are omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

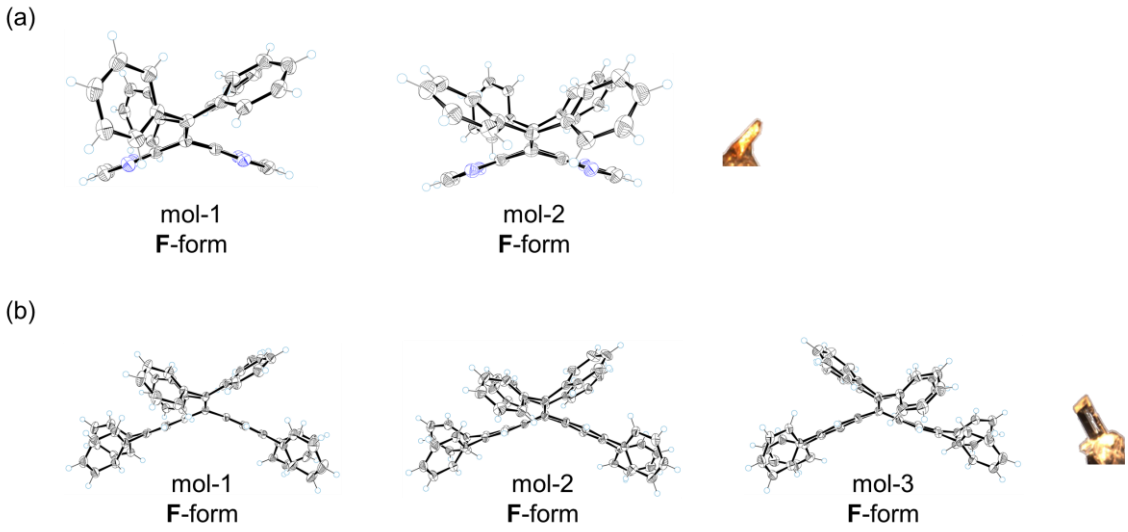


Figure S10. ORTEP drawings of (a) **III** [**F**-form (mol-1 and mol-2) without crystallisation solvent (recrystallised from $CHCl_3$/hexane)], and (b) **IV** [**F**-form (mol-1, mol-2, and mol-3) without crystallisation solvent (recrystallised from CH_2Cl_2/hexane)]. The solvent molecules are omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

Crystal Data

Method

A suitable crystal was selected and measured on a Rigaku XtaLAB Synergy (Cu-Kα radiation, λ = 1.54184 Å) with HyPix diffractometer. The crystal was kept at 150 K during data collection. Using Olex2,[10] the structure was solved with the SHELXT[11] structure solution program using Intrinsic Phasing and refined with the SHELXL[12] refinement package using Least Squares minimization.

Table S1. Crystal data of **III**, **IV**, and **1a**.

	III	**IV**	**(a) F-form**	**(b) F-form**	**(c) T-form**
Recrystallisation solvent	$CHCl_3$/hexane	CH_2Cl_2/hexane	CH_2Cl_2/hexane	$CHCl_3$/EtOH	CH_2Cl_2/EtOH
Colour and shape	Yellow block	Colourless plate	Yellow plate	Yellow plate	Red block
Solvate	Non	Non	CH_2Cl_2	$CHCl_3$	None
Empirical formula	$C_{36}H_{24}N_4$	$C_{64}H_{44}$	$C_{61}H_{42}N_4Cl_2$	$C_{61}H_{41}N_4Cl_3$	$C_{60}H_{40}N_4$
Formula weight	512.59	812.99	901.88	936.33	816.96
Temperature/K	150	150	150	150	150
Crystal system	triclinic	triclinic	monoclinic	monoclinic	triclinic
Space group	P-1	P-1	$P2_1/n$	$P2_1/n$	P-1
a [Å]	9.93699(14)	10.81378(14)	16.5930(3)	16.58736(14)	9.75804(18)
b [Å]	13.4375(2)	19.7207(2)	16.7981(3)	17.18100(13)	10.24335(19)
c [Å]	20.7105(3)	32.0682(4)	17.4925(3)	17.25022(14)	12.5631(2)
α [°]	100.7714(13)	87.3043(10)	90	90	109.5893(17)
β [°]	95.4569(12)	80.5761(11)	100.4761(18)	101.0383(8)	92.4238(15)
γ [°]	102.2024(12)	88.2988(10)	90	90	114.6339(18)
Volume [Å^3]	2629.12(7)	6737.26(15)	4794.45(16)	4825.14(7)	1050.81(4)
Z	4	6	4	4	1
ρ_{calc}g [cm^3]	1.295	1.202	1.249	1.289	1.291
μ [mm^{-1}]	0.6	0.515	1.559	2.066	0.582
Crystal size [mm^3]	0.2 × 0.15 × 0.1	0.3 × 0.1 × 0.05	0.2 × 0.1 × 0.05	0.6 × 0.5 × 0.05	0.4 × 0.2 × 0.2
Reflections collected	31474	85233	31137	31612	11871
Independent reflections	10588	27336	9524	9741	4276
R_{int}	0.0339	0.0332	0.0708	0.0311	0.0251
Data/restraints/parameters	10588/0/721	27336/0/1729	9524/0/604	9741/0/613	4276/0/289
GOF	1.035	1.032	1.158	1.54	1.034
R1 [I>=2σ (I)]	0.0613	0.0645	0.1134	0.0961	0.0436
wR2 [I>=2σ (I)]	0.1668	0.1753	0.2821	0.3134	0.1136
R1 [all data]	0.0664	0.0702	0.1534	0.1003	0.0458
wR2 [all data]	0.1720	0.1806	0.3074	0.3248	0.1155
CCDC	2176740	2176741	2176742	2176743	2176744

Table S2. Crystal data of **1b**.

	(a) F-form	(b) P-form	(c) P-form	(d) P-form	(e) TF-form	(f) TF-form	(g) TF-form	(h) TF-form	(i) T-form
Recrystallisation solvent	EtOAc/ EtOH	EtOAc/ EtOH	CH_2Cl_2/ hexane	$CHCl_3$/ EtOH	CH_2Cl_2/ hexane	EtOAc/ hexane	EtOAc/ EtOH	CH_2Cl_2/ EtOH	EtOAc/ hexane
Colour and shape	Yellow plate	Orange plate	Orange plate	Orange plate	Reddish-orange plate	Reddish-orange block	Reddish-orange plate	Reddish-orange plate	Red plate
Solvate	2EtOH	H_2O	CH_2Cl_2	0.5$CHCl_3$	0.5CH_2Cl_2	0.5hexane	0.5EtOAc	CH_2Cl_2	None
Empirical formula	$C_{68}H_{60}N_4O_2$	$C_{64}H_{50}N_4O$	$C_{65}H_{50}N_4Cl_2$	$C_{64.5}H_{48.5}N_4Cl_{1.5}$	$C_{64.5}H_{49}ClN_4$	$C_{67}H_{55}N_4$	$C_{66}H_{52}N_4O$	$C_{65}H_{50}Cl_2N_4$	$C_{64}H_{48}N_4$
Formula weight	965.2	891.08	957.99	932.75	915.52	916.15	917.11	957.99	873.06
Temperature/K	150	150	150	150	150	150	150	150	150
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	triclinic	triclinic	triclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	P-1	P-1	P-1	P-1	I2/a
a [Å]	13.73810(16)	13.0186(7)	13.06055(8)	13.15327(10)	13.8714(3)	13.8366(2)	13.83784(18)	13.8559(4)	28.1936(3)
b [Å]	19.2903(2)	15.5503(6)	15.93664(9)	15.80594(9)	14.3596(3)	14.3012(2)	14.3149(3)	14.3395(3)	5.66772(5)
c [Å]	20.7162(3)	25.0921(8)	24.82470(16)	25.12301(16)	15.5180(4)	15.4141(3)	15.3314(2)	15.2345(3)	32.3675(3)
α [°]	90	90	90	90	87.623(2)	73.7712(15)	73.8179(14)	73.943(2)	90
β [°]	105.0871(12)	103.288(4)	102.6521(6)	102.2740(7)	70.622(2)	71.2750(16)	71.4192(12)	71.145(2)	107.8392(11)
γ [°]	90	90	90	90	61.366(2)	61.2700(17)	61.3275(16)	61.450(3)	90
Volume [Å^3]	5300.81(11)	4943.7(4)	5041.58(5)	5103.68(6)	2533.36(11)	2504.14(9)	2496.59(8)	2488.83(13)	4923.45(9)
Z	4	4	4	4	2	2	2	2	4
ρ_{calc}g [cm^3]	1.209	1.197	1.262	1.214	1.2	1.215	1.22	1.278	1.178
μ [mm^{-1}]	0.562	0.549	1.511	1.245	1.008	0.539	0.558	1.531	0.526
Crystal size [mm^3]	0.5 × 0.1 × 0.02	0.2 × 0.05 × 0.02	0.5 × 0.2 × 0.03	0.4 × 0.2 × 0.05	0.8 × 0.4 × 0.1	0.4 × 0.2 × 0.15	0.3 × 0.2 × 0.03	0.6 × 0.2 × 0.03	0.6 × 0.1 × 0.05
Reflections collected	35360	35436	34101	34613	30266	28717	29691	30911	17160
Independent reflections	10752	10077	10179	10384	10267	10106	10091	10236	4926
R_{int}	0.0378	0.1381	0.0262	0.0189	0.0512	0.0330	0.0203	0.0416	0.0218
Data/restraints/ parameters	10752/0/675	10077/0/625	10179/0/653	10384/0/653	10267/0/662	10106/0/645	10091/0/657	10236/0/645	4926/0/309
GOF	1.016	1.023	1.045	1.065	1.038	1.044	1.034	1.034	1.069
R1 [I>=2σ (I)]	0.0487,	0.0888,	0.0516,	0.0725	0.0880	0.0480	0.0479	0.0718	0.0446
wR2 [I>=2σ (I)]	0.1270	0.2273	0.1413	0.2231	0.2615	0.1283	0.1367	0.2030	0.1160
R1 [all data]	0.0596	0.1802	0.0549	0.0755	0.0931	0.0514	0.0507	0.0770	0.0463
wR2 [all data]	0.1343	0.2836	0.1443	0.2264	0.2679	0.1315	0.1397	0.2083	0.1175
CCDC	2176745	2176746	2176747	2176748	2176749	2176750	2176751	2176752	2176753

Table S3. Crystal data of **1c**.

	(a) F-form	(b) F-form	(c) F-form	(d) F-form	(e) F-form + semi-P-form	(f) TP-form	(g) TP-form	(h) TP-form	(i) TF-form
Recrystallisation solvent	EtOAc	CH_2Cl_2/hexane	CH_2Cl_2/EtOH	$CHCl_3$/EtOH	$CHCl_3$/hexane	$CHCl_3$/hexane	CH_2Cl_2/hexane	EtOAc/EtOH	$CHCl_3$/hexane
Colour and shape	Yellow block	Yellow plate	Yellow plate	Yellow plate	Orange plate	Red needle	Red needle	Red needle	Reddish-orange plate
Solvate	EtOAc	$0.25CH_2Cl_2$	$1.25CH_2Cl_2$	$2CHCl_3$	H_2O	$CHCl_3$	CH_2Cl_2	EtOH	$CHCl_3$
Empirical formula	$C_{64}H_{44}N_4O_2F_4$	$C_{60.25}H_{36.5}Cl_{0.5}F_4N_4$	$C_{61.25}H_{38.5}Cl_{2.5}F_4N_4$	$C_{62}H_{38}Cl_6F_4N_4$	$C_{60}H_{38}F_4N_4O$	$C_{61}H_{37}Cl_3F_4N_4$	$C_{61}H_{38}Cl_2F_4N_4$	$C_{62}H_{42}F_4N_4O$	$C_{61}H_{37}N_4F_4Cl_3$
Formula weight	977.03	910.16	995.08	1127.66	906.94	1008.29	973.85	934.99	1008.29
Temperature/K	150	150	150	150	150	150	150	150	150
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	P-1	C2/c	$P2_1/n$	$P2_1/n$	P-1
a [Å]	12.75083(13)	12.66222(15)	12.7522(3)	12.86604(12)	13.3387(4)	25.6556(5)	25.5002(17)	25.5161(2)	10.12009(13)
b [Å]	22.3845(2)	21.9556(3)	22.7801(8)	24.1764(2)	16.6099(5)	9.8373(2)	9.7673(4)	9.80781(8)	13.5095(2)
c [Å]	17.88186(15)	17.6375(2)	17.1545(6)	17.28731(17)	18.4931(6)	40.0763(7)	40.489(4)	39.5463(4)	18.6161(3)
α [°]	90	90	90	90	108.333(3)	90	90	90	102.7568(13)
β [°]	98.8812(9)	99.1661(11)	97.596(3)	99.5946(9)	94.699(2)	96.4440(18)	95.796(7)	94.5123(9)	97.5345(12)
γ [°]	90	90	90	90	105.688(3)	90	90	90	91.2272(12)
Volume [Å^3]	5042.66(8)	4840.72(11)	4939.6(3)	5302.07(9)	3681.3(2)	10050.6(3)	10032.9(12)	9866.08(15)	2457.54(6)
Z	4	4	4	4	3	8	8	8	2
ρ_{calc}g [cm^3]	1.287	1.249	1.338	1.413	1.227	1.333	1.289	1.259	1.363
μ [mm^{-1}]	0.72	0.929	1.929	3.449	0.685	2.142	1.648	0.696	2.19
Crystal size [mm^3]	0.4 × 0.4 × 0.2	1.0 × 0.7 × 0.1	0.4 × 0.2 × 0.1	0.3 × 0.2 × 0.05	0.3 × 0.1 × 0.02	0.4 × 0.04 × 0.03	0.7 × 0.02 × 0.02	0.8 × 0.05 × 0.03	0.5 × 0.25 × 0.1
Reflections collected	32543	29221	30617	32287	41870	30470	62192	61118	29396
Independent reflections	10208	9726	9950	10723	14790	9912	20204	19771	9922
R_{int}	0.0228	0.0659	0.0303	0.0304	0.0299	0.0341	0.1222	0.0282	0.0360
Data/restraints/parameters	10208/0/657	9726/0/623	9950/0/666	10723/0/685	14790/0/932	9912/0/692	20204/0/1334	19771/0/1279	9922/0/649
GOF	1.04	1.075	1.086	1.013	1.036	1.036	1.088	1.044	1.064
R1 [I>=2σ (I)]	0.0670	0.0756	0.1064	0.1052	0.0527	0.0914	0.1267	0.0796	0.0854
wR2 [I>=2σ (I)]	0.1951	0.2183	0.2531	0.3110	0.1451	0.2775	0.3382	0.2347	0.2582
R1 [all data]	0.0700	0.0817	0.1123	0.1109	0.0609	0.1044	0.2382	0.0998	0.0898
wR2 [all data]	0.1979	0.2248	0.2561	0.3170	0.1508	0.2920	0.4033	0.2561	0.2632
CCDC	2176754	2176755	2176756	2176757	2176758	2176759	2176760	2176761	2176762

Table S4. Crystal data of **1d**.

	(a) P-form	(b) P-form	(c) TF-form	(d) T-form
Recrystallisation solvent	$CHCl_3$/EtOH	CH_2Cl_2/hexane	$CHCl_3$/hexane	$CHCl_3$/hexane
Colour and shape	Orange plate	Orange plate	Reddish-orange plate	Red needle
Solvate	$CHCl_3$	CH_2Cl_2	$CHCl_3$	None
Empirical formula	$C_{61}H_{37}N_4Cl_7$	$C_{61}H_{38}N_4Cl_6$	$C_{61}H_{37}Cl_7N_4$	$C_{60}H_{36}N_4Cl_4$
Formula weight	1074.09	1039.65	1074.09	954.73
Temperature/K	150	150	150	150
Crystal system	triclinic	monoclinic	triclinic	orthorhombic
Space group	P-1	$P2_1/n$	P-1	$P2_12_12$
a [Å]	13.2185(5)	13.13701(8)	13.8192(2)	17.5899(5)
b [Å]	15.7122(5)	15.53185(9)	14.2692(2)	24.5607(6)
c [Å]	25.1598(8)	25.04601(14)	15.4824(2)	5.46102(14)
α [°]	91.884(3)	90	74.8558(14)	90
β [°]	101.524(3)	102.7632(6)	70.7523(14)	90
γ [°]	93.318(3)	90	61.4238(16)	90
Volume [Å^3]	5106.3(3)	4984.17(5)	2511.37(8)	2359.26(11)
Z	4	4	2	2
ρ_{calc}g [cm^3]	1.397	1.385	1.42	1.344
μ [mm^{-1}]	3.907	3.502	3.972	2.634
Crystal size [mm^3]	0.15 × 0.15 × 0.01	0.4 × 0.2 × 0.1	0.15 × 0.15 × 0.05	0.5 × 0.05 × 0.05
Reflections collected	56442	30493	30619	8107
Independent reflections	20217	10068	10148	4279
R_{int}	0.0875	0.0210	0.0420	0.0299
Data/restraints/parameters	20217/0/1297	10068/0/640	10148/0/649	4279/0/307
GOF	1.019	1.024	1.056	1.074
R1 [I>=2σ (I)]	0.1065	0.0396	0.0952	0.0440
wR2 [I>=2σ (I)]	0.2955	0.0994	0.2723	0.1195
R1 [all data]	0.1454	0.0415	0.1061	0.0482
wR2 [all data]	0.3320	0.1008	0.2849	0.1219
CCDC	2176763	2176764	2176765	2176766

Molecular packing in the crystals

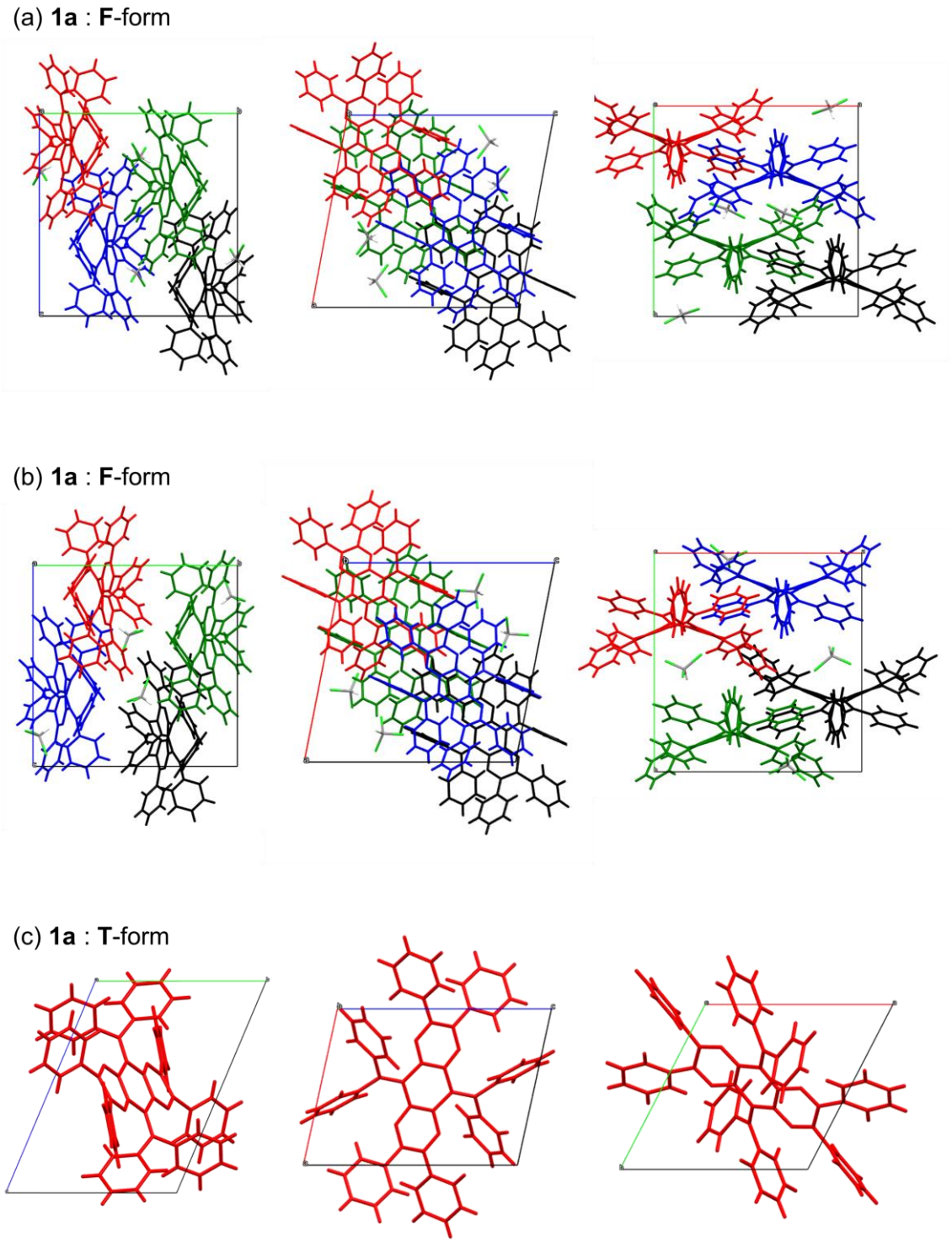


Figure S11. Molecular packing in the crystals of **1a** along the *a*-, *b*-, and *c*-axis (left, middle, and right, respectively) [(a) **F**-form in CH_2Cl_2 solvate (recrystallised from CH_2Cl_2/hexane), (b) **F**-form in $CHCl_3$ solvate (recrystallised from $CHCl_3$/EtOH), and (c) **T**-form without crystallisation solvent (recrystallised from CH_2Cl_2/EtOH)].

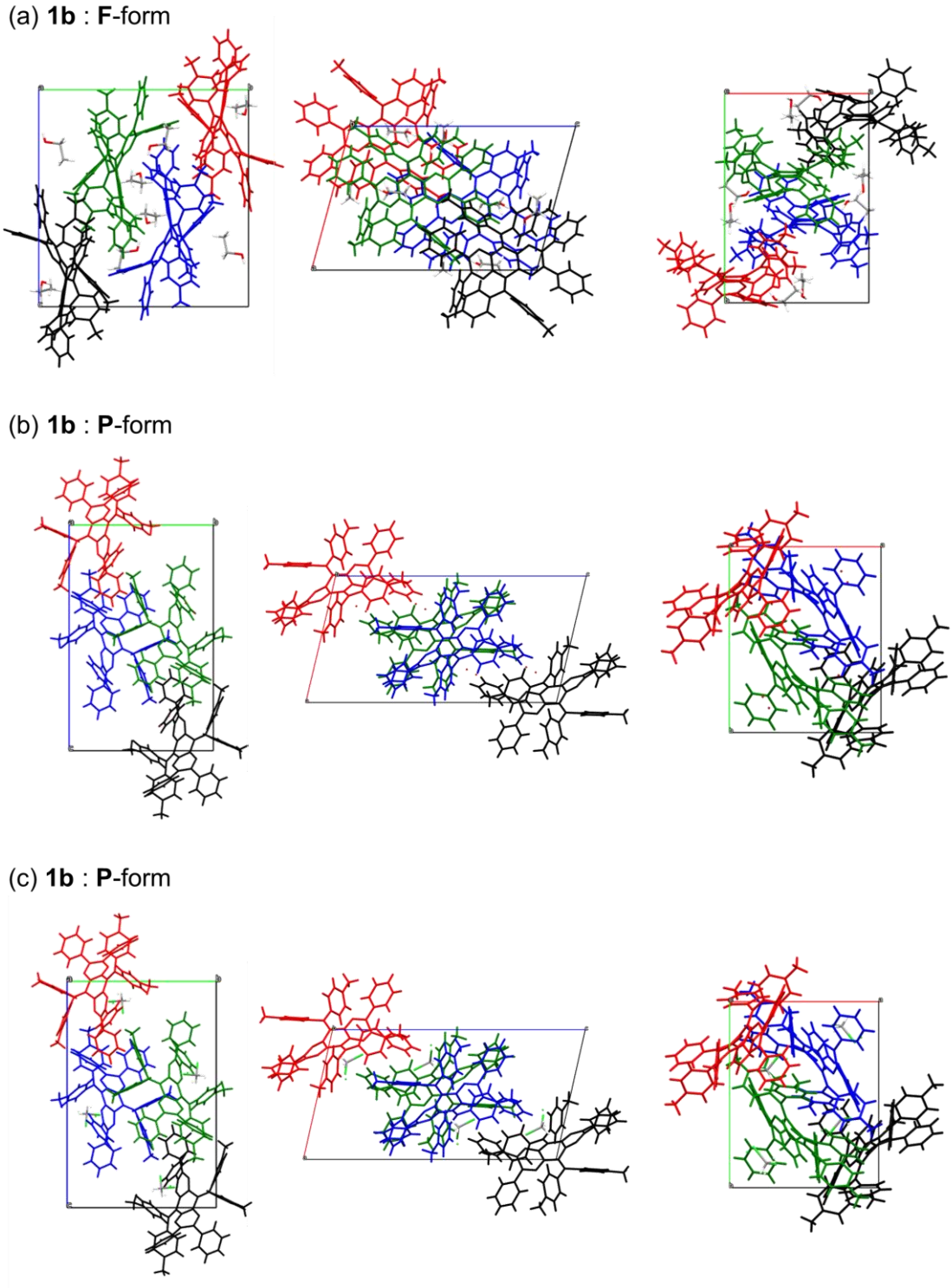
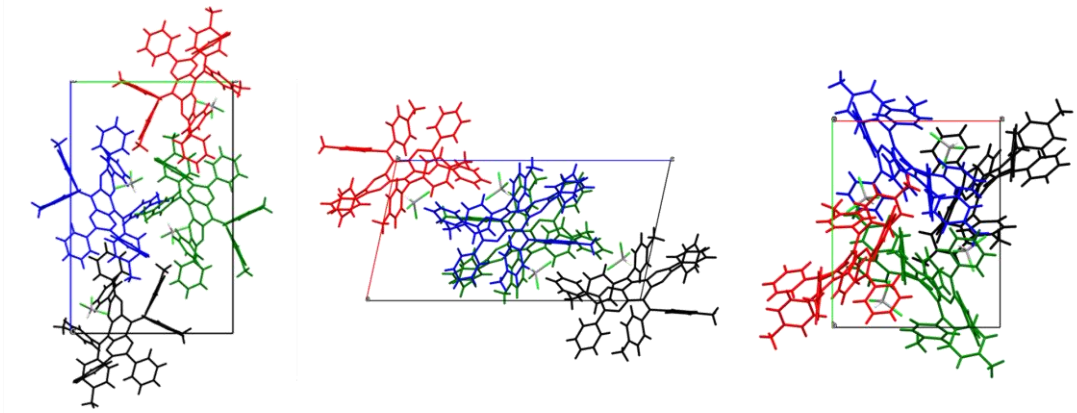
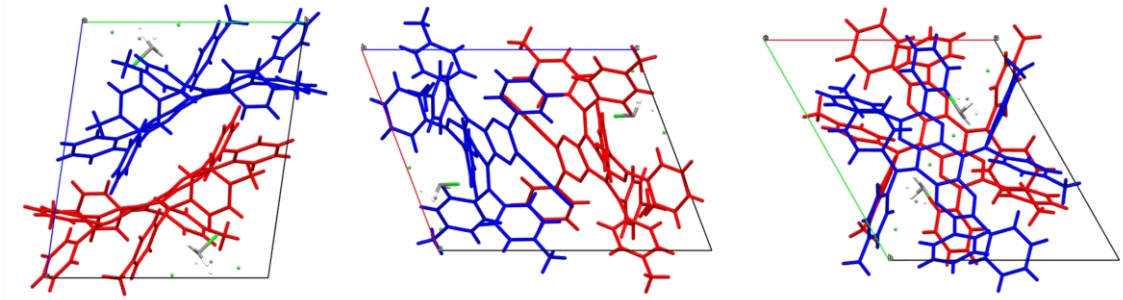


Figure S12. Molecular packing in the crystals of **1b** along the *a*-, *b*-, and *c*-axis (left, middle, and right, respectively) [(a) **F**-form in 2EtOH solvate (recrystallised from EtOAc/EtOH), (b) **P**-form in H_2O solvate (recrystallised from EtOAc/EtOH), and (c) **P**-form in CH_2Cl_2 solvate (recrystallised from CH_2Cl_2/hexane)].

(d) **1b** : **P**-form



(e) **1b** : **TF**-form



(f) **1b** : **TF**-form

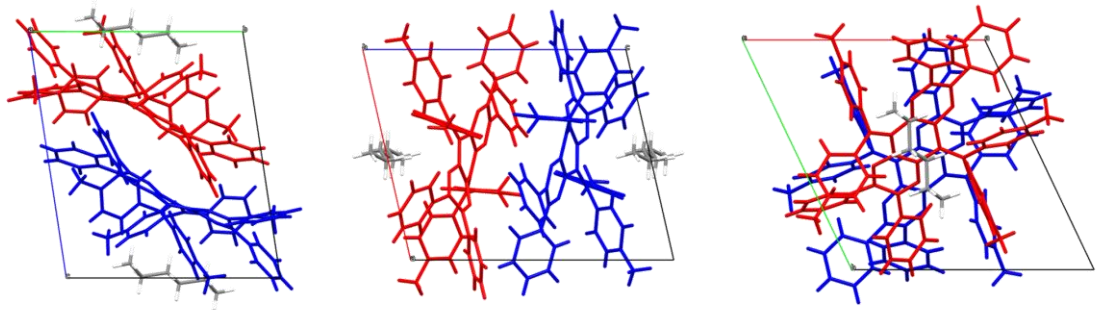


Figure S12. Molecular packing in the crystals of **1b** along the *a*-, *b*-, and *c*-axis (left, middle, and right, respectively) [(d) **P**-form in 0.5$CHCl_3$ solvate (recrystallised from $CHCl_3$/EtOH), (e) **TF**-form in 0.5CH_2Cl_2 solvate (recrystallised from CH_2Cl_2/hexane), and (f) **TF**-form in 0.5hexane solvate (recrystallised from EtOAc/hexane)].

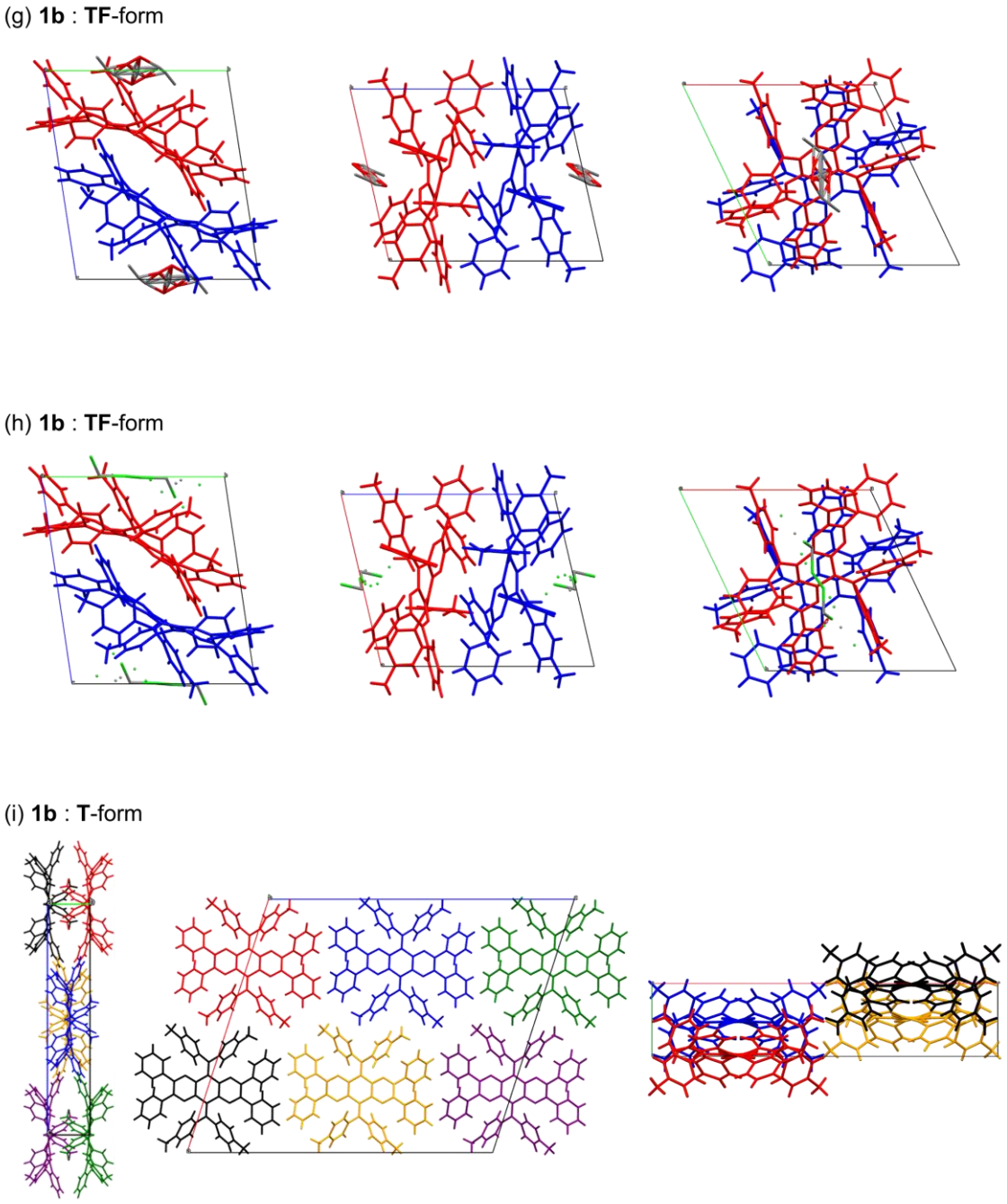


Figure S12. Molecular packing in the crystals of **1b** along the *a*-, *b*-, and *c*-axis (left, middle, and right, respectively) [(g) **TF**-form in 0.5EtOAc solvate (recrystallised from EtOAc/EtOH), (h) **TF**-form in CH_2Cl_2 solvate (recrystallised from CH_2Cl_2/EtOH), and (i) **T**-form without crystallisation solvent (recrystallised from EtOAc/hexane)].

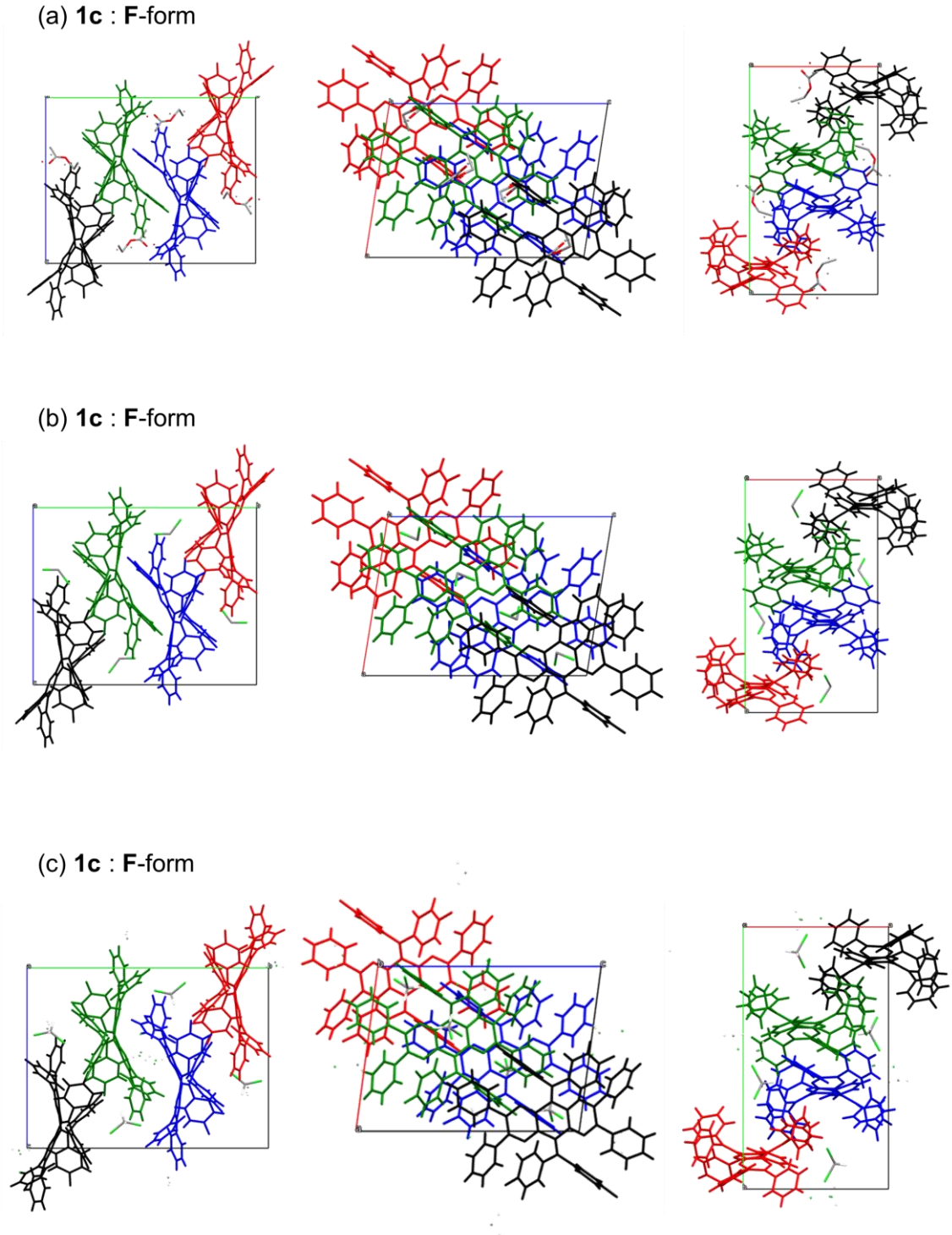
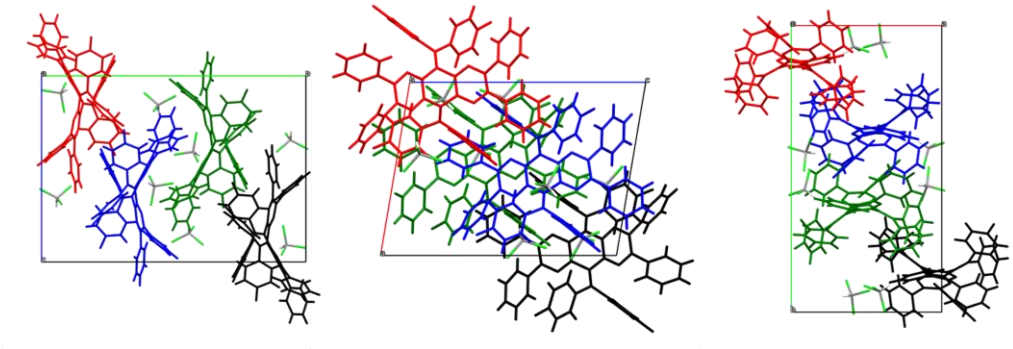
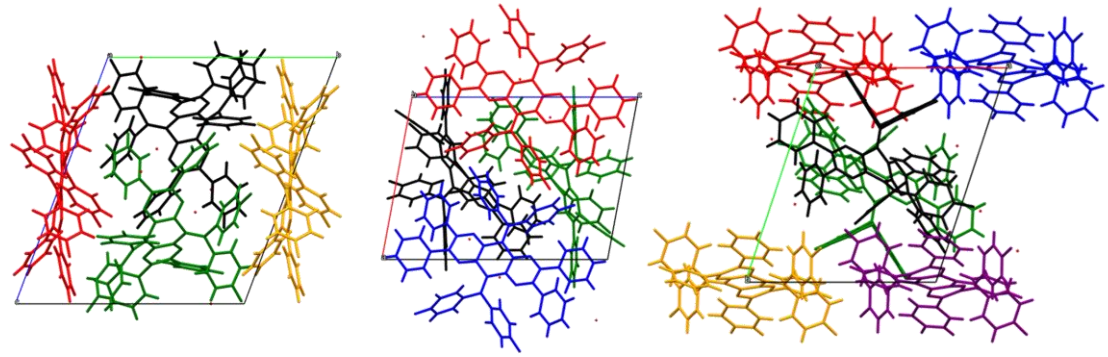


Figure S13. Molecular packing in the crystals of **1c** along the *a*-, *b*-, and *c*-axis (left, middle, and right, respectively) [(a) **F**-form in EtOAc solvate (recrystallised from EtOAc), (b) **F**-form in $0.25CH_2Cl_2$ solvate (recrystallised from CH_2Cl_2/hexane), and (c) **F**-form in $1.25CH_2Cl_2$ solvate (recrystallised from CH_2Cl_2/EtOH)].

(d) **1c** : **F**-form



(e) **1c** : **F**-form + semi-**P**-form



(f) **1c** : **TP**-form

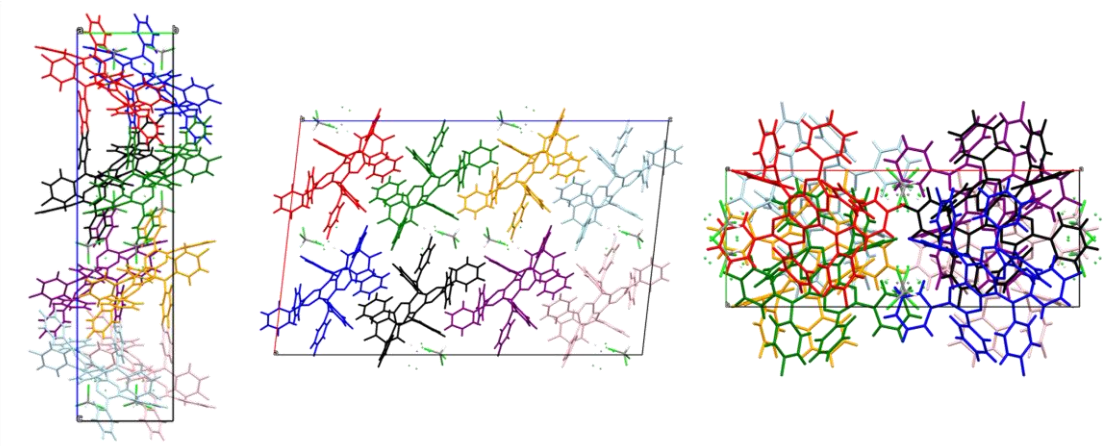
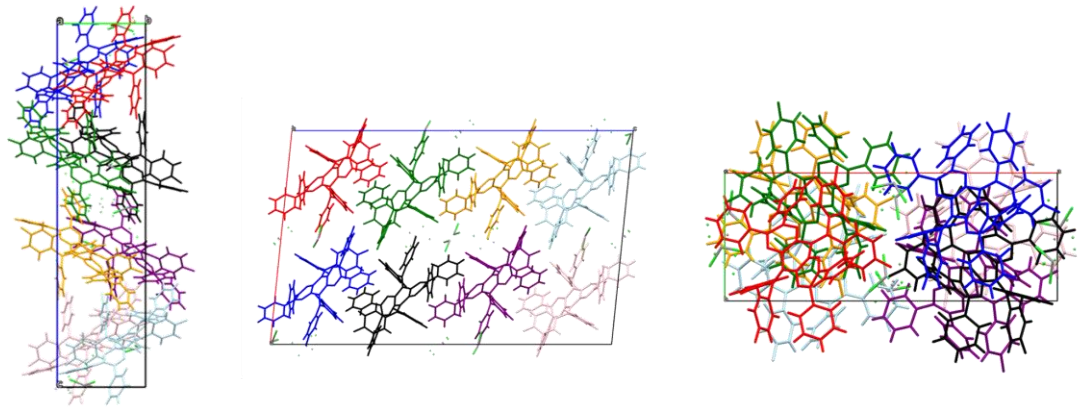
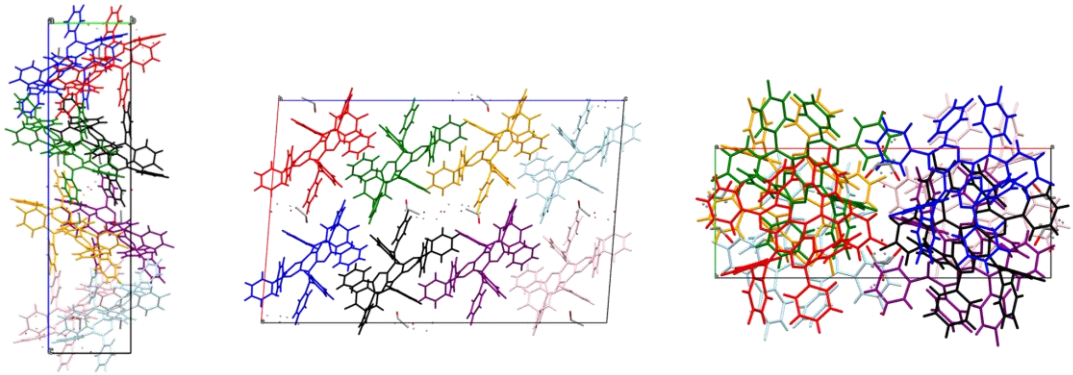


Figure S13. Molecular packing in the crystals of **1c** along the *a*-, *b*-, and *c*-axis (left, middle, and right, respectively) [(d) **F**-form in $2CHCl_3$ solvate (recrystallised from $CHCl_3$/EtOH), (e) **F**-form (mol-1) and semi-**P**-form (mol-2) in H_2O solvate (recrystallised from $CHCl_3$/hexane), and (f) **TP**-form in $CHCl_3$ solvate (recrystallised from $CHCl_3$/hexane)].

(g) **1c** : **TP**-form



(h) **1c** : **TP**-form



(i) **1c** : **TF**-form

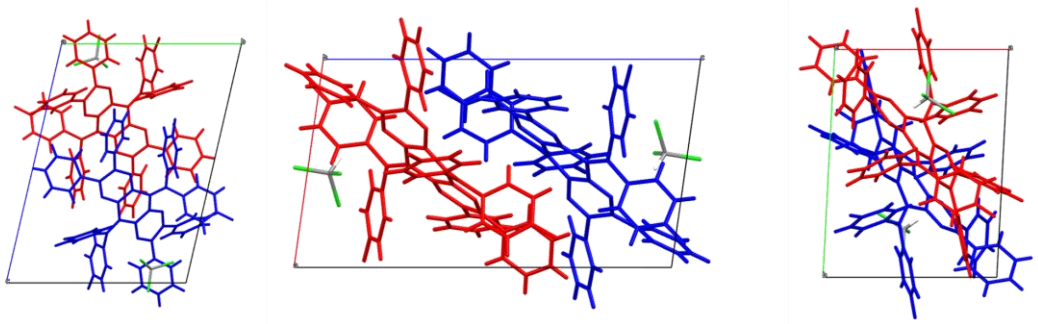


Figure S13. Molecular packing in the crystals of **1c** along the *a*-, *b*-, and *c*-axis (left, middle, and right, respectively) [(g) **TP**-form (mol-1 and mol-2) in CH_2Cl_2 solvate (recrystallised from CH_2Cl_2/hexane), (h) **TP**-form (mol-1 and mol-2) in EtOH solvate (recrystallised from EtOAc/EtOH), and (i) **TF**-form in $CHCl_3$ solvate (recrystallised from $CHCl_3$/hexane)].

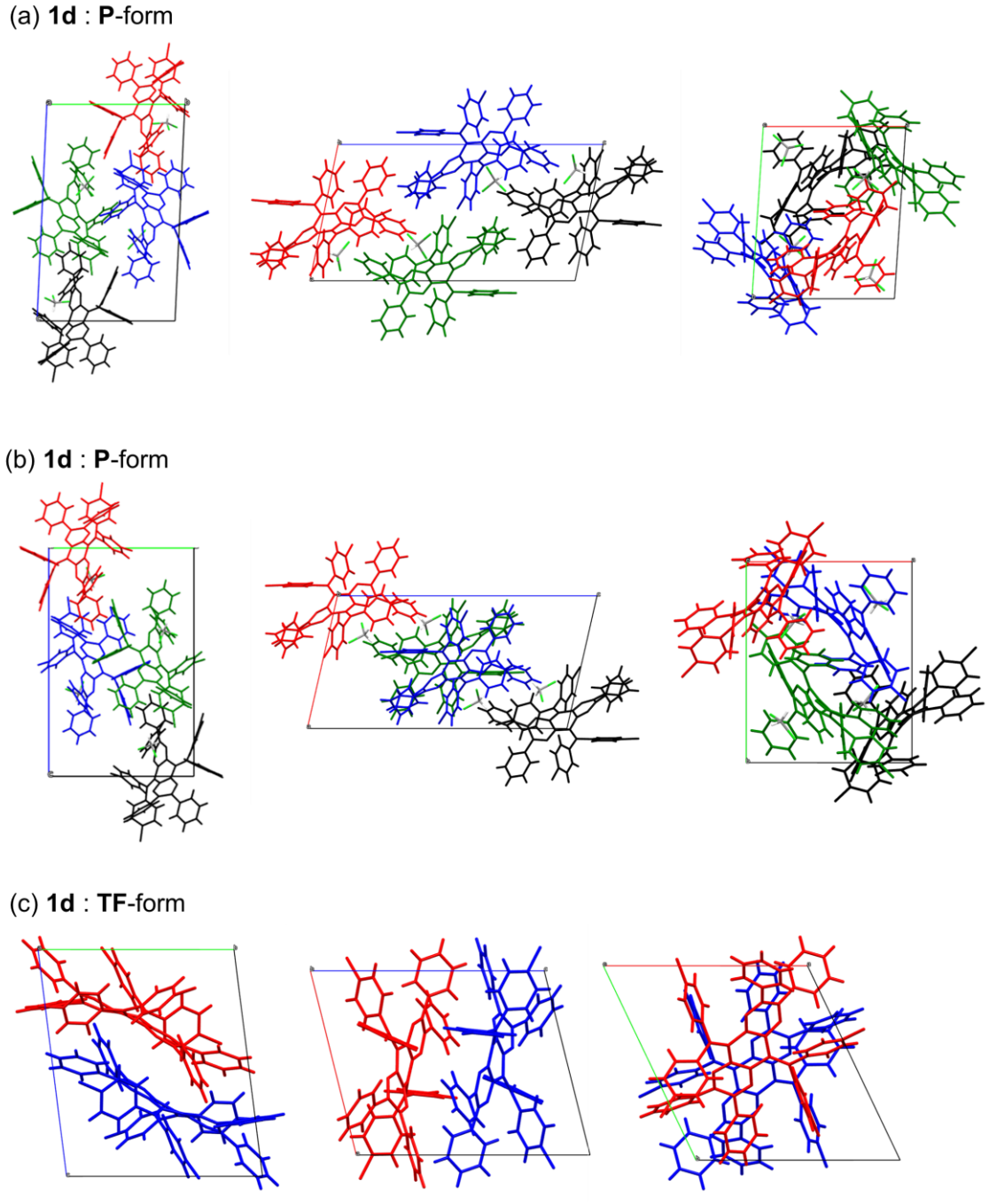


Figure S14. Molecular packing in the crystals of **1d** along the *a*-, *b*-, and *c*-axis (left, middle, and right, respectively) [(a) **P**-form (mol-1 and mol-2), $CHCl_3$ in solvate (recrystallised from $CHCl_3$/EtOH), (b) **P**-form in CH_2Cl_2 solvate (recrystallised from CH_2Cl_2/hexane), and (c) **TF**-form in $CHCl_3$ solvate (recrystallised from $CHCl_3$/hexane),].

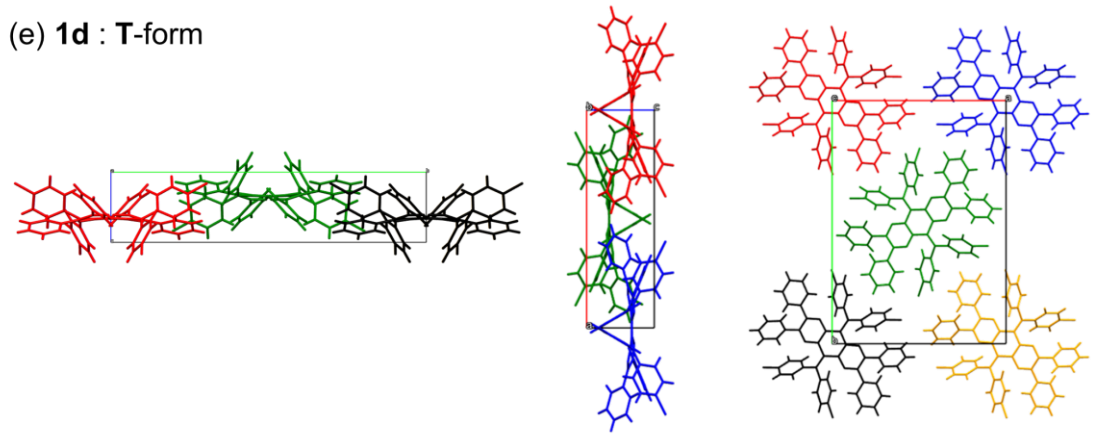
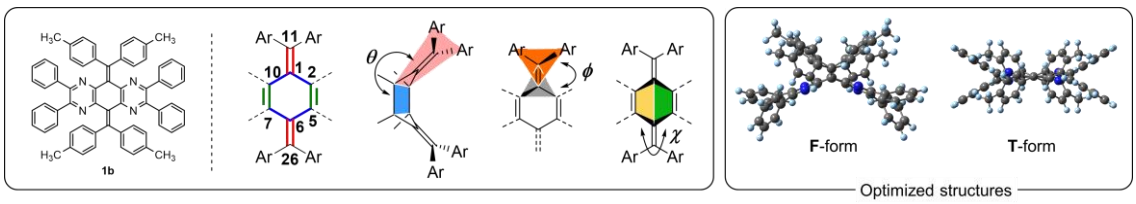


Figure S14. Molecular packing in the crystals of **1d** along the *a*-, *b*-, and *c*-axis (left, middle, and right, respectively) [(e) **T**-form without crystallisation solvent (recrystallised from $CHCl_3$/hexane)].

Structural parameters

Table S5. Structural parameters of **1b** obtained from X-ray structures (**F**-, **P**-, **TF**-, and **T**-forms) and from optimised structures (**F**-, and **T**-forms) calculated by the DFT method (B3LYP/6-31G*).

	C1-C2 [Å]	C5-C6 [Å]	C6-C7 [Å]	C10-C1 [Å]	C2-C5 [Å]	C7-C10 [Å]	C1-C11 [Å]	C6-C26 [Å]	θ [°]	ϕ [°]	χ [°]
F-form (Expt.)	1.4813(19)	1.483(2)	1.4870(19)	1.481(2)	1.410(2)	1.409(2)	1.357(2)	1.358(2)	29.91(8) 28.78(9)	8.89(7) 12.15(7)	35.86(11)
F-form (Calcd.)	*1.4869*	*1.4875*	-	-	*1.4202*	-	*1.3665*	-	*34.66*	*13.55* *13.55*	*40.79*
T-form (Expt.)	1.4650(12)	1.4636(17)	-	-	1.4158(15)	-	1.3898(15)	-	2.13(4)	32.77(5)	1.77(10)
T-form (Calcd.)	*1.4686*	*1.4686*	*1.4687*	*1.4686*	*1.4280*	-	*1.3900*	-	*3.92* *3.92*	*27.90*	*2.48*
P-form (Expt.)	1.475(6)	1.481(7)	1.479(6)	1.471(7)	1.408(6)	1.413(6)	1.370(6)	1.364(6)	13.0(3) 17.0(3)	15.0(2) 12.1(2)	17.5(4)
TF-form (Expt.)	1.481(4)	1.478(3)	1.467(4)	1.467(4)	1.411(4)	1.411(4)	1.370(4)	1.383(4)	21.34(15) 9.49(13)	17.64(13) 31.05(10)	17.66(18)



Hammett's σ_p Values

Table S6. Hammett's σ_p values[13] about CH_3, H, F, and Cl groups, which are the substituents at 4-position on the aryl groups of N_4AQDs **1**.

	gas phase σ_p	**benzene solution σ_p**	**aqueous solution σ_p**	σ_p^+
CH_3	-0.07	-0.11	-0.17	-0.31
H	0.00	0.00	0.00	0.00
F	0.19	0.17	0.06	-0.07
Cl	0.29	0.27	0.23	0.11

Spectroscopic Investigations

UV/Vis spectra

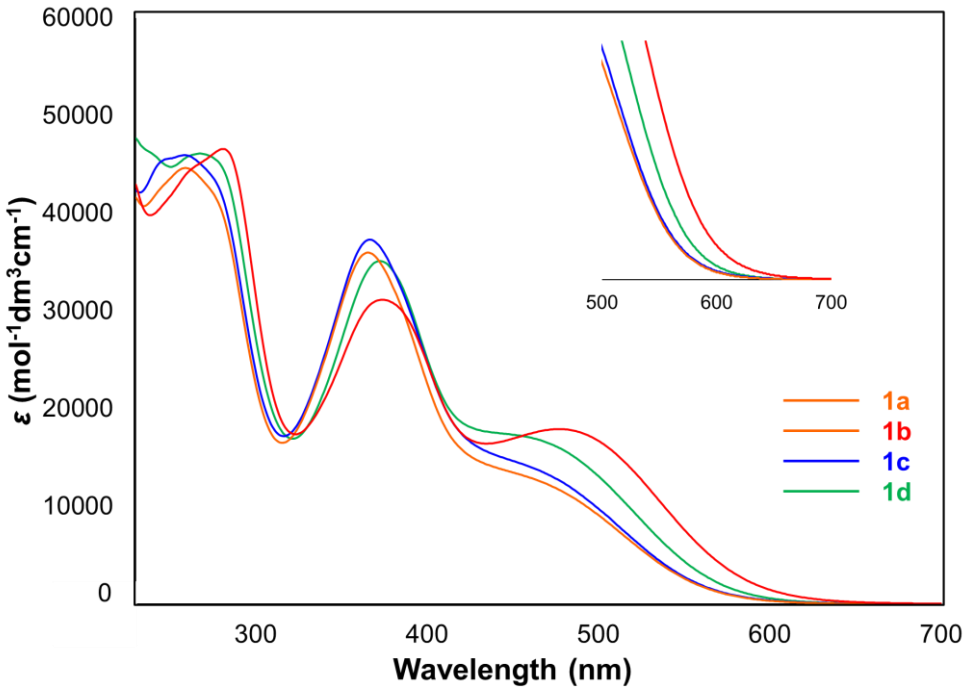


Figure S15. UV/Vis spectra of **1a**, **1b**, **1c**, and **1d** in CH_2Cl_2.

Table S7. Experimental and theoretical absorption properties of **1a**, **1b**, **1c**, and **1d**. Shoulder peaks are marked with "sh". The λ_{end} is the absorption end of each spectrum. The energy gap $\Delta E^{DFT}_{LUMO\text{-}HOMO}$ was estimated by DFT calculations (B3LYP/6-31G*).

	λ_{max} [nm] (log ε)	λ_{end} [nm]	$\Delta E^{DFT}_{LUMO\text{-}HOMO}$ [eV] / [nm]
1a	sh 470 (4.09) 366 (4.56) 259 (4.65)	657	3.50 / 354 (**F**-form) 2.38 / 520 (**T**-form)
1b	477 (4.25) 374 (4.49) 281 (4.67)	711	3.44 / 361 (**F**-form) 2.33 / 532 (**T**-form)
1c	sh 465 (4.14) 367 (4.57) 259 (4.66)	683	3.39 / 365 (**F**-form) 2.35 / 529 (**T**-form)
1d	sh 475 (4.21) 373 (4.55) 268 (4.66)	668	3.34 / 371 (**F**-form) 2.31 / 536 (**T**-form)

VT ^{1}H NMR

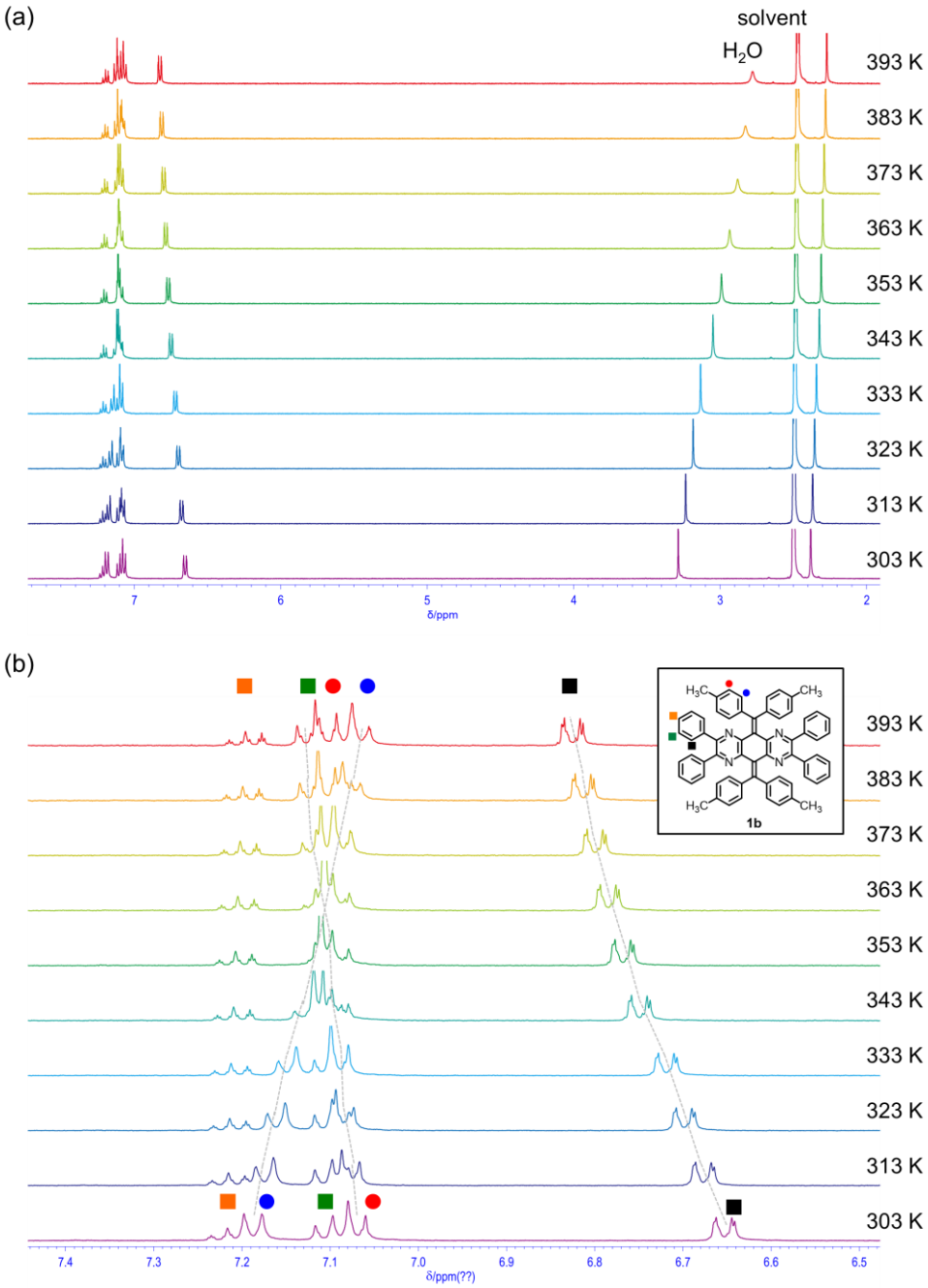


Figure S16. (a) VT ^{1}H NMR spectra of **1b** in DMSO-d_6 from 303 K to 393 K (every 10 K), and (b) enlarged view of aromatic region.

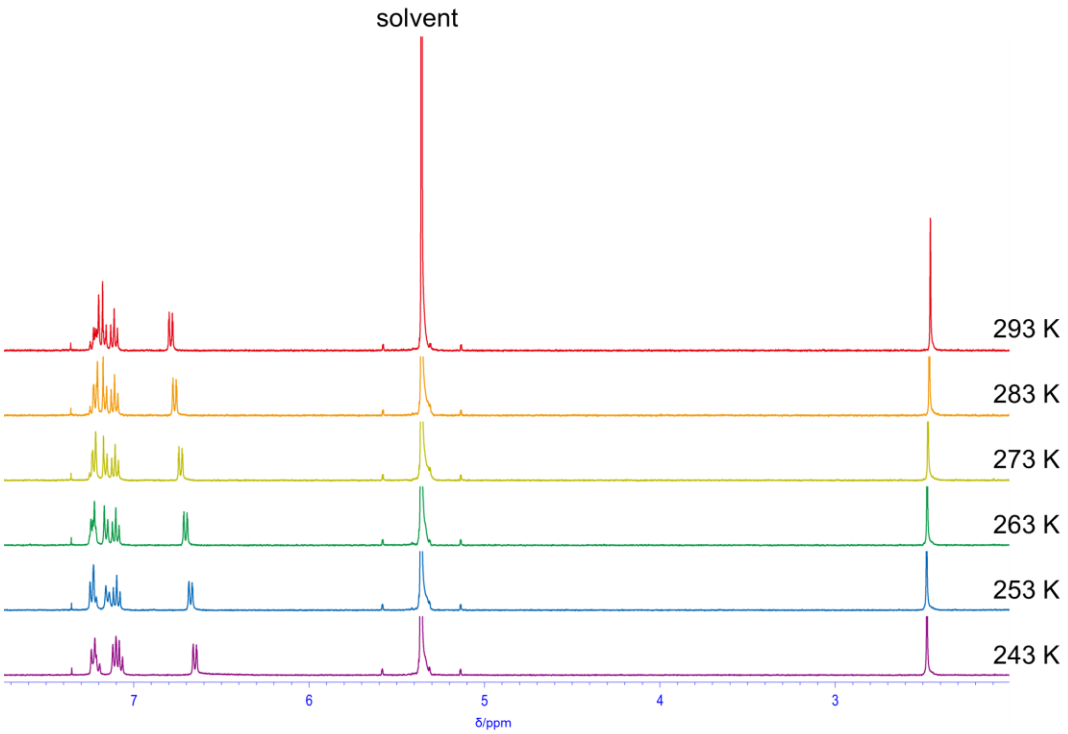


Figure S17. VT ^{1}H NMR spectra of **1b** in CD_2Cl_2 from 293 K to 203 K (every 10 K).

Excitation spectra

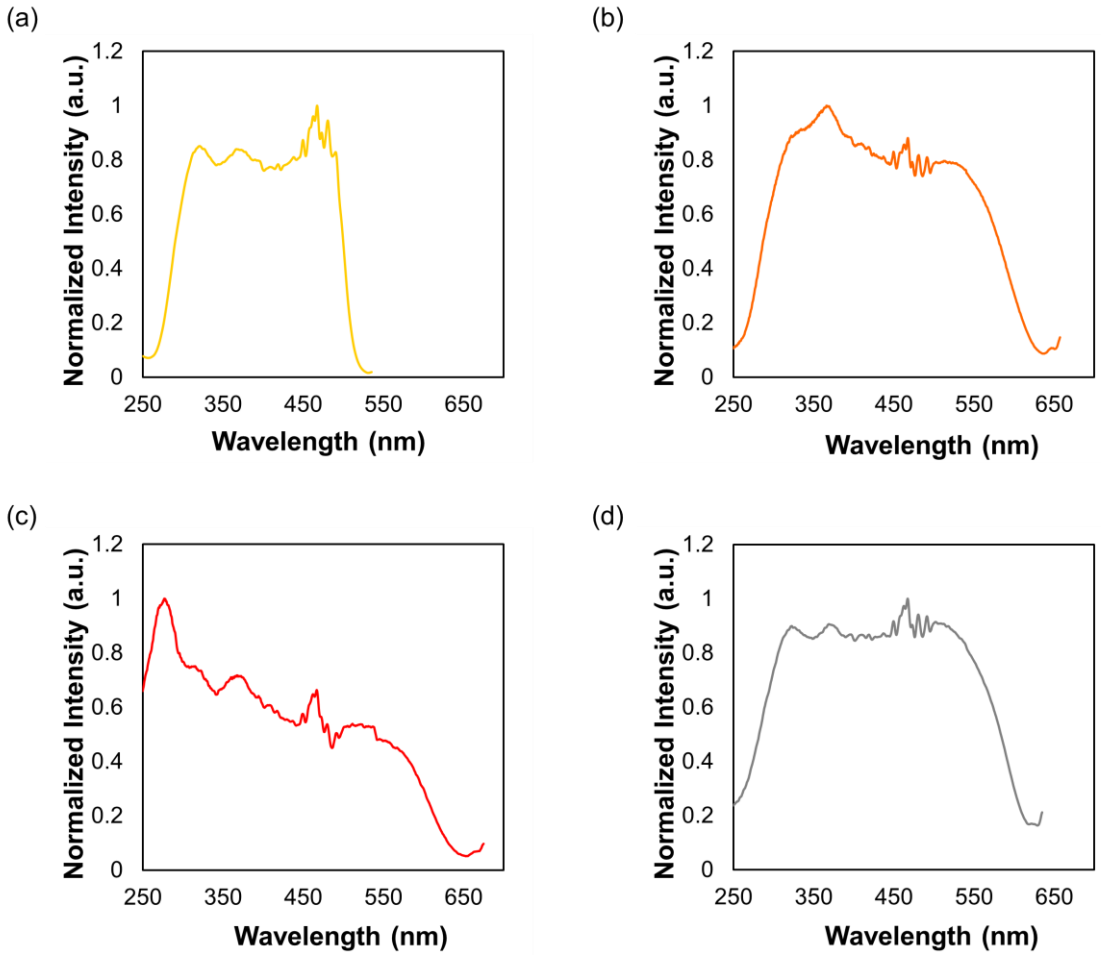


Figure S18. Excitation spectra of (a) **F**-form, (b) **TP**-form, (c) **TF**-form, and (d) **F**-form + semi-**P**-form of **1c**. All measurements were detected at the longer emission maximum.

Diffuse reflectance spectra

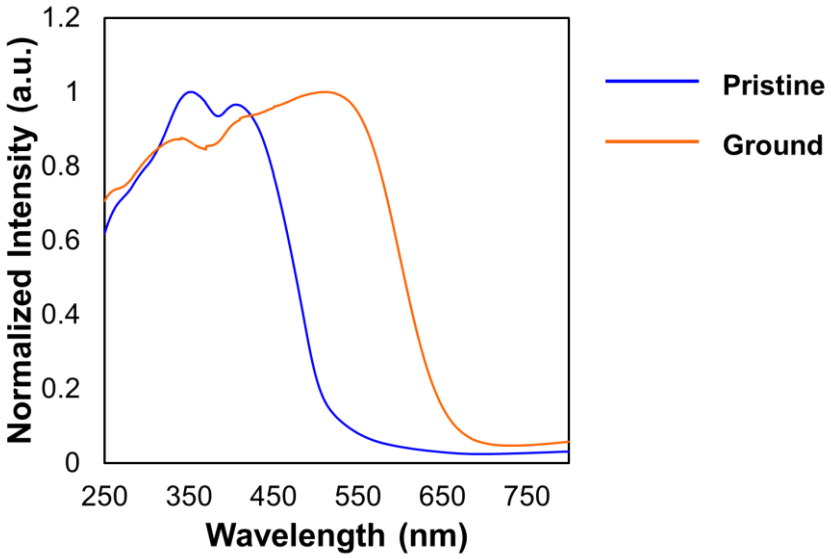


Figure S19. Diffuse reflectance spectra of **1c**.

Mechanofluorochromic Behaviour

Table S8. Luminescence properties of each state of **1c** were recorded in the solid state. All samples are excited at 380 nm. Emission lifetimes are detected at the longer emission maximum.

	λ_{em} [nm]	τ_1 [ns]	τ_2 [ns]	τ_{av} [ns]	Φ_{em} [%]
Pristine	544	0.901	2.491	1.810	5.9
Ground	636	0.311	1.303	0.674	1.0
Treated with EtOAc and drying	559	0.498	1.233	1.067	2.8

Theoretical Study

DFT calculations

Table S9. Relative energies of **1a**, **1b**, **1c**, and **1d** based on the optimised structures obtained by DFT calculations [(U)B3LYP/6-31G*].

ΔE_{rel} [kcal/mol]	F-form	T-form	T-form (Diradical)	
			Singlet	Triplet
1a (R = H)	3.15	0	10.9	13.9
1b (R = CH_3)	3.45	0	10.7	14.0
1c (R = F)	2.86	0	10.8	14.0
1d (R = Cl)	2.74	0	10.3	12.9

Table S10. Estimated LUMO and HOMO levels of **1a**, **1b**, **1c**, **1d**, **I**, **III**, and **IV** based on the optimised structures obtained by DFT calculations [(U)B3LYP/6-31G*].

		ΔE^{DFT}_{LUMO} [eV]	ΔE^{DFT}_{HOMO} [eV]	$\Delta E^{DFT}_{LUMO-HOMO}$ [eV]
1a (R = H)	**F**-form	-1.85	-5.34	3.50
	T-form	-2.36	-4.74	2.38
1b (R = CH_3)	**F**-form	-1.76	-5.20	3.44
	T-form	-2.26	-4.59	2.33
1c (R = F)	**F**-form	-2.06	-5.45	3.39
	T-form	-2.53	-4.87	2.35
1d (R = Cl)	**F**-form	-2.25	-5.59	3.34
	T-form	-2.74	-5.05	2.31
I (R = H)	**F**-form	-1.32	-5.43	4.11
III	**F**-form	-1.84	-5.51	3.67
IV	**F**-form	-1.48	-5.36	3.88

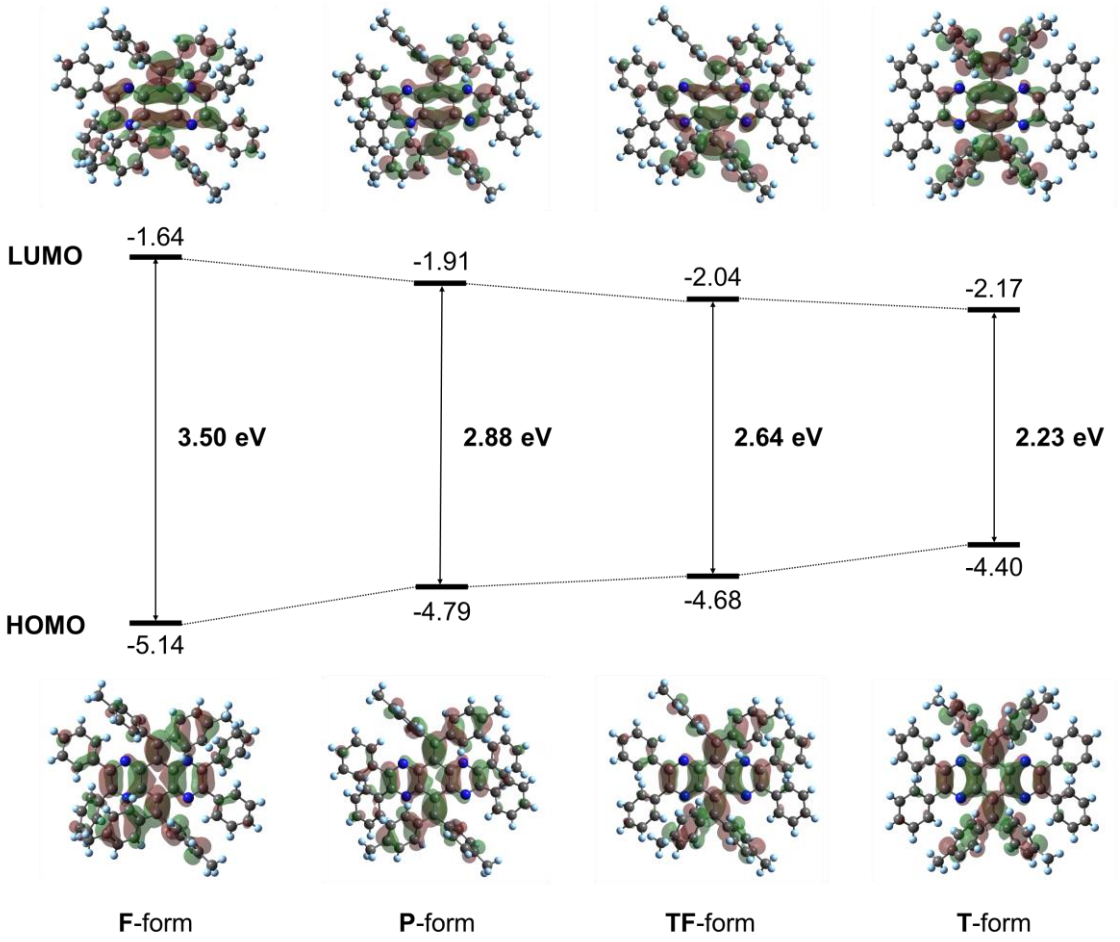


Figure S20. HOMO and LUMO levels calculated by the DFT method (B3LYP/6-31G*) based on the crystallographic coordinates of **1b**.

TD-DFT calculations

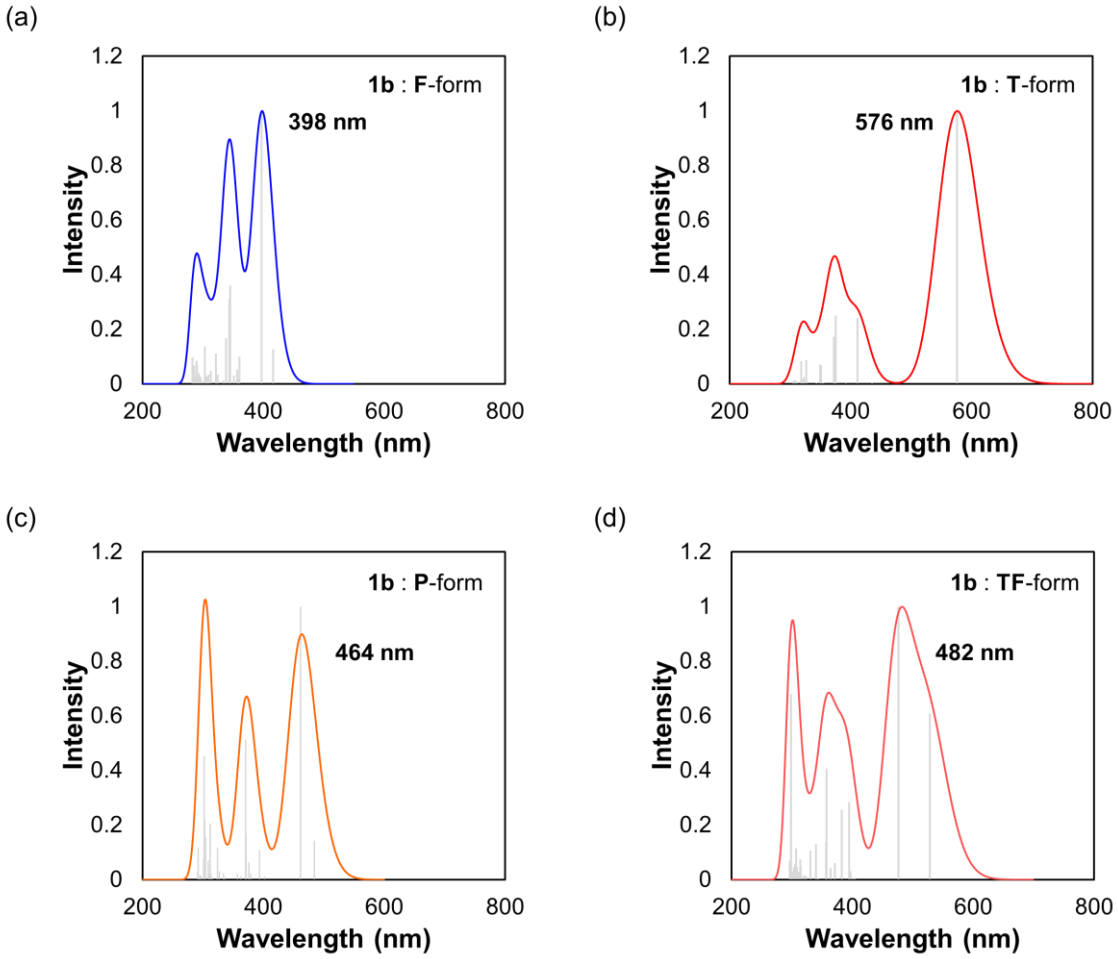


Figure S21. Simulated UV/Vis spectra of (a) **F**-form, (b) **T**-form, (c) **P**-form, and (d) **TF**-form of **1b** obtained by TD-DFT calculations (B3LYP/6-31G*) based on the crystallographic coordinates.

1b : **F**-form
HOMO : 230, LUMO : 231
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9768 eV 416.51 nm f=0.0669 <S**2>=0.000
230 -> 231 0.17115
230 -> 232 0.67988
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2685.66035965
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1218 eV 397.16 nm f=0.5265 <S**2>=0.000
230 -> 231 0.67321
230 -> 232 -0.17005

Excited State 3: Singlet-A 3.4410 eV 360.31 nm f=0.0520 <S**2>=0.000
226 -> 231 0.11022
227 -> 231 0.14430
227 -> 232 0.10540
227 -> 234 0.11583
228 -> 231 0.30120
228 -> 232 0.25587
229 -> 231 0.39406
229 -> 232 0.29006

Excited State 4: Singlet-A 3.4656 eV 357.76 nm f=0.0098 <S**2>=0.000
227 -> 231 0.32831
227 -> 232 0.53258
228 -> 232 -0.12970
229 -> 232 -0.14323

Excited State 5: Singlet-A 3.4750 eV 356.78 nm f=0.0276 <S**2>=0.000
224 -> 232 -0.11164
227 -> 231 -0.19952
227 -> 232 0.26263
228 -> 231 -0.20364
228 -> 232 0.23724
229 -> 231 -0.30418
229 -> 232 0.36230

Excited State 6: Singlet-A 3.5262 eV 351.61 nm f=0.0160 <S**2>=0.000
227 -> 231 0.51985
227 -> 232 -0.24643
228 -> 231 -0.11226
228 -> 232 0.21851
229 -> 231 -0.22223

Excited State 7: Singlet-A 3.5914 eV 345.22 nm f=0.1897 <S**2>=0.000
228 -> 231 0.45062
228 -> 232 0.26184

229 -> 231 -0.33141
229 -> 232 -0.28155

Excited State 8: Singlet-A 3.6071 eV 343.72 nm f=0.1632 <S**2>=0.000
228 -> 231 -0.32673
228 -> 232 0.41013
229 -> 231 0.24526
229 -> 232 -0.35702

Excited State 9: Singlet-A 3.6638 eV 338.41 nm f=0.0881 <S**2>=0.000
230 -> 233 0.31426
230 -> 234 0.60509

Excited State 10: Singlet-A 3.7139 eV 333.84 nm f=0.0066 <S**2>=0.000
230 -> 233 0.61765
230 -> 234 -0.31033

Excited State 11: Singlet-A 3.8145 eV 325.03 nm f=0.0181 <S**2>=0.000
220 -> 232 0.15457
222 -> 232 -0.11998
224 -> 232 -0.23503
225 -> 232 0.32211
226 -> 232 0.38917
227 -> 234 0.16086
228 -> 232 -0.20886
229 -> 232 -0.15694

Excited State 12: Singlet-A 3.8572 eV 321.44 nm f=0.0584 <S**2>=0.000
220 -> 231 0.13830
222 -> 231 -0.13246
224 -> 231 -0.23237
225 -> 231 0.34201
226 -> 231 0.42509
227 -> 233 -0.12348
228 -> 231 -0.16246
229 -> 231 -0.13602

Excited State 13: Singlet-A 3.9556 eV 313.44 nm f=0.0245 <S**2>=0.000
220 -> 231 -0.10391
222 -> 231 0.10390
224 -> 231 0.25589
224 -> 232 0.13685
225 -> 231 -0.21686
226 -> 231 0.47807
226 -> 232 0.27098

Excited State 14: Singlet-A 4.0107 eV 309.13 nm f=0.0178 <S**2>=0.000
224 -> 231 -0.21783
224 -> 232 0.20103
225 -> 232 -0.27501

226 -> 231 -0.16916
226 -> 232 0.47942

Excited State 15: Singlet-A 4.0509 eV 306.07 nm f=0.0142 <S**2>=0.000
224 -> 231 0.39065
225 -> 231 0.50404
225 -> 232 -0.10488

Excited State 16: Singlet-A 4.0836 eV 303.61 nm f=0.0717 <S**2>=0.000
223 -> 232 -0.14034
224 -> 232 0.40327
225 -> 231 0.12113
225 -> 232 0.48181

Excited State 17: Singlet-A 4.1426 eV 299.29 nm f=0.0046 <S**2>=0.000
222 -> 231 -0.10706
223 -> 231 0.55790
223 -> 232 0.25004
224 -> 231 0.23035
224 -> 232 0.14649

Excited State 18: Singlet-A 4.1805 eV 296.58 nm f=0.0132 <S**2>=0.000
220 -> 231 0.11795
220 -> 232 -0.16178
222 -> 231 -0.37264
222 -> 232 0.40865
223 -> 231 -0.11506
224 -> 231 0.13320
224 -> 232 -0.17925
225 -> 232 0.10313
227 -> 233 -0.10160

Excited State 19: Singlet-A 4.2263 eV 293.37 nm f=0.0201 <S**2>=0.000
216 -> 232 0.17745
217 -> 232 -0.17410
218 -> 232 0.10007
219 -> 232 0.25194
222 -> 231 0.19726
222 -> 232 -0.10524
227 -> 232 -0.17156
229 -> 233 0.23701
229 -> 234 0.32765

Excited State 20: Singlet-A 4.2427 eV 292.23 nm f=0.0073 <S**2>=0.000
218 -> 231 0.32789
218 -> 232 0.14979
219 -> 231 -0.21012
219 -> 232 -0.13201
220 -> 231 -0.18500
220 -> 232 -0.11310

221 -> 231 0.39643
221 -> 232 0.21201

Excited State 21: Singlet-A 4.2661 eV 290.63 nm f=0.0377 <S**2>=0.000
216 -> 231 0.12864
217 -> 231 -0.13931
219 -> 231 0.27173
221 -> 231 0.11327
221 -> 232 -0.11794
223 -> 231 -0.21735
223 -> 232 0.30395
224 -> 232 0.19700
229 -> 233 -0.19736
229 -> 234 0.25187

Excited State 22: Singlet-A 4.2731 eV 290.15 nm f=0.0085 <S**2>=0.000
217 -> 232 0.10050
219 -> 231 -0.23195
219 -> 232 0.15729
220 -> 231 -0.15965
220 -> 232 0.20706
221 -> 231 -0.21379
221 -> 232 0.27995
222 -> 231 -0.11161
223 -> 231 -0.16043
223 -> 232 0.31708
224 -> 232 0.14690

Excited State 23: Singlet-A 4.2824 eV 289.52 nm f=0.0440 <S**2>=0.000
216 -> 231 -0.13998
217 -> 231 0.18481
219 -> 232 -0.19568
220 -> 231 0.22923
221 -> 232 -0.16124
222 -> 232 -0.11516
223 -> 231 -0.15179
223 -> 232 0.17638
224 -> 232 0.16627
227 -> 233 0.11771
227 -> 234 0.10488
228 -> 233 0.17177
229 -> 233 0.31392

Excited State 24: Singlet-A 4.2935 eV 288.77 nm f=0.0141 <S**2>=0.000
219 -> 232 -0.10789
222 -> 231 0.33589
222 -> 232 0.40077
223 -> 231 0.14419
223 -> 232 0.17168
224 -> 231 -0.20459

227 -> 233 0.12860
228 -> 234 0.15694
229 -> 233 0.11872

Excited State 25: Singlet-A 4.3013 eV 288.25 nm f=0.0028 <S**2>=0.000
219 -> 231 -0.14162
219 -> 232 0.10074
220 -> 232 -0.19631
221 -> 232 -0.16566
222 -> 231 0.17098
223 -> 232 0.32537
227 -> 233 -0.15896
227 -> 234 -0.13812
228 -> 233 -0.17588
228 -> 234 -0.30152
229 -> 234 -0.14217

Excited State 26: Singlet-A 4.3379 eV 285.81 nm f=0.0353 <S**2>=0.000
218 -> 231 -0.20776
220 -> 231 0.29121
221 -> 231 0.20227
221 -> 232 0.24774
222 -> 231 0.15436
227 -> 234 -0.11006
228 -> 233 -0.18335
228 -> 234 0.29084
229 -> 233 -0.15468

Excited State 27: Singlet-A 4.3430 eV 285.48 nm f=0.0144 <S**2>=0.000
218 -> 231 0.11843
219 -> 231 -0.25530
220 -> 231 0.10652
220 -> 232 0.34932
221 -> 231 0.10877
221 -> 232 -0.27276
222 -> 231 0.11965
222 -> 232 0.19031
227 -> 233 -0.19034
227 -> 234 0.11314
228 -> 233 -0.11911
229 -> 234 0.13647

Excited State 28: Singlet-A 4.3580 eV 284.50 nm f=0.0159 <S**2>=0.000
217 -> 232 0.13679
219 -> 231 -0.15526
220 -> 231 -0.12659
220 -> 232 -0.13536
221 -> 231 -0.17004
221 -> 232 -0.32289
222 -> 231 -0.10647

222 -> 232 -0.16789
227 -> 234 -0.22037
228 -> 234 0.36569

Excited State 29: Singlet-A 4.3763 eV 283.31 nm f=0.0042 <S**2>=0.000
218 -> 231 0.30029
219 -> 232 -0.21063
220 -> 231 0.16922
221 -> 231 -0.28431
221 -> 232 0.16713
227 -> 233 -0.19345
227 -> 234 -0.17555
228 -> 233 -0.16516
229 -> 233 0.12609
230 -> 235 0.22709

Excited State 30: Singlet-A 4.3793 eV 283.11 nm f=0.0510 <S**2>=0.000
217 -> 231 -0.18311
218 -> 231 0.11451
218 -> 232 0.18246
219 -> 232 0.10068
220 -> 231 0.17146
222 -> 231 0.15307
227 -> 233 -0.21971
227 -> 234 0.14408
228 -> 233 0.36612
229 -> 233 -0.11963
229 -> 234 -0.26835

1b : **T**-form
HOMO : 230, LUMO : 231
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.1075 eV 588.30 nm f=0.0000 <S**2>=0.000
230 -> 232 0.70415
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2685.70155817
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.1517 eV 576.21 nm f=0.7683 <S**2>=0.000
230 -> 231 0.70903
230 <- 231 -0.10925

Excited State 3: Singlet-A 2.8474 eV 435.43 nm f=0.0034 <S**2>=0.000
229 -> 231 -0.12596
230 -> 233 0.69076

Excited State 4: Singlet-A 2.9363 eV 422.25 nm f=0.0002 <S**2>=0.000
227 -> 231 0.59954
230 -> 234 -0.35256

Excited State 5: Singlet-A 2.9628 eV 418.47 nm f=0.0007 <S**2>=0.000
228 -> 231 -0.22357
229 -> 231 0.65406
230 -> 233 0.10851

Excited State 6: Singlet-A 3.0045 eV 412.66 nm f=0.0006 <S**2>=0.000
224 -> 231 -0.10152
228 -> 231 0.65083
229 -> 231 0.22575

Excited State 7: Singlet-A 3.0147 eV 411.27 nm f=0.1852 <S**2>=0.000
227 -> 231 0.34578
230 -> 234 0.60486

Excited State 8: Singlet-A 3.1644 eV 391.81 nm f=0.0049 <S**2>=0.000
224 -> 234 -0.10660
225 -> 231 -0.11797
227 -> 232 0.67290

Excited State 9: Singlet-A 3.3041 eV 375.24 nm f=0.1914 <S**2>=0.000
224 -> 232 0.11117
228 -> 232 -0.30958
229 -> 232 0.60200

Excited State 10: Singlet-A 3.3278 eV 372.57 nm f=0.1327 <S**2>=0.000
224 -> 232 -0.14196
228 -> 232 0.58838
229 -> 232 0.32939

Excited State 11: Singlet-A 3.3768 eV 367.16 nm f=0.0000 <S**2>=0.000
224 -> 231 0.66890
228 -> 231 0.11786

Excited State 12: Singlet-A 3.4926 eV 354.99 nm f=0.0019 <S**2>=0.000
226 -> 231 0.67359
230 -> 235 -0.19221

Excited State 13: Singlet-A 3.5348 eV 350.75 nm f=0.0527 <S**2>=0.000
225 -> 231 0.67324
227 -> 232 0.11468

Excited State 14: Singlet-A 3.5489 eV 349.36 nm f=0.0549 <S**2>=0.000
221 -> 232 -0.11515
224 -> 232 0.61416
227 -> 234 -0.17871
228 -> 232 0.20796

Excited State 15: Singlet-A 3.6102 eV 343.43 nm f=0.0026 <S**2>=0.000
226 -> 231 0.19201
230 -> 235 0.67642

Excited State 16: Singlet-A 3.7143 eV 333.80 nm f=0.0018 <S**2>=0.000
219 -> 231 -0.22299
221 -> 232 0.13894
223 -> 231 0.63944

Excited State 17: Singlet-A 3.7569 eV 330.02 nm f=0.0002 <S**2>=0.000
219 -> 232 -0.12045
221 -> 231 0.65004
223 -> 232 0.12989

Excited State 18: Singlet-A 3.7802 eV 327.98 nm f=0.0012 <S**2>=0.000
216 -> 231 -0.12809
222 -> 231 0.66044
230 -> 236 -0.16497

Excited State 19: Singlet-A 3.7942 eV 326.77 nm f=0.0678 <S**2>=0.000
215 -> 231 0.11677
217 -> 231 -0.16614
225 -> 232 0.61824
230 -> 237 -0.15450
230 -> 241 0.11551

Excited State 20: Singlet-A 3.8275 eV 323.93 nm f=0.0000 <S**2>=0.000
218 -> 231 0.10869
226 -> 232 0.65410
230 -> 240 -0.13374

Excited State 21: Singlet-A 3.8389 eV 322.97 nm f=0.0197 <S**2>=0.000
217 -> 231 0.29195
220 -> 231 0.37922
225 -> 232 0.14456
230 -> 236 -0.12039
230 -> 237 0.43506

Excited State 22: Singlet-A 3.8720 eV 320.21 nm f=0.0006 <S**2>=0.000
216 -> 231 0.28460
222 -> 231 0.22329
230 -> 236 0.55881
230 -> 237 0.15353

Excited State 23: Singlet-A 3.8793 eV 319.60 nm f=0.0128 <S**2>=0.000
219 -> 231 0.61385
221 -> 232 -0.12759
223 -> 231 0.25609

Excited State 24: Singlet-A 3.8971 eV 318.15 nm f=0.0632 <S**2>=0.000
217 -> 231 -0.23314
219 -> 231 0.11293
220 -> 231 0.55730
225 -> 232 -0.18972
230 -> 237 -0.22589

Excited State 25: Singlet-A 3.9636 eV 312.80 nm f=0.0005 <S**2>=0.000
218 -> 231 0.59786
221 -> 231 -0.11173
223 -> 232 -0.10272
230 -> 240 0.25232
230 -> 242 -0.13523

Excited State 26: Singlet-A 3.9849 eV 311.13 nm f=0.0065 <S**2>=0.000
212 -> 231 -0.10944
214 -> 231 0.11965
215 -> 231 -0.15824
217 -> 231 0.47502
220 -> 231 0.10382
230 -> 236 0.11158
230 -> 237 -0.40347
230 -> 241 -0.10761

Excited State 27: Singlet-A 4.0112 eV 309.10 nm f=0.0074 <S**2>=0.000
212 -> 231 0.16110
215 -> 231 0.40848
217 -> 231 0.22637
222 -> 232 -0.13028
225 -> 232 -0.13206
228 -> 233 -0.10305
230 -> 237 -0.10412

230 -> 239 0.14478
230 -> 241 0.38283

Excited State 28: Singlet-A 4.0371 eV 307.11 nm f=0.0098 <S**2>=0.000
216 -> 231 0.43783
217 -> 232 0.11909
223 -> 232 -0.26987
227 -> 233 0.10402
230 -> 236 -0.29352
230 -> 238 -0.24575
230 -> 242 0.15023

Excited State 29: Singlet-A 4.0428 eV 306.68 nm f=0.0064 <S**2>=0.000
216 -> 231 0.19744
221 -> 231 -0.12706
223 -> 232 0.54019
226 -> 232 0.11431
227 -> 233 -0.11615
230 -> 236 -0.12776
230 -> 238 -0.19399
230 -> 240 0.20188

Excited State 30: Singlet-A 4.0700 eV 304.63 nm f=0.0079 <S**2>=0.000
216 -> 231 0.33868
223 -> 232 0.11355
230 -> 238 0.53674
230 -> 242 -0.13654

1b : **P**-form
HOMO : 230, LUMO : 231
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.5598 eV 484.35 nm f=0.0902 <S**2>=0.000
230 -> 231 0.37970
230 -> 232 0.59104
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2685.67064611
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.6849 eV 461.79 nm f=0.6327 <S**2>=0.000
230 -> 231 0.58842
230 -> 232 -0.37852

Excited State 3: Singlet-A 3.0814 eV 402.37 nm f=0.0068 <S**2>=0.000
229 -> 231 -0.30027
230 -> 233 0.63434

Excited State 4: Singlet-A 3.1497 eV 393.63 nm f=0.0690 <S**2>=0.000
229 -> 231 0.63540
230 -> 233 0.29930

Excited State 5: Singlet-A 3.2710 eV 379.04 nm f=0.0141 <S**2>=0.000
227 -> 231 0.32907
228 -> 231 0.57538
230 -> 234 -0.18347

Excited State 6: Singlet-A 3.2947 eV 376.31 nm f=0.0399 <S**2>=0.000
227 -> 231 -0.39346
228 -> 231 0.35995
229 -> 232 -0.11419
230 -> 234 0.41291

Excited State 7: Singlet-A 3.3337 eV 371.91 nm f=0.1039 <S**2>=0.000
227 -> 231 0.41760
230 -> 234 0.52608

Excited State 8: Singlet-A 3.3451 eV 370.64 nm f=0.3237 <S**2>=0.000
227 -> 231 -0.13688
229 -> 232 0.67247

Excited State 9: Singlet-A 3.4238 eV 362.13 nm f=0.0077 <S**2>=0.000
227 -> 232 0.58959
228 -> 232 0.29114

Excited State 10: Singlet-A 3.4720 eV 357.10 nm f=0.0128 <S**2>=0.000
227 -> 232 -0.28860
228 -> 232 0.59909

Excited State 11: Singlet-A 3.6824 eV 336.69 nm f=0.0049 <S**2>=0.000
224 -> 231 -0.11263
225 -> 231 0.28666
226 -> 231 0.58722
230 -> 235 -0.13514

Excited State 12: Singlet-A 3.7076 eV 334.40 nm f=0.0153 <S**2>=0.000
224 -> 231 -0.18821
225 -> 231 0.49964
225 -> 232 0.11341
226 -> 231 -0.33567
227 -> 233 -0.10934

Excited State 13: Singlet-A 3.7887 eV 327.25 nm f=0.0195 <S**2>=0.000
220 -> 232 0.12699
221 -> 232 0.10484
224 -> 232 0.18520
225 -> 231 0.15752
225 -> 232 -0.27905
226 -> 232 -0.12806
227 -> 234 -0.12198
228 -> 232 0.12925
229 -> 233 -0.11443
230 -> 235 0.48989

Excited State 14: Singlet-A 3.8226 eV 324.35 nm f=0.0734 <S**2>=0.000
220 -> 232 -0.14110
224 -> 232 -0.22919
225 -> 232 0.28687
226 -> 231 0.11747
226 -> 232 0.20720
227 -> 234 0.12844
230 -> 235 0.45295

Excited State 15: Singlet-A 3.8355 eV 323.26 nm f=0.0043 <S**2>=0.000
220 -> 231 0.11368
221 -> 231 0.13023
223 -> 231 -0.12582
224 -> 231 0.51094
225 -> 231 0.30054
226 -> 232 0.13499
227 -> 233 0.14412
230 -> 235 -0.13274

Excited State 16: Singlet-A 3.9238 eV 315.98 nm f=0.0035 <S**2>=0.000
224 -> 231 -0.19638
224 -> 232 0.11683
225 -> 232 -0.15891
226 -> 232 0.60280

Excited State 17: Singlet-A 3.9541 eV 313.56 nm f=0.0125 <S**2>=0.000
220 -> 231 -0.18908
222 -> 231 0.38830
223 -> 231 -0.33560
224 -> 232 0.24844
225 -> 232 0.25398
229 -> 233 -0.13992

Excited State 18: Singlet-A 3.9771 eV 311.75 nm f=0.1297 <S**2>=0.000
220 -> 231 -0.10805
222 -> 231 0.17000
225 -> 232 -0.10299
229 -> 233 0.63141

Excited State 19: Singlet-A 3.9942 eV 310.41 nm f=0.0129 <S**2>=0.000
220 -> 231 0.25907
220 -> 232 0.11383
221 -> 231 0.17428
222 -> 231 -0.29749
222 -> 232 -0.15056
224 -> 231 -0.12844
224 -> 232 0.24504
225 -> 232 0.33451
229 -> 233 0.16906

Excited State 20: Singlet-A 4.0130 eV 308.95 nm f=0.0447 <S**2>=0.000
220 -> 231 -0.11263
220 -> 232 0.16921
221 -> 231 -0.17334
221 -> 232 0.16015
223 -> 231 0.44405
223 -> 232 -0.15890
224 -> 231 0.22008
224 -> 232 0.10221
225 -> 232 0.23667
227 -> 233 -0.10762

Excited State 21: Singlet-A 4.0760 eV 304.18 nm f=0.0987 <S**2>=0.000
217 -> 231 -0.10278
220 -> 231 0.14257
221 -> 231 0.22391
222 -> 231 0.31700
223 -> 231 0.29200
224 -> 231 -0.10921
227 -> 233 0.25631
228 -> 233 0.24233
229 -> 234 0.16166

Excited State 22: Singlet-A 4.0891 eV 303.20 nm f=0.1392 <S**2>=0.000
217 -> 231 -0.13333

219 -> 231 0.23498
221 -> 231 -0.31289
223 -> 231 -0.12816
228 -> 233 0.47458
230 -> 237 0.11254

Excited State 23: Singlet-A 4.1012 eV 302.32 nm f=0.2866 <S**2>=0.000
217 -> 231 0.30958
219 -> 231 -0.27060
220 -> 231 -0.16753
221 -> 231 0.21118
222 -> 231 -0.12782
228 -> 233 0.38788

Excited State 24: Singlet-A 4.1169 eV 301.16 nm f=0.0489 <S**2>=0.000
216 -> 231 0.10130
217 -> 231 0.15513
220 -> 231 -0.31638
222 -> 231 -0.11473
227 -> 233 0.40441
228 -> 233 -0.14691
229 -> 234 0.29545

Excited State 25: Singlet-A 4.1554 eV 298.37 nm f=0.0037 <S**2>=0.000
217 -> 231 0.19397
218 -> 231 -0.13903
219 -> 231 0.43118
219 -> 232 -0.14478
220 -> 231 -0.15577
221 -> 231 0.15177
223 -> 231 0.14770
223 -> 232 0.29443
224 -> 232 0.10543

Excited State 26: Singlet-A 4.1729 eV 297.12 nm f=0.0095 <S**2>=0.000
217 -> 231 -0.23322
218 -> 231 0.12595
220 -> 231 -0.12905
221 -> 231 0.12163
221 -> 232 -0.10176
222 -> 231 -0.13831
227 -> 233 -0.33667
229 -> 234 0.42702

Excited State 27: Singlet-A 4.1991 eV 295.26 nm f=0.0099 <S**2>=0.000
216 -> 231 0.15886
217 -> 231 0.29720
220 -> 231 0.32275
221 -> 231 -0.23035
222 -> 231 0.18578

227 -> 233 -0.15052
229 -> 234 0.27271
230 -> 236 0.11805

Excited State 28: Singlet-A 4.2044 eV 294.89 nm f=0.0025 <S**2>=0.000
215 -> 231 -0.10593
219 -> 231 -0.25927
220 -> 232 -0.11767
221 -> 231 -0.25662
221 -> 232 -0.16993
222 -> 232 -0.10212
223 -> 232 0.42884
224 -> 231 0.14684
224 -> 232 0.22315

Excited State 29: Singlet-A 4.2432 eV 292.20 nm f=0.0743 <S**2>=0.000
215 -> 231 -0.26393
217 -> 231 0.16089
218 -> 231 0.50510
230 -> 236 -0.24168
230 -> 237 0.10899

Excited State 30: Singlet-A 4.2586 eV 291.14 nm f=0.0179 <S**2>=0.000
212 -> 231 -0.10083
215 -> 231 -0.29223
216 -> 231 -0.16345
220 -> 232 -0.11272
222 -> 232 0.24107
223 -> 232 -0.24121
224 -> 232 0.21649
229 -> 234 0.10332
230 -> 236 0.34847

1b : **TF**-form
HOMO : 230, LUMO : 231
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.3481 eV 528.02 nm f=0.2742 <S**2>=0.000
230 -> 231 0.62839
230 -> 232 0.31989
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2685.68892804
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.6013 eV 476.62 nm f=0.4511 <S**2>=0.000
230 -> 231 -0.31864
230 -> 232 0.62343

Excited State 3: Singlet-A 3.0632 eV 404.75 nm f=0.0022 <S**2>=0.000
227 -> 231 0.52112
229 -> 231 0.40769
230 -> 233 -0.16619

Excited State 4: Singlet-A 3.0917 eV 401.02 nm f=0.0021 <S**2>=0.000
227 -> 231 0.37137
229 -> 231 -0.32524
230 -> 233 0.48587

Excited State 5: Singlet-A 3.1214 eV 397.21 nm f=0.0140 <S**2>=0.000
224 -> 231 0.12407
227 -> 231 -0.12048
228 -> 231 0.64008
229 -> 231 0.14364
230 -> 233 0.12474

Excited State 6: Singlet-A 3.1426 eV 394.53 nm f=0.1281 <S**2>=0.000
227 -> 231 -0.17564
228 -> 231 -0.21217
229 -> 231 0.44721
230 -> 233 0.45921

Excited State 7: Singlet-A 3.2421 eV 382.42 nm f=0.1157 <S**2>=0.000
230 -> 234 0.68799

Excited State 8: Singlet-A 3.3425 eV 370.94 nm f=0.0274 <S**2>=0.000
227 -> 232 0.65991

Excited State 9: Singlet-A 3.4058 eV 364.04 nm f=0.0192 <S**2>=0.000
224 -> 232 0.12037
225 -> 231 -0.11142
227 -> 234 -0.11615
228 -> 232 0.57957
229 -> 232 0.26658

Excited State 10: Singlet-A 3.4674 eV 357.57 nm f=0.1837 <S**2>=0.000
224 -> 231 -0.18856
225 -> 231 0.12891
226 -> 231 -0.22799
228 -> 232 -0.13316
229 -> 232 0.57347

Excited State 11: Singlet-A 3.4782 eV 356.46 nm f=0.0624 <S**2>=0.000
224 -> 231 0.28606
225 -> 231 -0.26812
226 -> 231 0.36559
228 -> 231 -0.12537
228 -> 232 -0.28382
229 -> 232 0.27195

Excited State 12: Singlet-A 3.6069 eV 343.74 nm f=0.0023 <S**2>=0.000
224 -> 231 -0.20186
225 -> 231 0.38542
226 -> 231 0.52064

Excited State 13: Singlet-A 3.6475 eV 339.92 nm f=0.0586 <S**2>=0.000
224 -> 231 0.46064
225 -> 231 0.45654
226 -> 231 -0.12733

Excited State 14: Singlet-A 3.7492 eV 330.70 nm f=0.0477 <S**2>=0.000
220 -> 232 0.10882
222 -> 232 -0.13747
224 -> 232 0.41596
225 -> 232 -0.24866
226 -> 232 0.31522
227 -> 234 -0.19096
228 -> 232 -0.20621

Excited State 15: Singlet-A 3.8319 eV 323.56 nm f=0.0052 <S**2>=0.000
218 -> 231 -0.13542
220 -> 231 -0.23088
221 -> 231 0.12165
222 -> 231 0.21940
230 -> 235 0.57944

Excited State 16: Singlet-A 3.8410 eV 322.80 nm f=0.0011 <S**2>=0.000
218 -> 231 0.25207
219 -> 231 -0.14352
220 -> 231 0.34980
221 -> 231 -0.15747
222 -> 231 -0.25502
223 -> 231 0.22152
230 -> 235 0.34039

Excited State 17: Singlet-A 3.8661 eV 320.70 nm f=0.0072 <S**2>=0.000
222 -> 231 0.15014
223 -> 231 0.60341
223 -> 232 -0.12086
224 -> 231 0.19340
230 -> 235 -0.15937

Excited State 18: Singlet-A 3.9096 eV 317.13 nm f=0.0051 <S**2>=0.000
215 -> 231 0.12057
219 -> 231 -0.16084
220 -> 231 0.13712
221 -> 231 -0.38931
222 -> 231 0.46075
223 -> 231 -0.12419
224 -> 231 0.12507

Excited State 19: Singlet-A 3.9363 eV 314.97 nm f=0.0232 <S**2>=0.000
219 -> 231 0.18242
220 -> 231 0.18296
221 -> 231 0.19478
222 -> 232 -0.10561
224 -> 232 0.32739
225 -> 232 0.31618
226 -> 232 -0.32198

Excited State 20: Singlet-A 3.9530 eV 313.64 nm f=0.0332 <S**2>=0.000
215 -> 231 -0.14916
216 -> 231 -0.19360
217 -> 231 -0.13246
218 -> 231 0.30560
220 -> 231 0.20640
221 -> 231 0.36118
222 -> 231 0.23413
224 -> 232 -0.14916
225 -> 232 -0.14781
226 -> 232 0.10285

Excited State 21: Singlet-A 3.9726 eV 312.10 nm f=0.0090 <S**2>=0.000
225 -> 232 0.47133
226 -> 232 0.43897
227 -> 233 -0.10089
229 -> 234 -0.10168
230 -> 237 0.11002

Excited State 22: Singlet-A 3.9838 eV 311.22 nm f=0.0127 <S**2>=0.000
215 -> 231 0.24676
216 -> 231 0.17830
217 -> 231 0.29612
218 -> 231 -0.21682

219 -> 231 0.11866
220 -> 231 0.29637
221 -> 231 0.21418
222 -> 231 0.11045
224 -> 232 -0.12507
226 -> 232 0.14782
230 -> 236 0.14767

Excited State 23: Singlet-A 4.0202 eV 308.40 nm f=0.0211 <S**2>=0.000
215 -> 231 -0.21997
216 -> 231 -0.10184
217 -> 231 -0.13298
218 -> 231 -0.21725
219 -> 231 0.40991
220 -> 231 0.22515
221 -> 231 -0.25881
226 -> 232 0.10822
230 -> 236 -0.17808

Excited State 24: Singlet-A 4.0365 eV 307.16 nm f=0.0514 <S**2>=0.000
215 -> 231 0.24251
218 -> 231 0.36786
219 -> 231 0.42586
220 -> 231 -0.17336
230 -> 236 0.16563

Excited State 25: Singlet-A 4.0537 eV 305.85 nm f=0.0258 <S**2>=0.000
212 -> 231 -0.15237
215 -> 231 -0.28888
216 -> 231 0.31175
217 -> 231 0.28563
218 -> 231 0.18345
227 -> 233 -0.10410
229 -> 233 -0.14044
230 -> 236 -0.20327
230 -> 237 -0.11879

Excited State 26: Singlet-A 4.0905 eV 303.10 nm f=0.0203 <S**2>=0.000
216 -> 231 0.12120
219 -> 231 0.10163
222 -> 231 0.11206
227 -> 233 0.59327

Excited State 27: Singlet-A 4.1239 eV 300.65 nm f=0.0013 <S**2>=0.000
216 -> 231 0.19903
222 -> 232 0.16096
223 -> 231 0.10697
223 -> 232 0.56621
224 -> 232 0.19084

Excited State 28: Singlet-A 4.1326 eV 300.02 nm f=0.0127 <S**2>=0.000
215 -> 231 -0.14066
216 -> 231 -0.32426
217 -> 231 0.42444
220 -> 232 -0.11797
223 -> 232 0.14315
227 -> 233 0.14513
229 -> 233 0.16752
230 -> 237 -0.17032
230 -> 239 0.12854

Excited State 29: Singlet-A 4.1548 eV 298.41 nm f=0.3065 <S**2>=0.000
212 -> 231 -0.11134
227 -> 233 0.11015
228 -> 233 0.51483
228 -> 234 -0.13950
229 -> 233 0.30672

Excited State 30: Singlet-A 4.1852 eV 296.25 nm f=0.0310 <S**2>=0.000
215 -> 231 -0.27876
217 -> 231 -0.11284
222 -> 232 -0.10754
229 -> 233 -0.20065
230 -> 236 0.49343
230 -> 237 -0.23983

Optimised Coordinates

1a (Ar = C_6H_5) : **F**-form								
SCF Done: E(RB3LYP) = -2529.47502619 A.U. after 6 cycles								
Atom	X	Y	Z		Atom	X	Y	Z
C	-0.0024496	-1.4254025	0.2982725		C	-2.8196033	4.6746069	2.5423744
C	1.2232597	-0.688941	-0.1121038		C	-3.5033569	3.7514287	3.3361495
N	2.3074478	-1.3828897	-0.4569927		C	-3.0606723	2.428592	3.3903181
C	3.387739	-0.7371043	-0.9192072		C	-1.9526198	2.0293821	2.6452144
C	3.3292173	0.6654524	-1.1380531		C	1.1454482	3.4115371	1.3712895
N	2.2621941	1.3706679	-0.7248586		C	1.7730796	4.1456012	0.3539042
C	1.2224946	0.728282	-0.1881631		C	2.7936157	5.0489018	0.6579137
C	0.0024376	1.4254005	0.2982778		C	3.221661	5.2123273	1.9761672
C	-1.2232728	0.6889399	-0.1120976		C	2.6095631	4.4800711	2.9966361
N	-2.3074641	1.3828887	-0.4569755		C	1.5677967	3.6046914	2.6983692
C	-3.3877611	0.7371065	-0.9191818		C	4.5848586	-1.591448	-1.1512668
C	-3.3292373	-0.6654508	-1.1380403		C	4.3601125	1.4397979	-1.8842427
N	-2.2622112	-1.3706658	-0.7248519		C	-4.5848842	1.5914613	-1.1511914
C	-1.2225089	-0.7282822	-0.1881595		C	-4.3601073	-1.4398018	-1.8842608
C	0.0325433	-2.5379577	1.0888418		H	1.1658566	-5.0045874	1.2055909
C	1.2638446	-2.9451085	1.8327965		H	3.1540983	-5.7077593	2.497133
C	1.7020058	-4.2790157	1.8103535		H	3.5761983	-1.7055595	4.0170596
C	2.8196014	-4.6746232	2.5423343		H	1.6084549	-1.0002465	2.6962122
C	3.5033635	-3.7514494	3.3361072		H	-1.4548324	-4.0077815	-0.6726835
C	3.0606827	-2.4286117	3.3902835		H	-3.2558822	-5.622352	-0.1414636
C	1.9526251	-2.0293966	2.6451903		H	-2.9334932	-4.6024706	4.0268266
C	-1.1454573	-3.4115398	1.3712832		H	-1.0711078	-3.0619255	3.4979264
C	-1.7731018	-4.1455915	0.3538968		H	-1.1658695	5.0045798	1.2056193
C	-2.7936393	-5.0488902	0.6579075		H	-3.154103	5.7077423	2.4971797
C	-3.2216727	-5.2123261	1.9761635		H	-3.5761805	1.7055365	4.0170965
C	-2.609562	-4.480082	2.9966334		H	-1.6084459	1.000233	2.696231
C	-1.5677948	-3.6047039	2.698365		H	1.4548013	4.0077994	-0.6726743
C	-0.032552	2.5379532	1.0888517		H	3.2558487	5.6223728	-0.1414565
C	-1.2638485	2.9450983	1.8328176		H	2.9335034	4.6024517	4.0268274
C	-1.7020125	4.2790047	1.8103833		H	1.0711196	3.0619033	3.4979303

Atom	X	Y	Z		Atom	X	Y	Z
C	-4.4114234	2.904183	-1.6189807		C	6.2309145	2.9661583	-3.3228948
C	-5.8828872	1.1505683	-0.8470822		H	4.3815333	3.0561179	-0.4658154
C	-6.9775884	1.9952936	-1.0226467		H	6.0542688	4.3949649	-1.7166331
C	-5.5082429	3.7427295	-1.8057837		H	4.540232	0.0207114	-3.5005764
C	-6.7961404	3.2911876	-1.5097104		H	6.1783675	1.3656061	-4.7690193
H	-6.0357383	0.1482461	-0.4608722		H	6.9560564	3.5551662	-3.8783088
H	-7.9742089	1.6402438	-0.7740894		H	4.3695102	-4.0624443	3.9140324
H	-3.4062251	3.2562211	-1.8255883		H	-4.0209735	-5.9110475	2.2091346
H	-5.3567008	4.7522524	-2.1789933		H	-4.3694995	4.0624196	3.9140829
H	-7.6517079	3.946284	-1.6516772		H	4.0209606	5.9110504	2.2091372
C	-4.8734278	-0.9755702	-3.1057848					
C	-4.7881219	-2.6851719	-1.4004575					
C	-5.7233402	-3.4372757	-2.1104674					
C	-5.7978163	-1.7352859	-3.8205938					
C	-6.2308394	-2.966195	-3.3229711					
H	-4.3816233	-3.0560752	-0.4657824					
H	-6.0543029	-4.3949467	-1.7166488					
H	-4.5401041	-0.0207802	-3.5006661					
H	-6.1781812	-1.3656997	-4.7691546					
H	-6.9559548	-3.555215	-3.878407					
C	4.4113943	-2.9041893	-1.6189995					
C	5.8828738	-1.1505052	-0.8472852					
C	6.9775834	-1.9952085	-1.0229035					
C	5.508221	-3.7427147	-1.8058544					
C	6.79613	-3.2911279	-1.509898					
H	6.0357281	-0.1481588	-0.4611377					
H	7.9742149	-1.640121	-0.7744442					
H	3.4061892	-3.2562603	-1.8255183					
H	5.3566763	-4.7522554	-2.1790146					
H	7.6517035	-3.9462071	-1.6519072					
C	4.8735161	0.9755239	-3.1057149					
C	4.7880892	2.685187	-1.4004545					
C	5.7233393	3.4372766	-2.1104373					
C	5.7979385	1.7352243	-3.8204966					

1a (Ar = C_6H_5) : **T**-form								
SCF Done: E(RB3LYP) = -2529.48005336 A.U. after 9 cycles								
Atom	X	Y	Z		Atom	X	Y	Z
N	-2.3934712	1.2973596	-0.4062428		H	-1.391281	2.5120541	2.287945
N	-2.3933743	-1.2975036	0.4062956		H	-3.1952588	3.9199457	3.2259431
C	-0.0000505	1.5053067	-0.0000256		H	-2.9409084	6.514283	-0.198091
C	-1.2320105	0.7085687	-0.0829926		H	-1.1328702	5.1080935	-1.1259819
C	-3.5458746	0.6413493	-0.3209939		H	1.391056	2.5121157	-2.2880472
C	-3.5458191	-0.6415547	0.3211209		H	3.1948479	3.9201757	-3.2261488
C	-1.2319646	-0.7086522	0.0829695		H	2.9402861	6.5146242	0.1977853
C	-0.0001079	2.893464	-0.0000425		H	1.1324358	5.1082631	1.1257811
C	-1.145757	3.6918047	0.5006644		H	-5.6556898	-0.5875911	-1.5504956
C	-1.7439791	3.3786651	1.7365801		H	-7.563577	0.4869207	-2.6878028
C	-2.7558981	4.1754205	2.2652108		H	-7.7428258	2.9682739	-2.7584505
C	-3.1959619	5.3064173	1.5718547		H	-5.9741789	4.3600014	-1.6942653
C	-2.6077706	5.635564	0.3482187		H	-4.0494716	3.2747141	-0.5696732
C	-1.5872079	4.8439782	-0.176105		H	-4.0492676	-3.2749427	0.5698681
C	1.1454484	3.6919045	-0.5008034		H	-5.9738401	-4.3603123	1.6946108
C	1.7436719	3.3787868	-1.7367244		H	-7.74248	-2.9686602	2.7589062
C	2.7554845	4.1756377	-2.2654141		H	-7.5633592	-0.4872985	2.6882157
C	3.1954356	5.306714	-1.5721159		H	-5.6556075	0.5872938	1.5507589
C	2.6072378	5.6358427	-0.3484786		N	2.3934653	-1.2973559	-0.4062691
C	1.5867816	4.8441589	0.175905		N	2.3933718	1.2975016	0.4062916
C	-4.7275948	1.2717534	-0.9605569		C	0.0000475	-1.5053104	-0.0000367
C	-5.7275545	0.4951774	-1.5706688		C	1.2320075	-0.708571	-0.0829976
C	-6.8032676	1.1029229	-2.2148904		C	3.545867	-0.641342	-0.3210298
C	-6.9011899	2.4954033	-2.2590272		C	3.5458161	0.6415548	0.3211003
C	-5.9081806	3.2754777	-1.6623674		C	1.2319612	0.7086488	0.0829725
C	-4.8266926	2.6715529	-1.0243527		C	0.0001069	-2.8934683	-0.0000682
C	-4.7274625	-1.2720114	0.9607754		C	1.1457481	-3.6918127	0.5006516
C	-4.8264861	-2.6718149	1.0245954		C	1.743933	-3.3786998	1.7365922
C	-5.9078983	-3.2757858	1.6626951		C	2.7558404	-4.1754628	2.2652333
C	-6.9009037	-2.4957538	2.2594166		C	3.1959305	-5.3064406	1.5718626
C	-6.8030535	-1.1032691	2.2152562		C	2.6077769	-5.6355605	0.3482015
C	-5.7274169	-0.495478	1.5709499		C	1.5872249	-4.8439677	-0.1761326

Atom	X	Y	Z		Atom	X	Y	Z
C	-1.145435	-3.6919078	-0.5008648		H	7.5633861	0.4872958	2.6881447
C	-1.7436196	-3.3787907	-1.7368047		H	5.6556231	-0.5872954	1.5507058
C	-2.755412	-4.1756444	-2.2655286		H	-3.9831188	-5.9302922	-1.9865579
C	-3.1953817	-5.3067234	-1.5722465		H	3.9837586	-5.929938	1.9861084
C	-2.6072223	-5.6358518	-0.3485906		H	-3.9837986	5.929909	1.9860928
C	-1.5867858	-4.8441654	0.1758272		H	3.9831885	5.9302805	-1.986401
C	4.7275816	-1.2717374	-0.9606121					
C	5.7275337	-0.4951534	-1.5707262					
C	6.8032404	-1.1028905	-2.2149663					
C	6.9011641	-2.4953702	-2.2591197					
C	5.9081622	-3.2754525	-1.662458					
C	4.8266804	-2.6715361	-1.0244247					
C	4.7274658	1.2720105	0.9607438					
C	4.8264866	2.671814	1.0245698					
C	5.9079052	3.2757843	1.6626593					
C	6.90092	2.4957517	2.2593644					
C	6.8030729	1.103267	2.2151978					
C	5.7274299	0.4954764	1.5709016					
H	1.3912134	-2.5121046	2.2879681					
H	3.1951718	-3.9200091	3.2259847					
H	2.9409353	-6.5142645	-0.1981199					
H	1.1329161	-5.108063	-1.1260289					
H	-1.3909877	-2.5121186	-2.2881158					
H	-3.1947447	-3.9201829	-3.2262775					
H	-2.9402848	-6.5146355	0.1976609					
H	-1.1324689	-5.1082701	1.125717					
H	5.6556678	0.5876147	-1.5505404					
H	7.5635438	-0.4868818	-2.6878802					
H	7.7427949	-2.9682343	-2.7585576					
H	5.9741613	-4.3599758	-1.6943688					
H	4.0494647	-3.2747033	-0.569744					
H	4.0492609	3.2749422	0.5698551					
H	5.9738446	4.3603109	1.6945799					
H	7.7425013	2.9686576	2.7588461					

1b (Ar = $CH_3C_6H_4$) : **F**-form								
SCF Done: E(RB3LYP) = -2686.74801835 A.U. after 16 cycles								
Atom	X	Y	Z		Atom	X	Y	Z
C	0.071705	1.4221985	0.0673987		C	2.9429998	-2.5242057	3.1686989
C	-1.187896	0.7475001	-0.3458013		C	1.8548004	-2.0849042	2.4189989
N	-2.2375951	1.4927016	-0.6893014		C	-1.3066016	-3.3442	1.1554988
C	-3.345396	0.9003031	-1.1585014		C	-1.9887025	-4.0338991	0.1436987
C	-3.3493979	-0.500797	-1.3908014		C	-3.0475038	-4.8888978	0.4547987
N	-2.3189988	-1.2579985	-0.9753014		C	-3.481004	-5.0631972	1.7739988
C	-1.2545979	-0.6687999	-0.4267013		C	-2.7999031	-4.3678981	2.7842989
C	-0.0716989	-1.4222015	0.0673987		C	-1.7220019	-3.5416995	2.4846989
C	1.1879021	-0.7475032	-0.3458013		C	-4.5031948	1.8098047	-1.3809014
N	2.2376012	-1.4927046	-0.6893014		C	-4.4065989	-1.2196957	-2.1553015
C	3.3454021	-0.9003061	-1.1585014		C	4.5032009	-1.8098077	-1.3809014
C	3.349404	0.500794	-1.3908014		C	4.406605	1.2196926	-2.1553015
N	2.3190049	1.2579954	-0.9753014		H	-0.9262902	5.0450001	1.0476988
C	1.254604	0.6687968	-0.4267013		H	-2.8750893	5.8107028	2.3457989
C	0.0910065	2.5274985	0.8706988		H	-3.4890948	1.8118033	3.783399
C	-1.118493	2.9770002	1.6234988		H	-1.5617957	1.0394007	2.4583989
C	-1.4963912	4.3289008	1.6324988		H	1.6809084	3.9061965	-0.8872014
C	-2.5951907	4.7596023	2.3703989		H	3.5444106	5.4303941	-0.3474013
C	-3.342592	3.8665033	3.1498989		H	3.1084093	4.4898946	3.820499
C	-2.9429938	2.5242026	3.1686989		H	1.1884072	3.0410971	3.2880989
C	-1.8547943	2.0849011	2.4189989		H	0.9262963	-5.0450031	1.0476988
C	1.3065076	3.344197	1.1554988		H	2.8750954	-5.8107058	2.3457989
C	1.9887086	4.0338961	0.1437987		H	3.4890008	-1.8118064	3.783399
C	3.0475099	4.8889947	0.4548987		H	1.5618018	-1.0394037	2.4583989
C	3.4810101	5.0631941	1.7739988		H	-1.6809023	-3.9061995	-0.8872014
C	2.7999091	4.367895	2.7842989		H	-3.5444045	-5.4303971	-0.3475013
C	1.7220079	3.5416964	2.4846989		H	-3.1084032	-4.4898977	3.820499
C	-0.0910004	-2.5275016	0.8706988		H	-1.1884011	-3.0411001	3.2880989
C	1.1184991	-2.9770032	1.6234988		C	4.2716991	-3.1204075	-1.8291014
C	1.4963973	-4.3289039	1.6324988		C	5.8201015	-1.4220095	-1.0853014
C	2.5951968	-4.7596054	2.3703989		C	6.8766004	-2.316011	-1.2507014
C	3.3424981	-3.8666063	3.1498989		C	5.330498	-4.008809	-2.0053014

Atom	X	Y	Z		Atom	X	Y	Z
C	6.6376986	-3.6098107	-1.7184014		H	-6.2074988	-1.0205932	-5.0454017
H	6.0173029	-0.4218097	-0.7140014		H	-7.0730018	-3.1953922	-4.2003016
H	7.8884009	-2.0011123	-1.0096014		C	-4.5488914	4.3333049	3.929599
H	3.2515986	-3.4310062	-2.0285015		C	4.6504114	5.9610926	2.1035988
H	5.1339966	-5.0161088	-2.3634015		C	4.5487975	-4.333308	3.929599
H	7.4634978	-4.3036119	-1.8527014		C	-4.6504053	-5.9610957	2.1034988
C	4.8962044	0.7131919	-3.3699015		H	-5.5649046	-5.3775944	2.2753989
C	4.8844067	2.4569921	-1.6978014		H	-4.8585063	-6.6630954	1.2894988
C	5.8445077	3.1588908	-2.4257015		H	-4.4659061	-6.5432959	3.0134989
C	5.8462054	1.4226907	-4.1025016		H	4.4337961	-5.3694079	4.266599
C	6.3285071	2.6453901	-3.6306016		H	5.4579976	-4.2913092	3.3147989
H	4.4955072	2.8611926	-0.7694014		H	4.7242984	-3.7075082	4.811299
H	6.213209	4.1108904	-2.0522015		H	5.5649107	5.3775913	2.2754989
H	4.5241031	-0.2349076	-3.7455016		H	4.8585124	6.6630924	1.2894988
H	6.2075049	1.0205902	-5.0453017		H	4.4658122	6.5433929	3.0134989
H	7.0731079	3.1953892	-4.2002016		H	-4.43389	5.3694049	4.266599
C	-4.2716931	3.1204045	-1.8292014		H	-5.4580916	4.2913062	3.3146989
C	-5.8200954	1.4220064	-1.0853014		H	-4.7243923	3.7075051	4.811199
C	-6.8765943	2.3161079	-1.2507014					
C	-5.3304919	4.008806	-2.0053014					
C	-6.6376925	3.6098077	-1.7184014					
H	-6.0172968	0.4218066	-0.7140014					
H	-7.8883948	2.0011093	-1.0095014					
H	-3.2514926	3.4310031	-2.0285015					
H	-5.1339906	5.0161058	-2.3634015					
H	-7.4634917	4.3036089	-1.8527014					
C	-4.8961983	-0.713195	-3.3699015					
C	-4.8844006	-2.4569951	-1.6978014					
C	-5.8445016	-3.1588939	-2.4258015					
C	-5.8460993	-1.4226937	-4.1026016					
C	-6.328501	-2.6453932	-3.6307016					
H	-4.4955011	-2.8611957	-0.7695014					
H	-6.213203	-4.1108934	-2.0522015					
H	-4.523997	0.2349046	-3.7455016					

1b (Ar = $CH_3C_6H_4$) : **T**-form								
SCF Done: E(RB3LYP) = -2686.75352282 A.U. after 7 cycles								
Atom	X	Y	Z		Atom	X	Y	Z
N	-2.3925554	1.295833	-0.4098178		H	-1.4014985	2.4941796	2.2840075
N	-2.3925524	-1.2956354	0.4104654		H	-3.2037362	3.883251	3.2253987
C	0.0000757	1.50537	0.0000438		H	-2.9367678	6.5190099	-0.1554992
C	-1.231043	0.7090561	-0.084027		H	-1.1276036	5.1356566	-1.0917505
C	-3.5454444	0.6405357	-0.3223058		H	1.4019713	2.4925525	-2.284342
C	-3.5454216	-0.6402805	0.3231722		H	3.2049009	3.8804307	-3.2262411
C	-1.2310729	-0.7089174	0.0844434		H	2.9386174	6.5180086	0.1532822
C	0.0002596	2.8954201	-0.0002973		H	1.1288175	5.1358716	1.0900407
C	-1.1425379	3.6893532	0.5079837		H	-5.6682129	-0.5855297	-1.5358343
C	-1.7507177	3.3646919	1.7364582		H	-7.5727057	0.4919926	-2.6758547
C	-2.7644594	4.1534539	2.2673679		H	-7.7345216	2.9738159	-2.7694399
C	-3.2210856	5.2996449	1.5981707		H	-5.9509212	4.3624763	-1.7263614
C	-2.6094123	5.631767	0.382388		H	-4.0300718	3.2732066	-0.597137
C	-1.5845594	4.8512302	-0.1489725		H	-4.0300411	-3.2729051	0.5982065
C	1.1433716	3.6886886	-0.5089331		H	-5.9507221	-4.3621016	1.7278285
C	1.7515155	3.3631741	-1.7371656		H	-7.7341267	-2.9733689	2.7711341
C	2.7656572	4.1512728	-2.2683786		H	-7.5722832	-0.4915492	2.6773971
C	3.2227132	5.2975563	-1.5997138		H	-5.6679763	0.5858845	1.5370105
C	2.6109973	5.630594	-0.3841609		N	2.3925678	-1.2958488	-0.4097971
C	1.5857983	4.8507595	0.1474785		N	2.3925543	1.2956271	0.4104433
C	-4.7255056	1.2719606	-0.9644307		C	-0.0000687	-1.5053877	0.0000604
C	-5.7328594	0.4974634	-1.5648639		C	1.2310467	-0.7090729	-0.0840029
C	-6.8066122	1.1069619	-2.2108936		C	3.5454494	-0.6405528	-0.322308
C	-6.8948635	2.4995701	-2.2679485		C	3.545422	0.6402779	0.3231642
C	-5.8937599	3.2777888	-1.6823357		C	1.2310735	0.7088988	0.0844351
C	-4.8148811	2.6719824	-1.0416093		C	-0.0002425	-2.8954388	-0.0002695
C	-4.7253871	-1.2716388	0.9655363		C	1.1425525	-3.689355	0.5080427
C	-4.8147768	-2.6716587	1.0427881		C	1.750713	-3.3646717	1.7365145
C	-5.8935521	-3.2774229	1.6837264		C	2.7644535	-4.153416	2.2674543
C	-6.8945497	-2.4991557	2.2694811		C	3.221104	-5.2996051	1.5982865
C	-6.8062811	-1.1065551	2.2123465		C	2.6094435	-5.6317568	0.3824991
C	-5.7326243	-0.4971011	1.5661055		C	1.5845951	-4.8512438	-0.1488881

Atom	X	Y	Z		Atom	X	Y	Z
C	-1.1433253	-3.6887265	-0.5089407		H	7.5720926	0.4916698	2.6777609
C	-1.7514101	-3.3632496	-1.737205		H	5.667874	-0.5858313	1.5373084
C	-2.7655068	-4.1513831	-2.2684583		C	-4.3448797	-6.1326521	-2.1684993
C	-3.2225639	-5.297663	-1.5998027		C	4.3427838	-6.1354302	2.1670108
C	-2.610899	-5.6306717	-0.384213		C	-4.3427286	6.1355077	2.166911
C	-1.5857529	-4.8508017	0.1474702		C	4.3450669	6.1325073	-2.1683876
C	4.7254706	-1.2719418	-0.9645416		H	5.3227713	5.675673	-1.9636431
C	5.7327131	-0.4974305	-1.5651475		H	4.2594521	6.2331075	-3.2563113
C	6.8064086	-1.106913	-2.2112888		H	4.3567614	7.1380369	-1.7352517
C	6.8947138	-2.4995204	-2.2682897		H	-5.3202502	5.6747276	1.9704429
C	5.8937129	-3.2777603	-1.6825179		H	-4.2517764	6.2437741	3.2537011
C	4.8148872	-2.6719649	-1.0416822		H	-4.3592263	7.1380332	1.7270703
C	4.7253653	1.2716534	0.965563		H	5.320348	-5.6751112	1.9696607
C	4.8147665	2.6716805	1.0427231		H	4.2524044	-6.2428889	3.2539215
C	5.8934925	3.2774819	1.6837029		H	4.3587158	-7.1382788	1.7278639
C	6.8944276	2.4992507	2.2696035		H	-5.3226182	-5.676043	-1.9634606
C	6.806148	1.1066485	2.212585		H	-4.2594473	-6.2329615	-3.2564593
C	5.7325377	0.4971546	1.5662992		H	-4.3563369	-7.1383004	-1.7356191
H	1.4014798	-2.494149	2.2840501					
H	3.2037183	-3.8831854	3.2254858					
H	2.9368155	-6.5190116	-0.1553633					
H	1.1276462	-5.1356946	-1.0916625					
H	-1.4018607	-2.492633	-2.2843858					
H	-3.2047036	-3.8805655	-3.2263496					
H	-2.9385313	-6.5180911	0.1532271					
H	-1.128804	-5.135886	1.0900568					
H	5.6680262	0.5855536	-1.5361667					
H	7.5724145	-0.4919353	-2.6763702					
H	7.7343273	-2.9737542	-2.7698724					
H	5.9509072	-4.3624409	-1.7265131					
H	4.0301556	-3.2731992	-0.5970943					
H	4.0300732	3.2729024	0.5980264					
H	5.9506738	4.3621641	1.727725					
H	7.7339694	2.9734999	2.7712992					

1c (Ar = FC_6H_4) : **F**-form								
SCF Done: E(RB3LYP) = -2926.40978362 A.U. after 6 cycles								
Atom	X	Y	Z		Atom	X	Y	Z
C	-0.0736787	-1.4279583	0.0792547		C	-2.9270361	2.5565724	3.1776499
C	1.186587	-0.7471007	-0.3216723		C	-1.8371114	2.125472	2.4253906
N	2.2350864	-1.4961195	-0.665083		C	1.2867587	3.4102656	1.0856731
C	3.3538335	-0.9078971	-1.1108466		C	1.944564	4.060692	0.0295227
C	3.3793221	0.4993547	-1.3057715		C	2.989164	4.9521183	0.2747201
N	2.345043	1.2569598	-0.9040896		C	3.3909496	5.1693651	1.5869431
C	1.2604877	0.6684994	-0.3924773		C	2.7697885	4.5396732	2.6606833
C	0.0736536	1.4279585	0.0792739		C	1.706375	3.6794985	2.4014034
C	-1.1866151	0.7471056	-0.321657		C	4.4998038	-1.8272501	-1.3524872
N	-2.2351102	1.4961282	-0.6650731		C	4.4720859	1.225195	-2.0118344
C	-3.3538562	0.9079109	-1.1108467		C	-4.499822	1.8272675	-1.3524937
C	-3.3793485	-0.4993397	-1.3057768		C	-4.4721136	-1.2251722	-2.011846
N	-2.3450715	-1.256949	-0.9040978		H	0.967227	-5.0651254	0.9614962
C	-1.260517	-0.6684938	-0.3924769		H	2.9379467	-5.840073	2.278934
C	-0.0855444	-2.5588448	0.8485482		H	3.4784342	-1.8790295	3.8212029
C	1.1226251	-3.0117305	1.6014339		H	1.5287322	-1.085917	2.4830261
C	1.5188153	-4.3595844	1.5751647		H	-1.6310458	-3.8701323	-0.9893552
C	2.6154278	-4.8044999	2.3086769		H	-3.4920484	-5.4705262	-0.5350558
C	3.3042439	-3.8922329	3.0999496		H	-3.109648	-4.7388986	3.6716638
C	2.9271423	-2.5565983	3.1774617		H	-1.191589	-3.2053703	3.2319027
C	1.8371871	-2.1254906	2.4252503		H	-0.9672808	5.0650968	0.9615408
C	-1.2867642	-3.4102776	1.08566		H	-2.9379485	5.8400305	2.279064
C	-1.9446002	-4.0606843	0.0295165		H	-3.4782805	1.8790053	3.8214337
C	-2.9891919	-4.9521165	0.2747276		H	-1.5286313	1.0859065	2.4831737
C	-3.3909391	-5.1693882	1.5869582		H	1.6309798	3.8701598	-0.9893434
C	-2.7697477	-4.5397155	2.6606922		H	3.4919974	5.4705426	-0.5350683
C	-1.7063423	-3.6795353	2.4013975		H	3.1097183	4.7388371	3.6716488
C	0.0855327	2.5588364	0.8485813		H	1.1916459	3.205318	3.2319147
C	-1.122611	3.0117092	1.6015173		C	-4.2519838	3.1148375	-1.8555028
C	-1.5188253	4.3595558	1.5752485		C	-5.8184572	1.4743352	-1.023459
C	-2.6154094	4.8044637	2.3088081		C	-6.8612203	2.3807598	-1.2073896
C	-3.3041685	3.892198	3.1001314		C	-5.2974896	4.01464	-2.0510893

Atom	X	Y	Z		Atom	X	Y	Z
C	-6.6066386	3.6507411	-1.7286		H	6.3213448	1.1245271	-4.8754837
H	-6.0280832	0.4931165	-0.610715		H	7.2410627	3.218154	-3.8948175
H	-7.8743462	2.0943695	-0.9382769		F	4.3595921	-4.3182761	3.8246745
H	-3.2300023	3.3989038	-2.0837127		F	-4.4080814	-6.0229595	1.8286405
H	-5.0893652	5.0032775	-2.4518121		F	-4.3594867	4.3182346	3.8249039
H	-7.4219894	4.3538843	-1.8765812		F	4.4080997	6.0229309	1.8286118
C	-4.9682768	-0.7690065	-3.2432416					
C	-4.9821948	-2.4172276	-1.4766004					
C	-5.9790142	-3.1256996	-2.1466567					
C	-5.9545522	-1.4859252	-3.9185607					
C	-6.4675381	-2.6634986	-3.3703518					
H	-4.5918946	-2.7813153	-0.532477					
H	-6.3733719	-4.0408325	-1.7124577					
H	-4.573867	0.145162	-3.6762861					
H	-6.3213747	-1.1244738	-4.8754927					
H	-7.2410966	-3.2181077	-3.8948449					
C	4.2519728	-3.1148174	-1.855507					
C	5.8184347	-1.4743191	-1.0234339					
C	6.8612008	-2.3807417	-1.2073579					
C	5.2974816	-4.0146176	-2.0510872					
C	6.6066266	-3.6507195	-1.72858					
H	6.028055	-0.4931035	-0.6106797					
H	7.874323	-2.0943522	-0.9382307					
H	3.2299942	-3.3988831	-2.0837305					
H	5.0893629	-5.0032527	-2.4518188					
H	7.4219797	-4.3538611	-1.8765562					
C	4.9682491	0.7690418	-3.2432347					
C	4.9821639	2.4172473	-1.4765791					
C	5.9789814	3.1257276	-2.1466296					
C	5.9545222	1.4859688	-3.918548					
C	6.4675059	2.6635385	-3.3703288					
H	4.591863	2.7813262	-0.5324525					
H	6.3733369	4.0408577	-1.7124227					
H	4.5738406	-0.1451233	-3.6762874					

1c (Ar = FC_6H_4) : **T**-form								
SCF Done: E(RB3LYP) = -2926.41434740 A.U. after 7 cycles								
Atom	X	Y	Z		Atom	X	Y	Z
N	2.3939267	-1.2976774	-0.4052615		H	1.3912886	-2.4922061	2.2876346
N	2.3938229	1.2977211	0.4056316		H	3.2106432	-3.9074072	3.2412625
C	-0.0000163	-1.5049081	0.0000114		H	2.95425	-6.5305945	-0.1394677
C	1.2319364	-0.708695	-0.0825092		H	1.1313137	-5.1269767	-1.0985681
C	3.546303	-0.6415185	-0.321235		H	-1.3914437	-2.4914818	-2.2877881
C	3.5462307	0.6415928	0.3217988		H	-3.2108413	-3.9063649	-3.2417879
C	1.2319025	0.7087105	0.0826777		H	-2.9542888	-6.5306613	0.1380684
C	-0.0000376	-2.8943423	-0.0001554		H	-1.1313228	-5.1273495	1.0975519
C	1.1405678	-3.689769	0.5115035		H	5.6561091	0.5921584	-1.5463505
C	1.7414309	-3.3639933	1.7437805		H	7.5635796	-0.4778637	-2.6872495
C	2.7543647	-4.1478621	2.2865456		H	7.7441702	-2.9588306	-2.7657442
C	3.173271	-5.2764387	1.5882603		H	5.9766085	-4.3550906	-1.7067756
C	2.6024911	-5.6414237	0.3736798		H	4.0498993	-3.2735139	-0.5806734
C	1.5827928	-4.8505522	-0.1512917		H	4.0497464	3.2735985	0.5813111
C	-1.1406533	-3.6896051	-0.5120421		H	5.9762272	4.3552044	1.7077792
C	-1.74157	-3.3634354	-1.7441907		H	7.7435955	2.9589722	2.7671045
C	-2.7545268	-4.1471269	-2.2871657		H	7.5630474	0.4780032	2.6885962
C	-3.1734009	-5.2759333	-1.5892318		H	5.6558084	-0.5920492	1.547331
C	-2.6025612	-5.6413166	-0.3747994		N	-2.3939946	1.2976567	-0.4053273
C	-1.5828454	-4.8506119	0.1503882		N	-2.3938878	-1.2977166	0.4056465
C	4.7277905	-1.2695317	-0.9631545		C	-0.0000487	1.5049248	-0.0000119
C	5.7276248	-0.4905159	-1.570449		C	-1.2320073	0.7087062	-0.0825052
C	6.8034186	-1.0957705	-2.2167819		C	-3.5463649	0.6414832	-0.3213221
C	6.9019868	-2.4880175	-2.2655248		C	-3.5462992	-0.6416026	0.3217621
C	5.9092825	-3.2708346	-1.671951		C	-1.231967	-0.7086978	0.0827099
C	4.8275803	-2.6689523	-1.0326656		C	0.0000008	2.8943615	-0.000189
C	4.7275862	1.2696261	0.9639413		C	-1.1404971	3.6898402	0.5116319
C	4.8273469	2.6690486	1.0334584		C	-1.7411389	3.3641548	1.7440414
C	5.9089187	3.2709475	1.6729496		C	-2.7539264	4.1481011	2.2869662
C	6.9015153	2.4881459	2.2667239		C	-3.1729064	5.2766701	1.588712
C	6.8029715	1.0958974	2.2179746		C	-2.6023386	5.6415716	0.3740074
C	5.7273095	0.4906265	1.5714372		C	-1.5827829	4.8506219	-0.1511245

Atom	X	Y	Z		Atom	X	Y	Z
C	1.1405932	3.6895912	-0.5121802		H	-7.5632043	-0.478013	2.6884112
C	1.7413273	3.3634664	-1.7444298		H	-5.6559373	0.5920395	1.5471941
C	2.7542488	4.1471405	-2.2874953		F	4.1502959	6.0445782	-2.1125461
C	3.1732735	5.2758843	-1.5895503		F	-4.1497941	6.0456296	2.1115709
C	2.6026145	5.641224	-0.3750202		F	4.1503019	-6.0453215	2.110964
C	1.5829297	4.8505386	0.1502571		F	-4.1504594	-6.0446415	-2.112139
C	-4.7278327	1.2694346	-0.9633385					
C	-5.7276156	0.4903603	-1.5706425					
C	-6.80339	1.0955516	-2.217067					
C	-6.9019896	2.4877934	-2.265894					
C	-5.909335	3.2706682	-1.6723134					
C	-4.8276521	2.6688484	-1.0329364					
C	-4.7276712	-1.269636	0.9638744					
C	-4.8274171	-2.6690583	1.033417					
C	-5.9090046	-3.2709575	1.6728813					
C	-6.9016323	-2.4881561	2.2666039					
C	-6.8031039	-1.0959075	2.2178296					
C	-5.7274258	-0.4906364	1.5713191					
H	-1.3909306	2.4923808	2.2878736					
H	-3.2100313	3.9077153	3.2417834					
H	-2.9541443	6.5307416	-0.1391095					
H	-1.1314635	5.1269875	-1.0984941					
H	1.3910829	2.4915645	-2.288034					
H	3.210421	3.9064138	-3.2421944					
H	2.9544537	6.530522	0.1378522					
H	1.1315465	5.127244	1.0974966					
H	-5.6560749	-0.592311	-1.546478					
H	-7.5635111	0.4775995	-2.6875397					
H	-7.7441578	2.9585575	-2.7661851					
H	-5.9766846	4.3549206	-1.7072042					
H	-4.0500093	3.2734546	-0.5809403					
H	-4.0497932	-3.2736077	0.5813092					
H	-5.9763014	-4.3552146	1.7077303					
H	-7.743725	-2.9589827	2.7669633					

1d (Ar = ClC_6H_4) : **F**-form								
SCF Done: E(RB3LYP) = -4367.86049443 A.U. after 6 cycles								
Atom	X	Y	Z		Atom	X	Y	Z
C	0.1839289	1.4230656	-0.1258576		C	2.7005362	-2.867709	2.9594621
C	-1.1261334	0.8362603	-0.514126		C	1.6557594	-2.3326518	2.2101635
N	-2.1159796	1.6642454	-0.853299		C	-1.5428842	-3.3390859	0.8242363
C	-3.2848544	1.1654009	-1.2769527		C	-2.2293518	-3.9272682	-0.2486131
C	-3.4306611	-0.2386844	-1.4465747		C	-3.3356975	-4.7479099	-0.0308754
N	-2.4518848	-1.0717943	-1.0589208		C	-3.7787167	-4.9627183	1.2728799
C	-1.3116214	-0.5685079	-0.5771151		C	-3.1219879	-4.3865537	2.3604766
C	-0.1839212	-1.4230691	-0.1258409		C	-1.9984086	-3.5973945	2.1286206
C	1.1261424	-0.8362678	-0.5141151		C	-4.3518558	2.1735701	-1.5249707
N	2.1159861	-1.6642545	-0.8532916		C	-4.6001478	-0.8841594	-2.1062537
C	3.2848583	-1.1654118	-1.2769554		C	4.3518597	-2.173576	-1.5249895
C	3.4306655	0.2386707	-1.4465841		C	4.600162	0.8841353	-2.1062548
N	2.4518906	1.0717838	-1.0589344		H	-0.5847197	5.1531893	0.652174
C	1.3116301	0.5685002	-0.5771193		H	-2.4607479	6.1132597	1.9519706
C	0.2818037	2.5707744	0.6116925		H	-3.2844588	2.2392473	3.6233878
C	-0.8852816	3.1360607	1.353698		H	-1.4280361	1.2744629	2.2978421
C	-1.179531	4.5075138	1.2910273		H	1.8921804	3.7439087	-1.2615745
C	-2.2305966	5.0554781	2.0215711		H	3.8524909	5.2078862	-0.8663126
C	-2.984845	4.228428	2.8529309		H	3.4762775	4.5656743	3.3699468
C	-2.7006273	2.8677578	2.9593012		H	1.4658762	3.1726548	2.9746866
C	-1.6558285	2.3326854	2.2100435		H	0.5847784	-5.1531634	0.6522209
C	1.5428902	3.3390837	0.8242168		H	2.4607704	-6.1132062	1.9520901
C	2.2293962	3.9272224	-0.2486317		H	3.2843232	-2.2391927	3.6235825
C	3.3357479	4.7478543	-0.0308887		H	1.427938	-1.274436	2.2979662
C	3.7787337	4.9626971	1.2728725		H	-1.8921093	-3.7439831	-1.2615519
C	3.1219664	4.3865755	2.3604687		H	-3.8524094	-5.2079761	-0.8662996
C	1.9983824	3.5974248	2.1286056		H	-3.4763246	-4.565627	3.3699503
C	-0.2818003	-2.570769	0.6117253		H	-1.4659315	-3.1725913	2.9747034
C	0.8852694	-3.136034	1.3537727		C	4.0027808	-3.4215024	-2.0663068
C	1.1795488	-4.507481	1.2911052		C	5.6898499	-1.9439349	-1.1665254
C	2.2305943	-5.0554299	2.0216898		C	6.6536195	-2.9323977	-1.3583455
C	2.9847889	-4.2283718	2.8530903		C	4.970282	-4.4029282	-2.2702197

Atom	X	Y	Z		Atom	X	Y	Z
C	6.2998282	-4.161775	-1.9175063		H	-6.5061609	-0.7031053	-4.9278572
H	5.9759277	-0.9954528	-0.72432		H	-7.5805627	-2.6772676	-3.8610908
H	7.6825405	-2.7419865	-1.0654842		Cl	-4.3015194	4.9142799	3.7948438
H	2.9645019	-3.6103105	-2.318602		Cl	5.183866	5.9837038	1.5531491
H	4.6852164	-5.359259	-2.7007768		Cl	4.3014351	-4.914205	3.7950561
H	7.0540598	-4.9288842	-2.0713553		Cl	-5.1838417	-5.983737	1.5531492
C	5.0855346	0.4210608	-3.3391971					
C	5.1992194	2.0098149	-1.5217802					
C	6.2714768	2.6464834	-2.1458946					
C	6.1478844	1.0674635	-3.9688481					
C	6.748	2.1784715	-3.3721551					
H	4.8194888	2.3789096	-0.5753241					
H	6.7332085	3.5095762	-1.6735634					
H	4.6241035	-0.4421963	-3.8090059					
H	6.5062616	0.7029812	-4.927793					
H	7.5806135	2.6771967	-3.8610758					
C	-4.0027823	3.4214772	-2.0663354					
C	-5.6898324	1.9439633	-1.1664319					
C	-6.6535949	2.9324366	-1.3582342					
C	-4.9702771	4.402913	-2.2702312					
C	-6.2998106	4.1617913	-1.9174491					
H	-5.9759041	0.9955015	-0.72418					
H	-7.6825044	2.7420516	-1.0653156					
H	-2.964512	3.610262	-2.3186832					
H	-4.6852161	5.3592272	-2.700828					
H	-7.0540368	4.9289088	-2.0712836					
C	-5.0854793	-0.4211323	-3.3392301					
C	-5.1992293	-2.0098135	-1.5217543					
C	-6.2714747	-2.6464972	-2.1458736					
C	-6.147816	-1.0675514	-3.9688864					
C	-6.7479593	-2.1785297	-3.3721659					
H	-4.8195283	-2.3788743	-0.5752731					
H	-6.7332269	-3.5095679	-1.6735218					
H	-4.6240257	0.4420997	-3.8090623					

1d (Ar = ClC_6H_4) : **T**-form								
SCF Done: E(RB3LYP) = -4367.86485871 A.U. after 7 cycles								
Atom	X	Y	Z		Atom	X	Y	Z
N	2.3943284	1.2991948	0.4018258		H	1.3950652	2.5026996	-2.290012
N	2.3941885	-1.2993627	-0.4020685		H	3.1953103	3.9135447	-3.2397734
C	0.0000411	1.5039173	-0.0000169		H	2.9380871	6.5280329	0.1651214
C	1.2323392	0.7082715	0.0814276		H	1.1348132	5.121139	1.1090374
C	3.5462685	0.6425789	0.3203115		H	-1.3949483	2.5024707	2.2900712
C	3.5461855	-0.642829	-0.3206864		H	-3.1951022	3.9133038	3.2400199
C	1.2322774	-0.7083612	-0.0815267		H	-2.9376454	6.5282827	-0.16448
C	0.0000804	2.8925282	0.0000599		H	-1.1344721	5.1213941	-1.1085887
C	1.1420924	3.6897573	-0.5068397		H	5.6512793	-0.5931295	1.5500757
C	1.7420268	3.372461	-1.7406344		H	7.5596551	0.475123	2.6904983
C	2.750623	4.1628512	-2.2821475		H	7.7473316	2.9557464	2.7607744
C	3.1758763	5.2955738	-1.5861634		H	5.9857726	4.3539817	1.6947483
C	2.5991603	5.6440567	-0.3648064		H	4.0564874	3.2749506	0.5717389
C	1.5833276	4.8479242	0.15925		H	4.0561933	-3.2752335	-0.5722213
C	-1.1418747	3.6897676	0.5070712		H	5.9852619	-4.354378	-1.6954947
C	-1.741843	3.3723365	1.7408169		H	7.7467828	-2.9562445	-2.7617175
C	-2.7503874	4.1627185	2.2824352		H	7.5592859	-0.4756097	-2.6913728
C	-3.1755506	5.2955769	1.5866155		H	5.6511282	0.5927541	-1.5506873
C	-2.5987931	5.6442012	0.3653196		N	-2.3943605	-1.299175	0.4018805
C	-1.5830153	4.8480693	-0.1588468		N	-2.3942231	1.2993701	-0.4020533
C	4.7282508	1.2698841	0.9611978		C	-0.0000739	-1.503926	-0.0000009
C	5.7252656	0.4894245	1.5714386		C	-1.2323751	-0.7082759	0.081421
C	6.8017337	1.0936559	2.2173877		C	-3.546297	-0.6425469	0.3203982
C	6.9041107	2.4858108	2.2615717		C	-3.5462242	0.6428501	-0.3206211
C	5.9145835	3.2699568	1.6645107		C	-1.232309	0.7083559	-0.0815497
C	4.8315611	2.6692103	1.0264999		C	-0.0001024	-2.892541	0.0000869
C	4.7280436	-1.2702063	-0.9617326		C	-1.1420268	-3.689794	-0.5069712
C	4.8312515	-2.6695388	-1.0270695		C	-1.7417312	-3.3725767	-1.7408998
C	5.9141513	-3.2703485	-1.6652287		C	-2.7502115	-4.1630113	-2.2825617
C	6.9036569	-2.48626	-2.2624004		C	-3.1755812	-5.2957028	-1.5865964
C	6.8013811	-1.0940984	-2.2181785		C	-2.5990915	-5.6441103	-0.3651119
C	5.7250361	-0.4898045	-1.5720827		C	-1.583369	-4.847934	0.1590935

Atom	X	Y	Z		Atom	X	Y	Z
C	1.141801	-3.6897648	0.5072388		H	-7.5594148	0.4756696	-2.6911597
C	1.741552	-3.3723886	1.7411042		H	-5.651227	-0.5927127	-1.5505431
C	2.7500264	-4.1627733	2.282849		Cl	4.4434066	-6.3047479	2.2665293
C	3.1753412	-5.2955789	1.5870364		Cl	-4.4436563	-6.3049329	-2.2659806
C	2.5987987	-5.6441502	0.3656234		Cl	4.4440952	6.3047494	-2.2653615
C	1.5830847	-4.8480194	-0.1586671		Cl	-4.4437026	6.3047423	2.2659521
C	-4.7282583	-1.2698142	0.9613631					
C	-5.7252306	-0.489318	1.5716255					
C	-6.8016767	-1.0935102	2.2176479					
C	-6.9040749	-2.4856623	2.2618825					
C	-5.9145899	-3.2698444	1.6647997					
C	-4.831588	-2.6691367	1.0267173					
C	-4.7280997	1.2702381	-0.9616236					
C	-4.8312926	2.6695712	-1.0269618					
C	-5.9142107	3.2703917	-1.6650807					
C	-6.9037477	2.4863135	-2.2622141					
C	-6.8014856	1.0941511	-2.2179942					
C	-5.7251241	0.4898465	-1.5719361					
H	-1.3946707	-2.5028465	-2.2902639					
H	-3.1947183	-3.9137653	-3.2402871					
H	-2.9381029	-6.528063	0.1647997					
H	-1.1350282	-5.1210946	1.1089781					
H	1.3945359	-2.5025691	2.2903545					
H	3.1945694	-3.9134002	3.2405244					
H	2.9377648	-6.528193	-0.1641681					
H	1.1347074	-5.1213046	-1.1084984					
H	-5.6512277	0.5932342	1.5502213					
H	-7.5595651	-0.4749492	2.6907744					
H	-7.7472795	-2.9555674	2.7611412					
H	-5.9857947	-4.353867	1.6950762					
H	-4.0565458	-3.274904	0.5719401					
H	-4.0562111	3.275258	-0.5721428					
H	-5.98531	4.3544213	-1.6953461					
H	-7.7468868	2.9563062	-2.761501					

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