Supporting Information

Long-Lived Singlet and Triplet Charge Separated States in Small Cyclophane Bridged Triarylamine-Naphthalene Diimide Dyads

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Synthesis

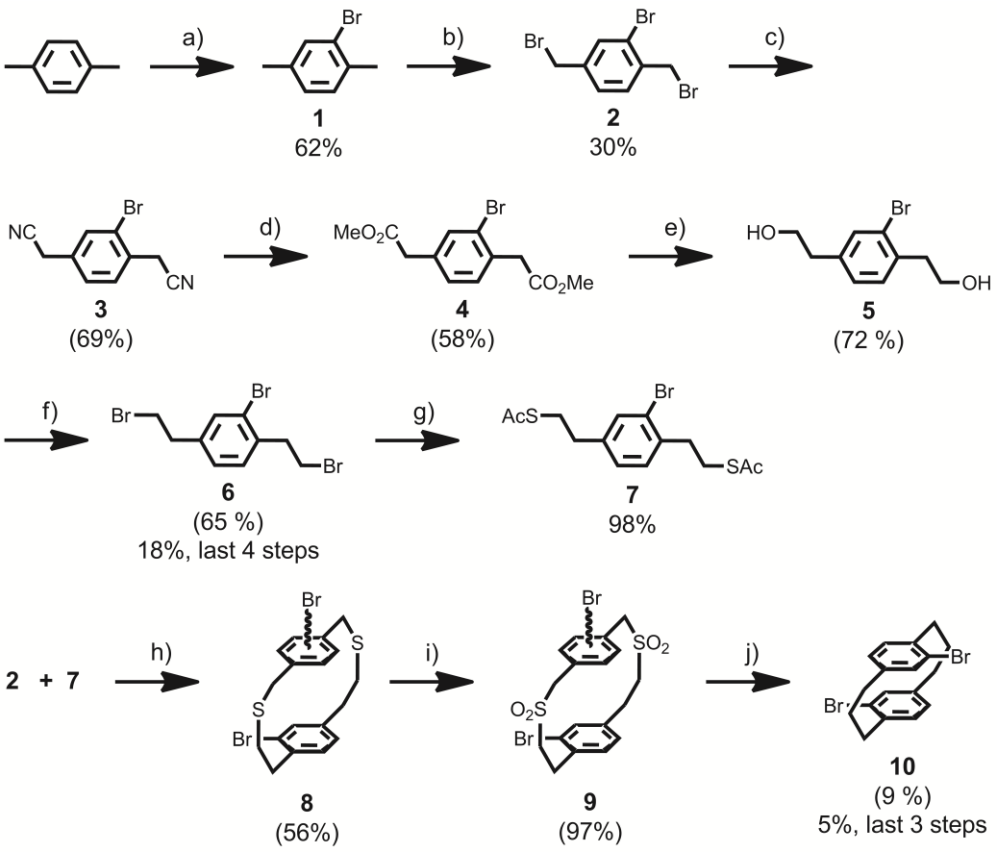
All commercial compounds including solvents were purchased from Fluka, Sigma-Aldrich, Merck, Acros or Chempur and used without further purification.

All reactions specified as being performed under nitrogen atmosphere were performed in air-free conditions (nitrogen, dried with Sicapent® from Merck, oxygen was removed by copper oxide catalyst R3-11 from BASF) using solvents freshly dried by standard procedures.

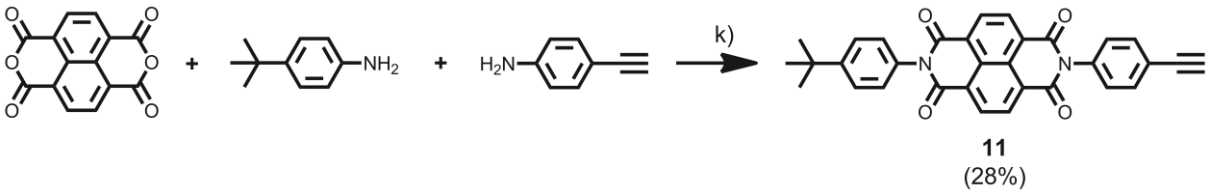
Flash column chromatography was performed on standard silica gel, 60 Å, 40–63 μm (Merck). Wherever specified products were purified by preparative size exclusion gel permeation chromatography with two sequential columns 10 μm, 50 Å and 500 Å (PSS) in a recycling set-up.

Proton and carbon nuclear magnetic resonance spectra (^{1}H NMR, ^{13}C-NMR) were measured on a Bruker AVANCE 400 FT-NMR spectrometer and an AVANCE DMX 600 FT-NMR spectrometer at the temperatures indicated. The residual signal of the respective solvent was used as the internal reference and the chemical shifts are given in ppm (δ-scale).

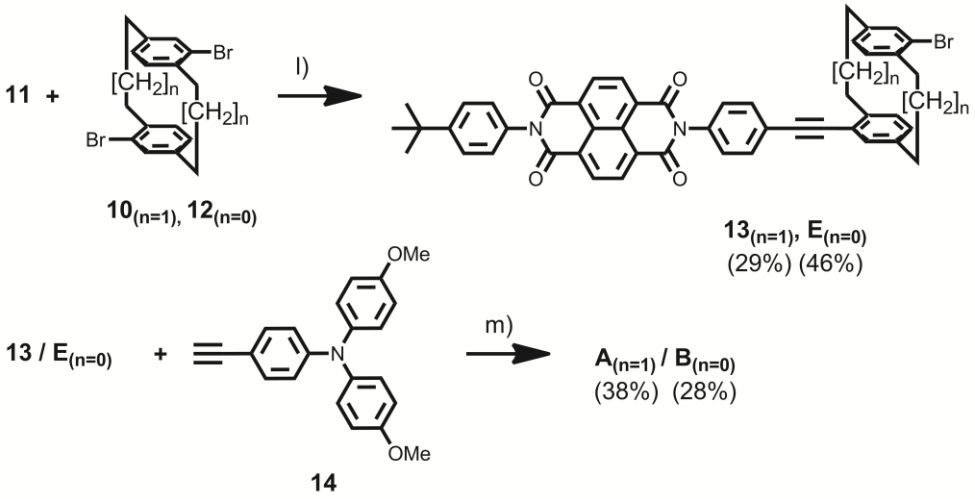
Mass spectrometry was performed on a Finnigan MAT 90 and Bruker Daltronik microTOF focus.



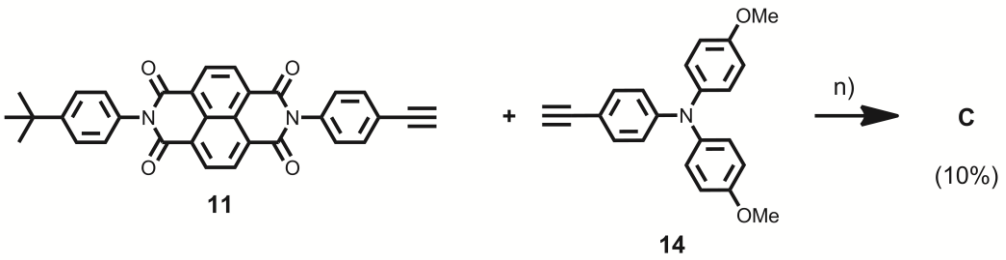
Scheme 1. Synthesis of [3.3]paracyclophane **10**: a) Br_2, Fe (1.8 mol%), 10–15°C → rt, 23 h; b) NBS, AIBN, CCl_4, reflux, 80 min; c) KCN, EtOH/H_2O 2:1, 70°C, 3.5 h; d) H_2SO_4 (98% in water), MeOH, reflux, 2 d; e) $LiAlH_4$, THF, rt → 50°C, 2 h; f) HBr (33% in AcOH),110°C, 16 h; g) KSAc, THF, 40°C, 16 h; h) KOH, MeOH/THF 1:1, reflux, 19 h; i) H_2O_2 (35% in H_2O), AcOH, 100°C, 16 h; j) vacuum flash pyrolysis, 0.015 mbar, 550°C. Yields in brackets are estimated by NMR of the crude product and refer in case of **8** and **9** to not fully characterized isomeric mixtures.



Scheme 2. Synthesis of acceptor **11** k) pyridine, 165°C (microwave reactor), 2 h.

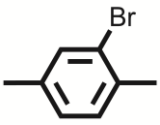


Scheme 3. Synthesis of donor-acceptor dyads **A**, **B**, and fragment **E**: l) $Pd(C_6H_5CN)_2Cl_2$ (15 mol%), CuI, tri-*tert*-butylphosphane (1M in toluene), Et_3N, dioxane, 25°C, 7 d for **13** and 16 h for **E**; m) $Pd(C_6H_5CN)_2Cl_2$ (30 mol%), CuI, tri-*tert*-butylphosphane (1M in toluene), Et_3N, dioxane, 60°C, 10 d for **A** and 5 d for **B**.



Scheme 4. Synthesis of donor-acceptor dyad **C**: n) $Pd(C_6H_5CN)_2Cl_2$ (7.1 mol%), CuI, Et_3N, atmospheric air as oxidant, dioxane, 50°C, 3 d.

2-Bromo-1,4-dimethylbenzene (1)



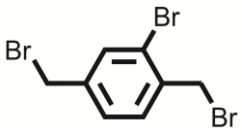
CAS: 553-94-6.

Bromine (416 ml, 8.17 mol) was added dropwise to a suspension of 1,4-dimethylbenzene (1.00 l, 8.17 mol) and *ferrum reductum* (7.99 g, 143 mmol) within 7 h at 10-15°C. The mixture was stirred for 16 h at rt. The crude product was purified by fractional distillation under reduced pressure using a Vigreux column (15 cm).

Yield: 942 g (5.09 mol, 62.3 %) colorless liquid (0.34 mbar, 86°C) C_8H_9Br [185.1 g/mol].

^{1}H-NMR (400 MHz, $CDCl_3$, 300 K): δ / ppm = 7.37–7.34 (m, 1H, C$H_{arom.}$), 7.12–7.08 (m, 1H, C$H_{arom.}$), 7.02–6.98 (m, 1H, C$H_{arom.}$), 2.35 (s, 3H, CH_3), 2.29 (s, 3H, CH_3)

2-Bromo-1,4-bis(bromomethyl)benzene (2)



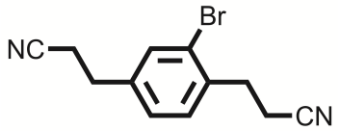
CAS: 19900-52-8

2-Bromo-1,4-dimethylbenzene (**1**) (206 g, 1.11 mol) was added to absolute carbon tetrachloride (1l) and heated to reflux. *N*-Bromosuccinimide (396 g, 1.29 mol) and azo-bis-isobutyronitrile (1.37 g, 8.34 mmol) were added in small portions during 50 min at reflux. The reaction mixture was stirred for 30 min under reflux. The hot mixture was filtered and the solvent was removed under reduced pressure. The residue was purified by recrystallization (chloroform) and dried in HV.

Yield: 114 g (334 mmol, 30%) colorless solid $C_8H_7Br_3$ [342.9 g/mol].

^{1}H-NMR (400 MHz, $CDCl_3$, 300 K): δ / ppm = 7.63–7.60 (m, 1H, C$H_{arom.}$), 7.45–7.41 (m, 1H, C$H_{arom.}$), 7.34–7.30 (m, 1H, C$H_{arom.}$), 4.58 (s, 2H, CH_2), 4.41 (s, 2H, CH_2)

3,3'-(2-bromo-1,4-phenylene)dipropanenitrile (3)



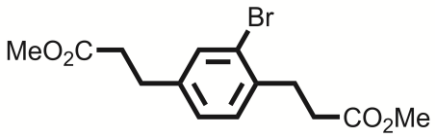
CAS:56403-39-5

2-Bromo-1,4-bis(bromomethyl)benzene (**2**) (80.0 g, 233 mmol) and potassium cyanide (39.6 g , 583 mmol) were suspended in a mixture of ethanol (800 ml) and water (400 ml) and stirred at 70°C for 3.5 h. More water was added and the reaction mixture was extracted with dichloromethane. The combined organic phases were washed with water and dried over magnesium sulfate. The solvent was removed *in vacuo* and the yellowish solid (46.1 g) dried in HV. An analytical sample was purified by flash chromatography (dichloromethane) and dried in HV to yield a colorless solid.

^{1}H-NMR (400 MHz, $CDCl_3$, 300 K): δ / ppm = 7.64–7.60 (m, 1H, C$H_{arom.}$), 7.59–7.53 (m, 1H, C$H_{arom.}$), 7.38–7.32 (m, 1H, C$H_{arom.}$), 3.84 (s, 4H, CH_2), 3.76 (s, 4H, CH_2).

^{13}C-NMR (101 MHz, $CDCl_3$, 300 K) δ / ppm = 132.6 (tert.), 132.2 (quart.), 130.4 (tert.), 130.3 (quart.), 127.9 (tert.), 124.4 (quart.), 116.9 (quart.), 116.6 (quart.), 24.7 (2C, sec.), 23.0 (2C, sec.)

Dimethyl-3,3'-(2-bromo-1,4-phenylene)dipropanoate (4)



Crude 3,3'-(2-bromo-1,4-phenylene)dipropanenitrile (**3**) (46.1 g, 156 mmol) was dissolved in dry methanol (500 ml). Sulfuric acid (107 ml, 1.96 mol, 98% in water) was added dropwise within 30 min. Then the solution was stirred for 2 d under reflux conditions. The mixture was hydrolyzed with water and extracted with dichloromethane. The combined organic phases were dried over magnesium sulfate and the solvent was removed *in vacuo*. The residue was purified by fractional distillation (124°C, 0.01 mbar) to yield a yellowish solid (30.1 g). An analytical sample was purified by recrystallization (methanol) to yield a colorless solid.

^{1}H-NMR (400 MHz, acetone, 300 K): δ / ppm = 7.58–7.55 (m, 1H, C$H_{arom.}$), 7.38–7.34 (m, 1H, C$H_{arom.}$), 7.31–7.26 (m, 1H, C$H_{arom.}$), 3.81 (s, 4H, CH_2), 3.68 (s, 4H, CH_2), 3.661 (s, 3H, CH_3), 3.658 (s, 3H, CH_3).

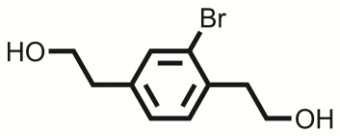
^{13}C-NMR (101 MHz, $CDCl_3$, 300 K) δ / ppm = 171.4 (quart.), 171.0 (quart.), 135.0 (quart.), 133.7(tert.), 133.2 (quart.), 131.6 (tert.) 128.7 (tert.), 125.1 (quart.), 52.33 (prim), 52.32 (prim.), 41.2 (2C, sec.), 40.4 (2C, sec.).

High Resolution Mass (EI): calc.: 221.08084 $[M–Br]^+$

found: 221.08077 $[M–Br]^+$

Δ: –0.30 ppm

2,2'-(2-bromo-1,4-phenylene)diethanol (5)



Lithium aluminum hydride (4.93 g, 130 mmol) was suspended in tetrahydrofuran (400 ml). The crude dimethyl-2,2'-(2-bromo-1,4-phenylene)diacetate (**4**) (30.1 g, 90.5 mmol) dissolved in tetrahydrofuran (80 ml) was added dropwise within 1 h to the suspension at rt. The reaction mixture was heated to 50°C and further lithium aluminum hydride (986 mg, 26.0 mmol) was added. The suspension was stirred for 1h at rt. The reaction mixture was hydrolyzed by slowly adding water. The solution was concentrated to 100 ml by removing the solvent *in vacuo*. Sulfuric acid (400 ml, 5% in water) was slowly added and the product extracted with dichloromethane. The combined organic phases were dried over magnesium sulfate and the solvent was removed *in vacuo*. The residue was dried in HV to yield a colorless oil (17.0 g). An analytical sample was purified by flash chromatography (DCM/EtOAc 1/1) to yield a colorless solid.

^{1}H-NMR (400 MHz, $CDCl_3$, 300 K): δ / ppm = 7.47–7.42 (m, 1H, C$H_{arom.}$), 7.23–7.20 (m, 1H, C$H_{arom.}$), 7.15–7.10 (m, 1H, C$H_{arom.}$), 3.89–3.82 (—, 4H, CH_2), 3.00 (t, $^{3}J_H$=6.68 Hz, 2H, CH_2), 2.82 (t, 2H, CH_2).

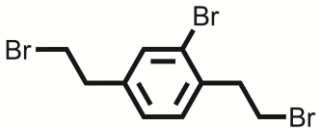
^{13}C-NMR (101 MHz, $CDCl_3$, 300 K) δ / ppm = 139.2 (quart.), 136.0 (quart.), 133.5 (tert.), 131.4(tert.), 128.4 (tert.), 124.9 (quart.), 63.5 (sec.), 62.3 (sec.), 39.1 (sec.), 38.4 (sec.).

High Resolution Mass (EI): calc.: 244.00934 M^+

found: 244.00739 M^+

Δ: 0.19 ppm

2-Bromo-1,4-bis(2-bromoethyl)benzene (6)



In three batches the crude 2,2'-(2-bromo-1,4-phenylene)diethanol (**5**) (16.7 g, 59.0 mmol) was added to hydrogen bromide (47.0 ml, 273 mmol, 33% in acetic acid) and stirred for 16 h in a high pressure glass tube at 110°C. The reaction mixture was hydrolyzed with water and extracted with dichloromethane. The combined organic phases were washed with water and dried over anhydrous magnesium sulfate. The solvent was removed *in vacuo*. The residue was purified by flash chromatography on silica gel (dichloromethane/petrol ether 5:95 → dichloromethane/petrol ether 8:92).

Yield: 15.8 g (42.5 mmol, 18 % over the last 4 steps) colorless solid $C_{10}H_{11}Br_3$ [370.9].

^{1}H-NMR (400 MHz, $CDCl_3$, 300 K): δ / ppm = 7.44–7.41 (m, 1H, C$H_{arom.}$), 7.24–7.20 (m, 1H, C$H_{arom.}$), 7.15–7.10 (m, 1H, C$H_{arom.}$), 3.61–3.52 (—, 4H, CH_2), 3.27 (t, ^3J_H=7.52 Hz, 2H, CH_2), 3.12 (t, ^3J_H=7.45 Hz, 2H, CH_2).

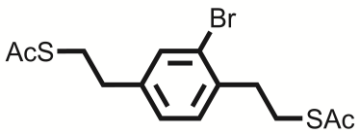
^{13}C-NMR (101 MHz, $CDCl_3$, 300 K) δ / ppm = 139.9 (quart.), 136.8 (quart.), 133.3 (tert.), 131.3 (tert.), 128.0 (tert.), 124.5 (quart.), 39.3 (sec.), 38.5 (sec.), 32.3 (sec.), 31.1 (sec.)

High Resolution Mass (EI): calc.: 367.84054 M^+

found: 367.84028 M^+

Δ: –0.71 ppm

S,S'-[(2-Bromo-1,4-phenylene)bis(ethane-2,1-diyl)] diethanethioate (7)



Under nitrogen atmosphere potassium thioacetate (4.90 g, 42.9 mmol) was added to a suspension of 2-bromo-1,4-bis(2-bromoethyl)benzene (5.71 g, 14.3 mmol) (**2**) in tetrahydrofuran (250 ml). The reaction mixture was stirred for 16 h at 40°C. The solvent was removed *in vacuo*. The residue was extracted with dichloromethane (200 ml) at 40°C and filtered. The solvent was removed from the filtrate *in vacuo*. The resulting product was dried in HV.

Yield: 5.47 g (14.1 mmol, 98 %) white solid $C_{14}H_{17}BrO_2S_2$ [361.3].

^{1}H-NMR (400 MHz, $CDCl_3$, 300 K): δ / ppm = 7.44–7.39 (m, 1H, C$H_{arom.}$), 7.21–7.17 (m, 1H, C$H_{arom.}$), 7.12–7.08 (m, 1H, C$H_{arom.}$), 3.15–3.05 (—, 4H, CH_2), 3.00–2.94 (m, 2H, CH_2), 2.84–2.78 (m, 2H, CH_2), 2.34 (s, 3H, CH_3), 2.33 (s, 3H, CH_3).

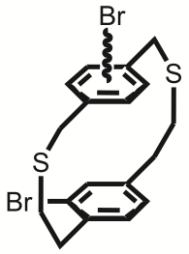
^{13}C-NMR (101 MHz, $CDCl_3$, 300 K) δ / ppm = 195.7 (quart.), 195.6 (quart.), 140.5 (quart.), 137.5 (quart.), 133.0 (tert.), 130.9 (tert.), 127.9 (tert.), 124.5 (quart.), 35.7 (sec.), 35.1 (sec.), 30.81 (prim.), 30.79 (prim.), 30.3 (sec.), 29.0 (sec.)

High Resolution Mass (ESI): calc.: 382.97455 $[M+Na]^+$

found: 382.97250 $[M+Na]^+$

Δ: 0.02 ppm

Dithia-cyclophane (8)

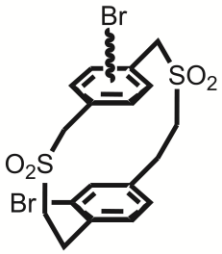


Under nitrogen atmosphere potassium hydroxide (12.2 g, 187 mmol) was dissolved in methanol (1 l) and tetrahydrofuran (1 l). A solution of 2-bromo-1,4-bis(bromomethyl)benzene (**2**) (12.8 g, 37.4 mmol) and *S*,*S*'-[(2-bromo-1,4-phenylene)bis(ethane-2,1-diyl)] diethanethioate (**7**) (13.5 g, 37.4 mmol) in tetrahydrofuran (60 ml) was added dropwise via a dilution elbow within 19 h under reflux conditions. Then the solution was stirred for 3h under reflux conditions.

The solvents were removed *in vacuo* and the residue was purified by flash chromatography on silica gel (3:1 petrol ether:dichloromethane). The dithia-cyclophane (**8**) containing fraction (9.60 g, colorless solid) was dried in HV.

^{1}H-NMR (400 Mhz, CD_2Cl_2, 300 K): δ / ppm = 7.27–6.70 (—, 6H, CH_{arom}), 3.80–2.20 (—, 12 H, CH_2)

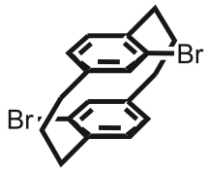
Bis-sulfone-cyclophane (9)



Crude dithia-cyclophane (**8**) (9.44 g) was suspended in acetic acid (150 ml). Then hydrogen peroxide solution in water (220 ml, 2.27 mol, 35%) was added to the suspension within 15 min at 80°C. The reaction mixture was stirred for 16 h at 100°C. The reaction mixture was cooled to rt. The solvent was reduced *in vacuo* to 50 ml. The suspension was filtered. The residue containing the bis-sulfone-cyclophane (**9**) was washed with diethyl ether and then dried in HV (10.5 g, white solid).

MS (EI, 70 eV): m/z (%) = M^+ : 526 (0.2 %), 525 (0.5 %), 524 (2.2 %), 523 (0.9 %), 522 (3.9 %), 521 (0.4 %), 520 (1.9 %)

5,18-dibromo-[3.3]paracyclophane (10)



The crude bis-sulfone-cyclophane (**9**) (10.2 g, 19.5 mmol) was subjected in portions of 230 mg–1300 mg to vacuum flash pyrolysis (550°C, 0.015 mbar).

The resulting condensate was dissolved in dichloromethane and filtered. The solvent was removed *in vacuo* from the filtrate. The residue was purified by flash chromatography (petrol ether). The product was isolated from the other regioisomers by recrystallization (chloroform) and dried in HV.

Yield: 661 mg (1.68 μmol, (ca. 9%) 5% over the last 3 steps) colorless solid $C_{18}H_{18}Br_2$ [394.1].

^{1}H-NMR (400 MHz, $CDCl_3$, 300K): δ / ppm = 6.98–6.96 (m, 2H, C$H_{arom.}$), 6.93–6.87 (m, 2H, C$H_{arom.}$), 6.68–6.64 (m, 2H, C$H_{arom.}$), 3.15–3.06 (m, 2H, CH_2), 2.84–2.73 (m, 2H, CH_2), 2.69–2.56 (—, 4H, CH_2), 2.40–2.27 (m, 2H, CH_2), 1.98–1.86 (m, 2H, CH_2).

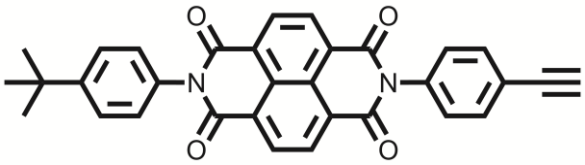
^{13}C-NMR (101 MHz, $CDCl_3$, 300 K): δ / ppm = 141.3 (quart.), 136.9 (quart.), 133.3 (tert.), 132.8 (tert.), 126.9 (tert.), 124.2 (quart.), 35.6 (sec.), 34.8 (sec.), 26.9 (sec.)

High Resolution Mass (ESI): calc.: 391.97698 M^+

found: 391.97660 M^+

Δ: –0.96 ppm

ACCEPTOR 11



Dry pyridine (20 ml) was added to a mixture of 1,4,5,8-naphthalenetetracarboxylic dianhydride (1.61 g, 6.00 mmol) and 4-*tert*-butylaniline (810 µl, 5.10 mmol). The reaction mixture was stirred in a high pressure glass tube for one hour in a microwave oven at 165°C. The mixture was allowed to cool down to 110°C and 4-ethynylaniline (703 mg, 6.00 mmol) was added. The reaction mixture was stirred for one hour in the microwave oven at 165°C. Subsequently the mixture was cooled to 110°C and filtered. The solvent of the filtrate was removed *in vacuo*. Acetone (300 ml) was added to the residue and stirred at reflux, allowed to cool to rt and filtered again. The residue was washed with acetone (100 ml). The residue was purified by flash chromatography on silica gel (dichloromethane). The product was dried in HV.

Yield: 700 mg (1.40 mmol, 28%) yellow solid $C_{32}H_{22}N_2O_4$ [498.5].

^{1}H-NMR (600 MHz, CD_2Cl_2, 298.8 K): δ / ppm = 8.82 (—, 4H, C$H_{naphth.}$), 7.73–7.69 (AA', 2H, C$H_{arom.}$), 7.64–7.61 (AA', 2H, C$H_{arom.}$), 7.35–7.33 (BB', 2H, C$H_{arom.}$), 7.28–7.25 (BB', 2H, C$H_{arom.}$), 3.26 (s, 1H, CH_{alkin}), 1.43 (s, 9H, CH_3)

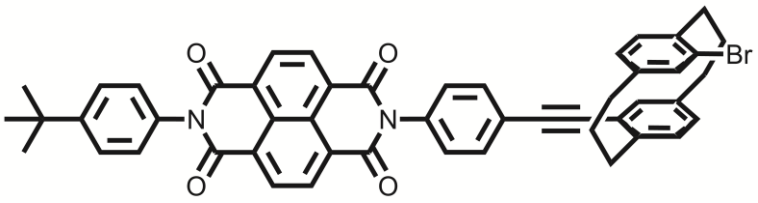
^{13}C-NMR (151 MHz, CD_2Cl_2, 298.8 K) δ / ppm = 163.5 (2C, quart.), 163.2 (2C, quart.), 152.6 (1C, quart.), 135.7 (1C, quart.), 133.5 (2C, tert.), 132.6 (1C, quart.), 131.7 (2C, tert.), 131.6 (2C, tert.), 129.2 (2C, tert.), 128.4 (2C, tert.), 127.63 (2C, quart.). 127.570 (1C, quart.), 127.566 (1C, quart.), 127.2 (2C, quart.), 126.9 (2C, tert.), 123.4 (1C, quart.), 82.9 (1C, quart.), 78.8 (1C, tert.), 35.1 (1C, quart.), 31.5 (3C, prim.)

High Resolution Mass (ESI): calc.: 499.16523 $(M+H)^+$

found: 499.16516 $(M+H)^+$

Δ: 0.15 ppm

COMPOUND 13



Under nitrogen atmosphere absolute dioxane (3 ml) was added to a mixture of compound **11** (116 mg, 232 *µ*mol), cyclophane **10** (60.9 mg, 155 *µ*mol), bis(benzonitrile)palladium(II)chloride (8.89 mg, 23.2 *µ*mol) and copper(I)iodide (2.94 mg, 15.5 *µ*mol). A solution of tri-*tert*-butylphosphane in toluene (46.4 *µ*l, 155 *µ*mol, 1 M) and triethylamine (43.7 *µ*l, 309 *µ*mol) were added. The reaction mixture was stirred at 25°C for 7 d under exclusion of light. The mixture was hydrolyzed by adding water and extracted with dichloromethane. The combined organic phases were dried over magnesium sulfate. The solvents were removed *in vacuo*. The residue was purified by flash chromatography on silica gel (dichloromethane). The product was rinsed with pentane (3×10 ml) in an ultrasonic bath, and the solvent was removed by centrifugation and decantation. The product was dried in HV.

Yield: 36.3 mg (45 *µ*mol, 29%) yellow solid $C_{50}H_{39}BrN_2O_4$ [811.8].

^{1}H-NMR (600 MHz, CD_2Cl_2, 298.8 K): δ / ppm = 8.86–8.81 (—, 4H, C*H*$_{naphth.}$), 7.83–7.78 (AA', 2H, C*H*$_{arom.}$), 7.65–7.61 (AA', 2H, C*H*$_{arom.}$), 7.42–7.38 (BB', 2H, C*H*$_{arom.}$), 7.29–7.25 (BB', 2H, C*H*$_{arom.}$), 7.04–6.98 (—, 3H, C*H*$_{cyc}$), 6.95–6.90 (—, 1H, C*H*$_{cyc}$), 6.76–6.71 (—, 2H, C*H*$_{cyc}$), 3.36–3.29 (—, 1H, C*H*$_{2cyc}$), 3.15–3.06 (—, 1H, C*H*$_{2cyc}$), 2.88–2.58 (—, 6H, C*H*$_{2cyc}$), 2.49–2.29 (—, 2H, C*H*$_{2cyc}$), 2.08–1.93 (—, 2H, C*H*$_{2cyc}$), 1.43 (s, 9H, C*H*$_3$)

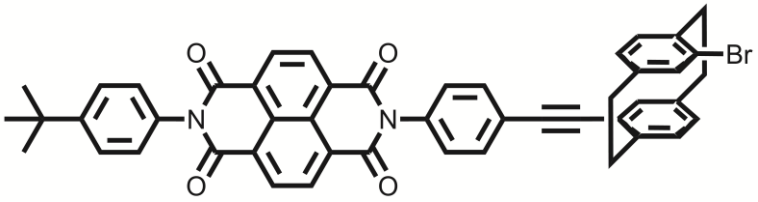
^{13}C-NMR (151 MHz, CD_2Cl_2, 298.8 K) δ / ppm = 163.5 (2C, quart.), 163.3 (2C, quart.), 152.5 (1C, quart.), 141.7 (1C, quart.), 141.1 (1C, quart.), 139.4 (1C, quart.), 137.3 (1C, quart.), 134.9 (1C, quart.), 133.6 (1C, tert.), 133.5 (1C, tert.), 133.0 (1C, tert.), 132.70 (2C, tert.), 132.66 (1C, quart.), 131.7 (2C, tert.), 131.6 (2C, tert.), 131.5 (1C, tert.), 129.2 (2C, tert), 128.7 (1C, tert.), 128.4 (2C, tert.), 128.1 (1C, tert.), 127.62 (2C, quart.), 127.59 (2C, quart.), 127.3 (2C, quart.), 126.9 (2C, tert.), 125.3 (1C, quart.), 124.3 (1C, quart.), 122.0 (1C, quart.), 91.8 (1C, quart.), 91.2 (1C, quart.), 35.8 (1C, sec), 35.3 (1C, sec.), 35.13 (1C, quart.), 35.11 (1C, sec.), 34.6 (1C, sec.), 31.5 (3C, prim), 28.2 (1C, sec.), 27.1 (1C, sec.)

High Resolution Mass (ESI): calc.: 811.21660 $(M+H)^+$

found: 811.21637 $(M+H)^+$

Δ: 0.28 ppm

FRAGMENT E



Under nitrogen atmosphere absolute dioxane (7.5 ml) was added to a mixture of compound **11** (245 mg, 492 μmol), cyclophane **12** (150 mg, 410 μmol), bis(benzonitrile)palladium(II)chloride (23.6 mg, 61.5 μmol) and copper(I)iodide (7.80 mg, 41.0 μmol). A solution of tri-*tert*-butylphosphane in toluene (123 μl, 155 μmol, 1 M) and triethylamine (63.7 μl, 45.6 mg, 451 µmol) were added. The reaction mixture was stirred for 16 h at 25°C under exclusion of light. The mixture was hydrolyzed with water and extracted with dichloromethane. The combined organic phases were dried over magnesium sulfate and the solvents were removed *in vacuo*. The residue was purified by flash chromatography on silica gel (dichloromethane). The product fraction was rinsed with acetone (2×10 ml) in an ultrasonic bath and the solvent was removed by centrifugation and decantation. The product was dried in HV.

Yield: 148 mg (189 μmol, 46%) yellow solid $C_{48}H_{35}BrN_2O_4$ [783.7].

^{1}H-NMR (600 MHz, CD_2Cl_2, 298.8 K): δ / ppm = 8.87–8.81 (—, 4H, C$H_{naphth.}$), 7.84–7.78 (AA', 2H, C$H_{arom.}$), 7.66–7.60 (AA', 2H, C$H_{arom.}$), 7.43–7.37 (BB', 2H, C$H_{arom.}$), 7.30–7.25 (BB', 2H, C$H_{arom.}$), 7.22–7.18 (—, 1H, CH_{cyc}), 7.08–7.04 (—, 1H, CH_{cyc}), 6.66–6.63 (—, 1H, CH_{cyc}), 6.58–6.56 (—, 1H, C$H_{cyc.}$), 6.54–5.51 (—, 2H, CH_{cyc}), 3.75–3.68 (—, 1H, C$H_{2cyc.}$), 3.52–3.45 (—, 1H, C$H_{2cyc.}$), 3.28–3.16 (—, 2H, CH_{2cyc}), 3.08–2.94 (—, 3H, CH_{2cyc}), 2.94–2.87(—, 1H, CH_{2cyc}), 1.43 (s, 9H, CH_3).

^{13}C-NMR (151 MHz, CD_2Cl_2, 298.8 K): δ / ppm = 163.5 (2C, quart.), 163.4 (2C, quart.), 152.6 (1C,quart.), 142.6 (1C, quart.), 142.0 (1C, quart.), 140.0 (1C, quart.), 139.3 (1C, quart.), 137.7 (1C, tert.), 137.6 (1C, tert.), 135.0 (1C, quart.), 134.8 (1C, tert.), 133.4(1C, tert.), 132.8 (2C, tert.), 132.7(1C, quart.), 131.7 (2C, tert.), 131.6 (2C, tert.), 129.9 (1C, tert.), 129.7(1C, tert.),

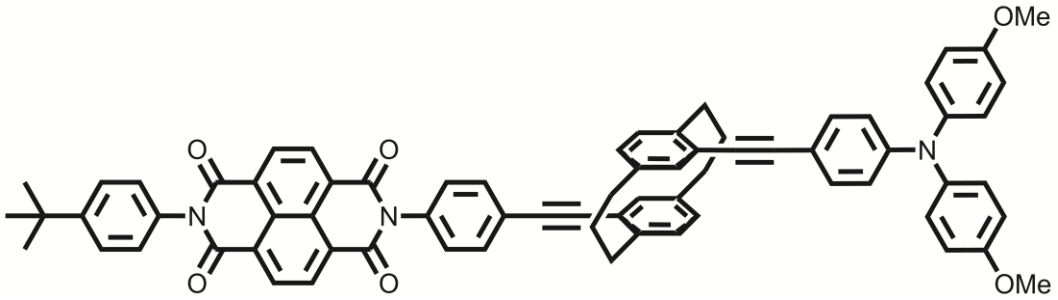
129.3 (2C, tert.), 128.4 (2C, tert.), 127.64 (2C, quart.), 127.59 (2C, quart.), 127.3 (2C, quart.), 126.94 (1C, quart.), 126.86 (2C, tert.), 125.1 (1C, quart.), 124.8 (1C, quart.), 92.3 (1C, quart.), 91.2 (1C, quart.), 35.7 (1C, sec.), 35.1 (1C, quart.), 34.4 (1C, sec.), 34.0 (1C, sec.), 33.4 (1C, sec.), 31.5 (3C, prim.)

High Resolution Mass (ESI): calc.: 783.18530 $(M+H)^+$

found: 783.18503 $(M+H)^+$

Δ: 0.34 ppm

DYAD A



Under nitrogen atmosphere dry dioxane (2.5 ml) was added to a mixture of compound **13** (36.3 mg, 44.7 μmol), compound **14** (58.9 mg, 179 μmol), bis(benzonitrile)palladium(II)chloride (5.15 mg, 13.4 μmol) and copper(I)iodide (1.70 mg, 8.94 μmol). A solution of tri-*tert*-butylphosphane in toluene (26.8 μl, 27.0 μmol, 1.0 M) and triethylamine (316 μl, 2.24 mmol) were added. The reaction mixture was stirred for 10 d at 60°C under exclusion of light. The solvent was evaporated *in vacuo*, the residue hydrolyzed with water and extracted with dichloromethane. The combined organic phases were dried over magnesium sulfate and the solvent was removed *in vacuo*. The residue was purified by flash column chromatography on silica gel (ethyl acetate/dichloromethane 100:1) followed by gel permeation chromatography (chloroform). The product fraction was rinsed with hot acetone (10 ml) in an ultrasonic bath, and the solvent was removed by centrifugation and decantation. This procedure was repeated with cold acetone (10 ml). The product was dried in HV.

Yield: 18.0 mg (17.0 μmol, 38%) yellowish solid $C_{72}H_{57}N_3O_4$ [1060.2].

^{1}H-NMR (400 MHz, CD_2Cl_2, 300 K): δ / ppm = 8.88–8.82 (—, 4H, C$H_{napht.}$), 7.87–7.79 (AA', 2H, C$H_{arom.}$), 7.67–7.60 (AA', 2H, C$H_{arom.}$), 7.43–7.35 (–, 4H, C$H_{arom.+TAA}$), 7.31–7.25 (BB', 2H, C$H_{arom.}$), 7.15–7.07 (—, 4H, CH_{TAA}), 7.03–6.92 (—, 4H, C$H_{cyc.}$), 6.91–6.86 (—, 6H, CH_{TAA}), 6.79–6.72 (—, 2H, C$H_{cyc.}$), 3.81 (—, 6H, CH_3), 3.39–3.24 (—, 2H, C$H_{2cyc.}$), 2.87–2.60 (—, 6H, C$H_{2cyc.}$), 2.51–2.38 (—, 2H, CH_{2cyc}), 2.13–1.98 (—, 2H, CH_{2cyc}), 1.44 (s, 9H, CH_3).

^{13}C-NMR (151 MHz, CD_2Cl_2, 298.8 K): δ / ppm = 163.5 (2C, quart.), 163.4 (2C, quart.), 156.9 (2C, quart.), 152.6 (1C, quart.), 149.1 (1C, quart.), 141.2 (1C, quart.), 140.6 (1C, quart.), 140.5 (2C, quart.), 139.5 (1C, quart.), 139.3 (1C, quart.), 134.8 (1C, quart.), 133.6 (1C, tert.), 133.3 (1C, tert.), 132.69 (2C, tert.), 132.67 (1C, quart.), 132.5 (2C, tert.), 131.7 (2C, tert.), 131.6 (2C, tert.),131.5 (2C, tert.), 129.5 (1C, tert.), 129.2 (2C, tert.), 128.8 (1C, tert.), 128.4 (2C, tert.), 127.62 (2C, quart.), 127.60 (2C, quart.), 127.5 (4C, tert.), 127.31 (2C, quart.), 126.9 (2C, tert.), 125.3 (1C, quart.), 122.8 (1C, quart.), 121.9 (1C, quart.), 119.5 (2C, tert.), 115.1 (4C, tert.),

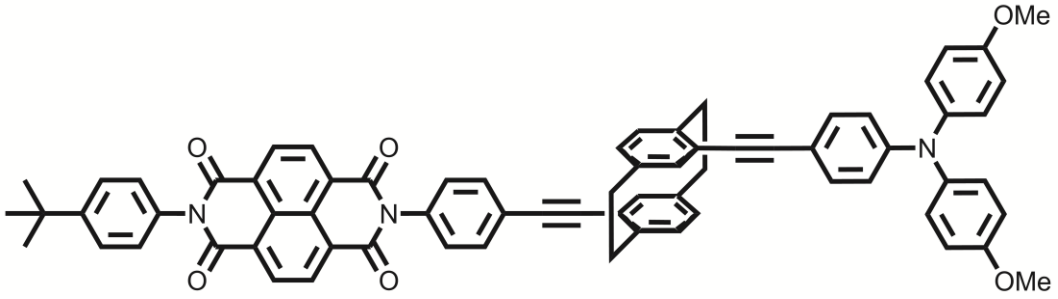
114.8 (1C, quart.), 93.2 (1C, quart.), 91.7 (1C, quart.), 91.4 (1C, quart.), 88.5 (1C, quart.), 55.8 (2C, prim.), 35.5 (1C, sec), 35.4 (1C, sec.), 35.1 (1C, quart.), 34.7 (2C, sec.), 31.5 (3C, prim.), 28.1 (2C, sec.)

High Resolution Mass (ESI): calc.: 1059.42419 M^+

found: 1059.42446 M^+

Δ: 0.25 ppm

DYAD B



Under nitrogen atmosphere absolute dioxane (2.5 ml) was added to a mixture of compound **E** (30.0 mg, 38.3 μmol), compound **14** (50.4 mg, 153 μmol), bis(benzonitrile)palladium(II)chloride (4.40 mg, 11.5 μmol) and copper(I) iodide (3.96 mg, 7.66 μmol). A solution of tri-*tert*-butylphosphane (23.0 μl, 23.0 μmol, 1M) in toluene and triethylamine (8.11 μl, 57.4 μmol) were added. The reaction mixture was stirred at 60°C under exclusion of light for 5 d. The mixture was hydrolyzed by adding water and extracted with dichloromethane. The combined organic phases were dried over magnesium sulfate and the solvents were evaporated *in vacuo*. The residue was purified by flash column chromatography on silica gel (gradient: dichloromethane →1:100 ethyl acetate/dichloromethane) followed by gel permeation chromatography (chloroform). The product fraction was heated to reflux in acetone (12 ml), cooled to rt and the solvent was removed by decantation. The product was dried in HV.

Yield: 11.0 mg (10.7 μmol, 28%) yellowish solid $C_{70}H_{53}N_3O_6$ [1032.2].

^{1}H-NMR (400 MHz, CD_2Cl_2, 300 K): δ / ppm = 8.87–8.82 (—, 4H, C$H_{naphth.}$), 7.86–7.79 (AA', 2H, C$H_{arom.}$), 7.66–7.61 (AA', 2H, C$H_{arom.}$), 7.43–7.36 (—, 4H, C$H_{arom.+TAA}$), 7.30–7.25 (BB', 2H, C$H_{arom.}$), 7.13–7.02 (—, 6H, C$H_{TAA+cyc}$), 6.91–6.86 (—, 6H, CH_{TAA}), 6.67–6.64 (—, 1H, C$H_{cyc.}$),

6.69–6.51 (—, 3H, C$H_{cyc.}$), 3.81 (s, 6H, CH_3), 3.75–3.62 (—, 2H, C$H_{2cyc.}$), 3.31–3.19 (—, 2H, C$H_{2cyc.}$), 3.12–3.03 (—, 2H, CH_{2cyc}), 3.02–2.89 (—, 2H, CH_{2cyc}), 1.44 (s, 9H, CH_3).

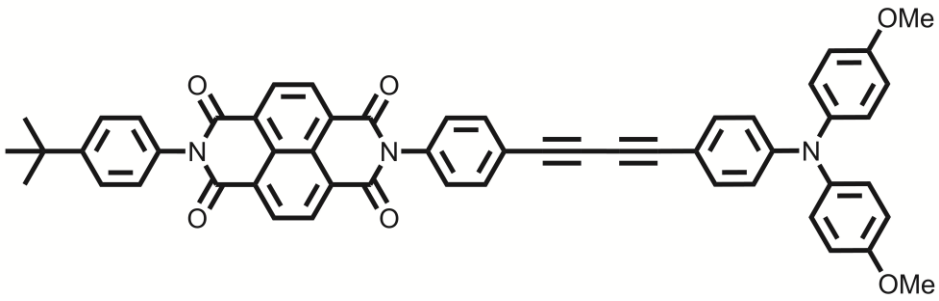
^{13}C-NMR (151 MHz, CD_2Cl_2, 298.8 K): δ / ppm = 163.5 (2C, quart.), 163.4 (2C, quart.), 156.9 (2C, quart.), 152.6 (1C, quart.), 149.2 (1C, quart.), 142.9 (1C, quart.), 142.3.6 (1C, quart.), 140.5 (2C, quart.), 140.2 (1C, quart.), 140.0 (1C, quart.), 137.6 (1C, tert.), 137.3 (1C, tert.), 135.0 (1C, quart.), 133.6 (1C, tert.), 133.5 (1C, tert.), 132.74 (2C, tert.), 132.67 (1C, quart.), 132.5 (2C, tert.), 131.7 (2C, tert.), 131.6 (2C, tert.), 131.0 (1C, tert.), 130.3 (1C, tert.),129.3 (2C, tert.), 128.4 (2C, tert.), 127.63 (2C, quart.),127.60 (2C, quart.), 127.58 (4C, tert.), 127.3 (2C, quart.), 126.9 (2C, tert.), 125.6 (1C, quart.), 125.2 (1C, quart.), 124,6 (1C, quart.), 119.3 (2C, tert.), 115.1 (4C, tert.), 114.53 (1C, quart.), 93.9 (1C, quart.), 92.2 (1C, quart.), 91.5 (1C, quart.), 88.7 (1C, quart.), 55.8 (2C, prim), 35.1 (1C, quart.), 34.4 (2C, sec.), 34.3 (1C, sec), 34.2 (1C, sec), 31.5 (3C, prim)

High Resolution Mass (ESI): calc.: 1031.39289 M^+

found: 1031.39236 M^+

Δ: 0.51 ppm

DYAD C



Dry dioxane (8 ml) and triethylamine (2 ml) were added to a mixture of compound **11** (75.8 mg, 152 μmol), compound **14** (50.0 mg, 152 μmol), bis(triphenylphosphine)palladium(II) dichloride (7.56 mg, 10.8 μmol) and copper(I) iodide (2.89 mg, 15.2 μmol). The mixture was stirred for 3 d at 50°C under exclusion of light but atmospheric conditions where oxygen acts as the oxidant. The solvent was removed *in vacuo*, the residue was hydrolyzed with water and extracted with dichloromethane. The combined organic phases were dried over anhydrous magnesium sulfate and the solvent was removed *in vacuo*. The residue was purified by flash chromatography on silica gel (dichloromethane) followed by gel permeation chromatography (chloroform). The product was dried in HV.

Yield: 12.0 mg (14.5 μmol, 10%) yellowish solid $C_{54}H_{39}N_3O_6$ [825.9].

^{1}H-NMR (600 MHz, CD_2Cl_2, 298.8 K): δ / ppm = 8.83–8.81 (—, 4H, C$H_{naphth.}$), 7.74–7.70 (AA', 2H, C$H_{arom.}$), 7.64–7.60 (AA', 2 H, C$H_{arom.}$), 7.36–7.33 (BB', 2H, C$H_{arom.}$), 7.33–7.30 (AA', 2H, CH_{TAA}), 7.28–7.25 (BB', 2H, C$H_{arom.}$), 7.12–7.07 (AA', 4H, CH_{TAA}), 6.90–6.86 (BB', 4H, CH_{TAA}), 6.79–6.75 (BB', 2H, CH_{TAA}), 3.79 (s, 6H, CH_{TAA}), 1.43 (s, 9H, CH_3).

^{13}C-NMR (151 MHz, CD_2Cl_2, 298.8 K): δ / ppm = 163.5 (2C, quart.), 163.2 (2C, quart.), 157.3 (2C, quart.), 152.6 (1C, quart.), 150.4 (1C, quart.), 139.8 (2C, quart.), 135.7 (1C, quart.), 133.9 (2C, tert.), 133.7 (2C, tert.), 132.6 (1C, quart.) , 131.7 (2C, tert.), 131.6 (2C, tert.), 129.3 (2C, tert.), 128.4 (2C, tert.), 128.0 (4C, tert.), 127.64 (2C, quart.), 127.576 (1C, quart.), 127.572 (1C, quart.), 127.2 (2C, quart.), 126.9 (2C, tert.), 123.4 (1C, quart.), 118.3 (2C, tert.), 115.2 (4C, tert.), 111.0 (1C, quart.), 83.9 (1C, quart.), 80.3 (1C, quart.), 75.9 (1C, quart.), 72.5 (1C, quart.), 55.8 (2C, prim.), 35.1 (1C, quart.), 31.5 (3C, prim.)

High Resolution Mass (ESI): calc.: 825.28334 M^+

found: 825.28313 M^+

Δ: 0.25 ppm

Table S1. Lifetimes and ratio of the amplitudes of ns-transient absorption experiments at the given molarity and given laser pulse energy in toluene at 28 200 cm^{-1} (355 nm) excitation assuming biexponential decay.

	c/ M	E_{laser} /mJ	A_{long}/A_{short}	τ_{long} /μs	τ_{short} /ns
A (ns)	1.3×10^{-6}	5.2	0.72	6.9	340
	1.3×10^{-6} [a]	1.6[a]	0.72[a]	7.0[a]	350[a]
	1.3×10^{-6}	0.80	0.61	7.1	360
	1.8×10^{-5}	1.6	0.70	4.5	320
	1.4×10^{-5} [b]	0.90[b]	0.62[b]	5.4[b]	330[b]
	5.8×10^{-6} [a, c]	1.6[a, c]	0.20[a, c]	0.14[a, c]	21[a, c]
B (ns)	9.8×10^{-7}	5.2	0.63	6.8	330
	9.8×10^{-7} [a]	1.6[a]	0.62[a]	6.9[a]	360[a]
	9.8×10^{-7}	0.80	0.63	6.9	340
	1.8×10^{-5}	1.6	0.664	4.3	300
	9.4×10^{-6} [b]	10[b]	0.57[b]	5.7[b]	320[b]
C (ns)	1.0×10^{-5}	5.2	0.025	3.2	4.2
	1.0×10^{-5} [a]	1.6[a]	0.022[a]	4.2[a]	4.0[a]
	2.4×10^{-5}	1.6	0.025	3.3	3.8
	2.3×10^{-5} [b]	0.90[b]	0.013[b]	3.2[b]	3.8[b]
	5.8×10^{-5} [b, d]	0.75[b, d]	1.0[b, d]	0.034[b, d]	2.2[b, d]

[a] used for fits of rate constants and triplet CS state population maxima with TENUA[1]

[b] excitation at 24 000 cm^{-1} (416 nm). [c] in MeCN. [d] in oxygen saturated toluene.

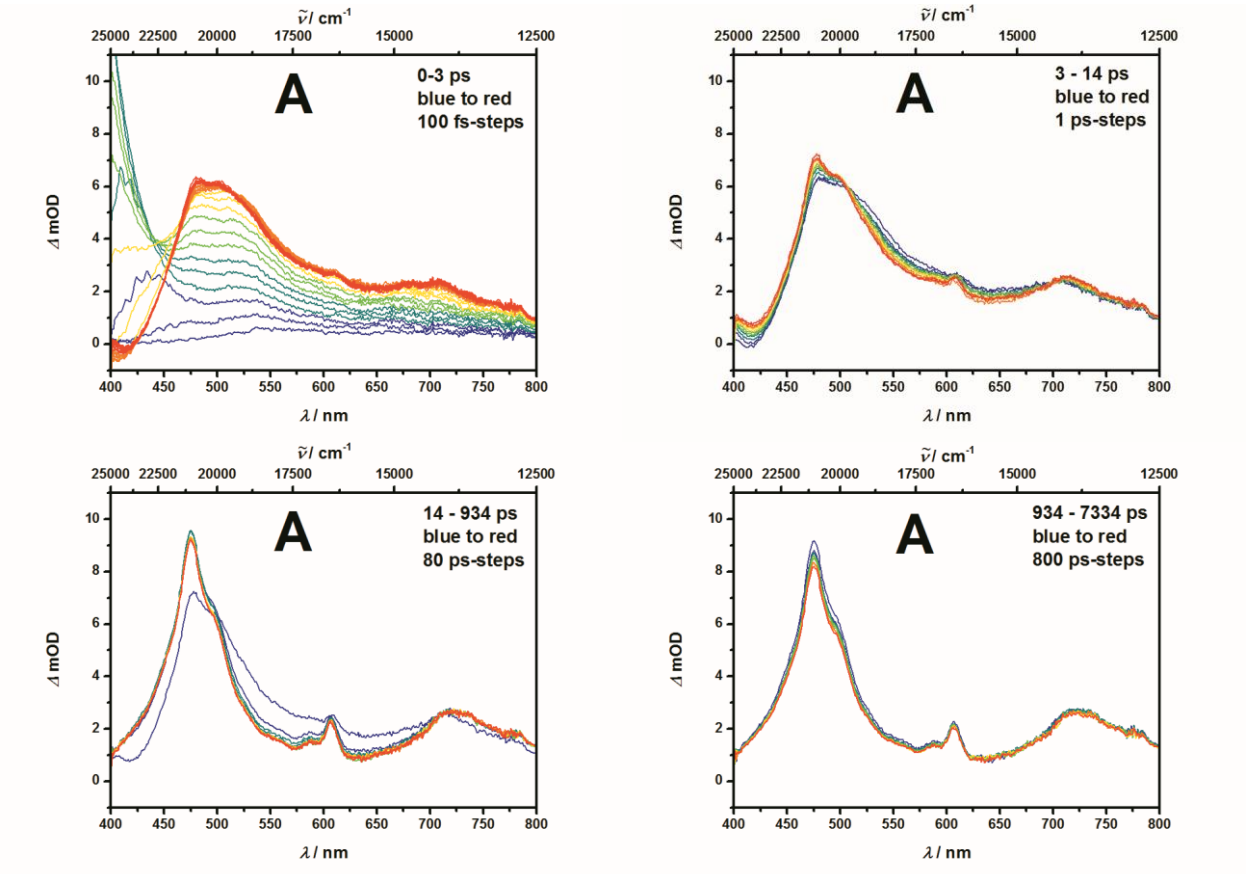


Figure S1. Original raw data of fs-transient absorption data only corrected for chirp and scattered light (excitation at 28200 cm^{-1} [355 nm]) of **A** in toluene.

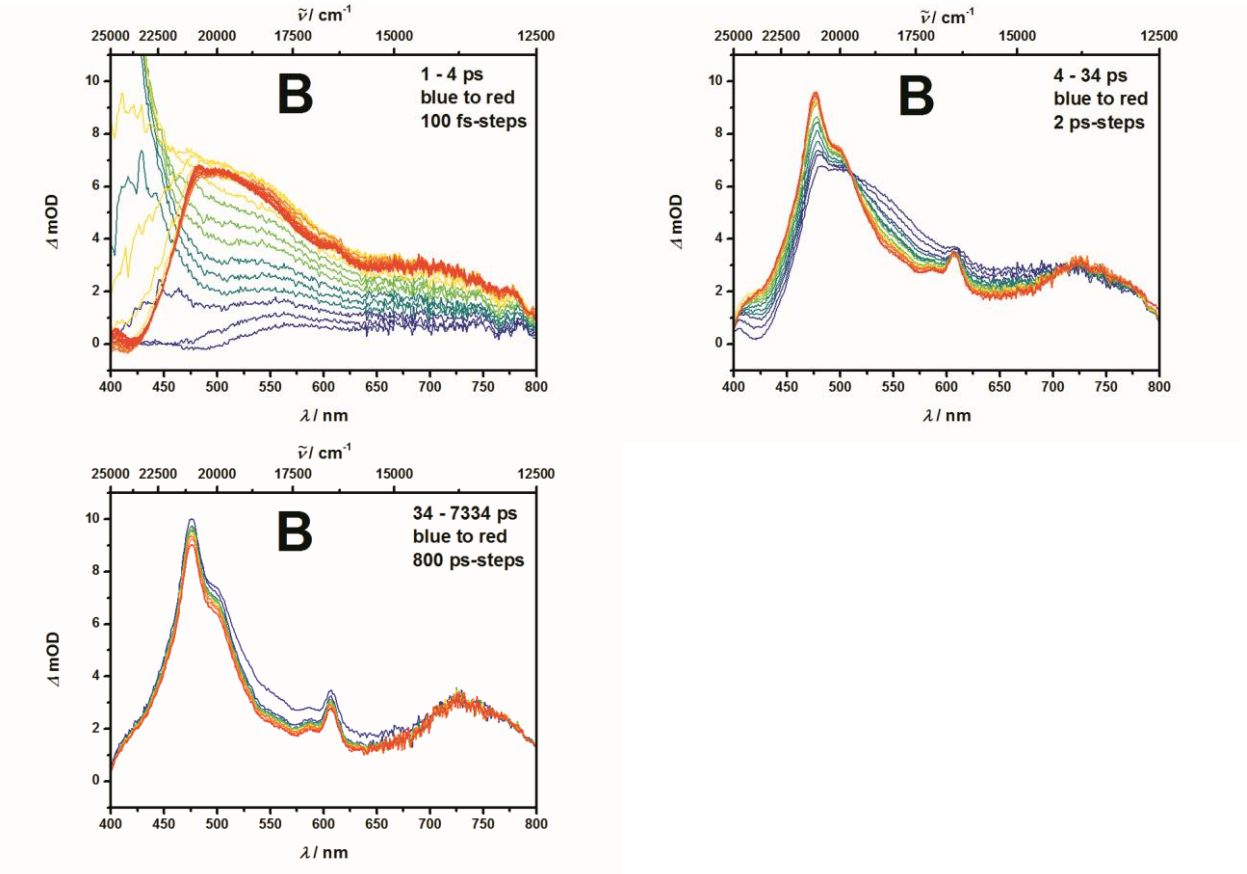


Figure S2. Original raw data of fs-transient absorption data only corrected for chirp and scattered light (excitation at 28200 cm^{-1} [355 nm]) of **B** in toluene.

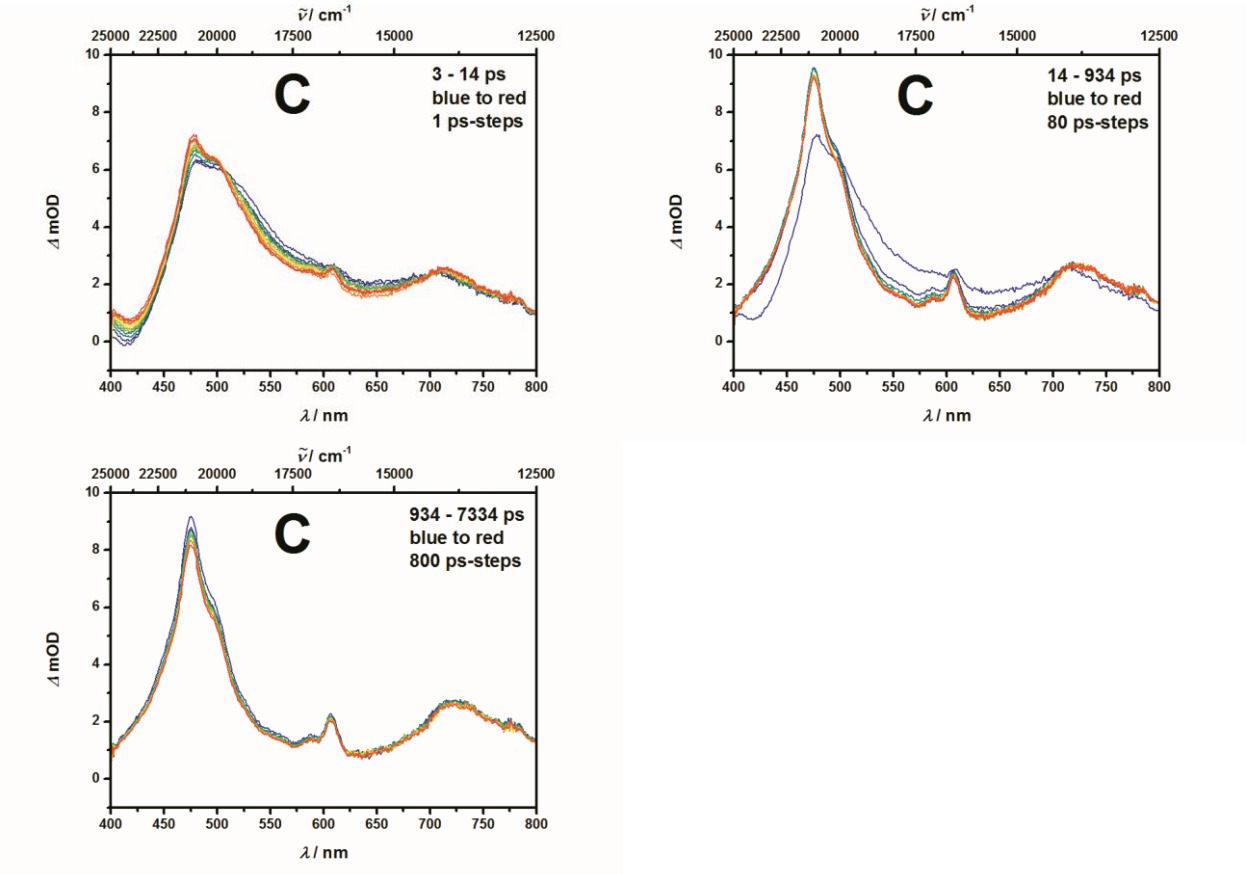


Figure S3. Original raw data of fs-transient absorption data only corrected for chirp and scattered light (excitation at 28200 cm^{-1} [355 nm]) of **C** in toluene.

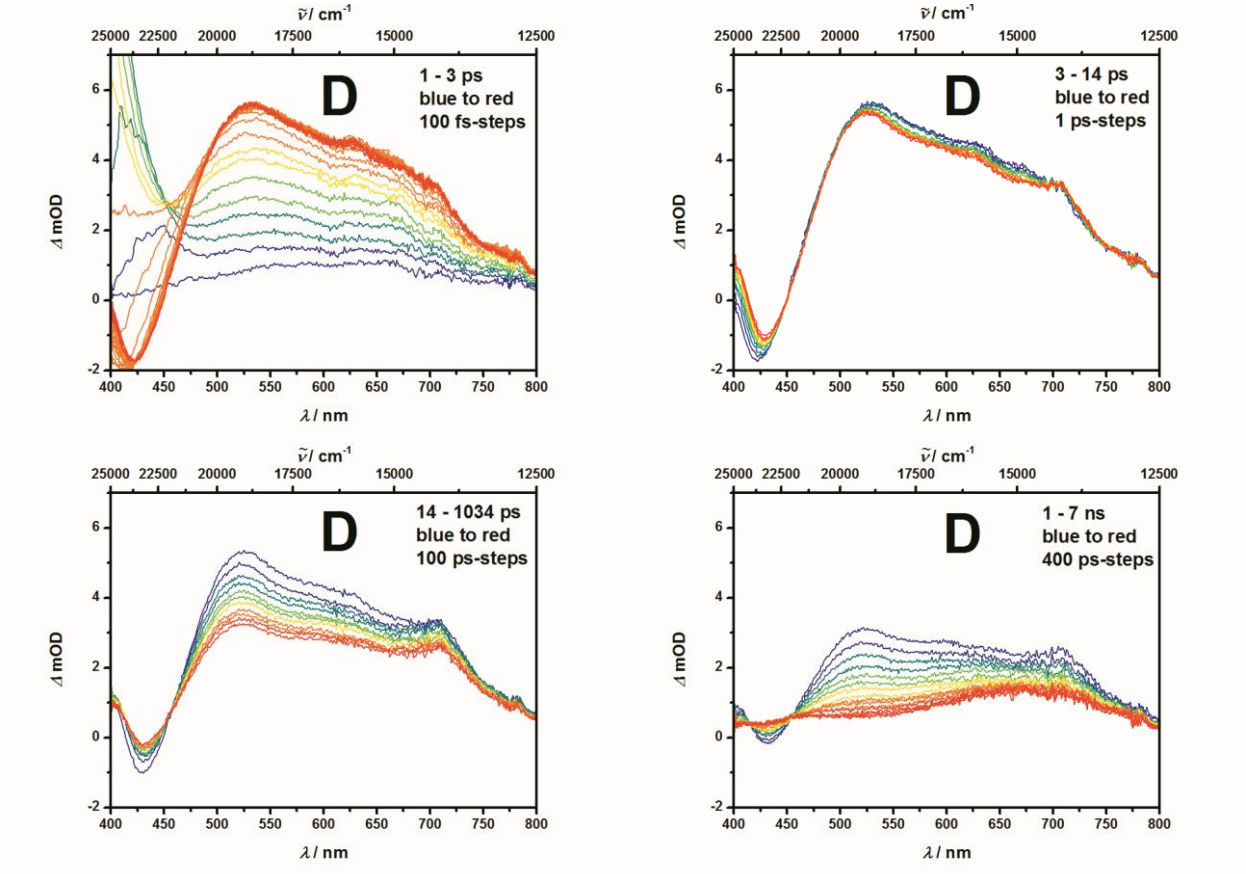


Figure S4. Original raw data of fs-transient absorption data only corrected for chirp and scattered light (excitation at 28200 cm^{-1} [355 nm]) of **D** in toluene.

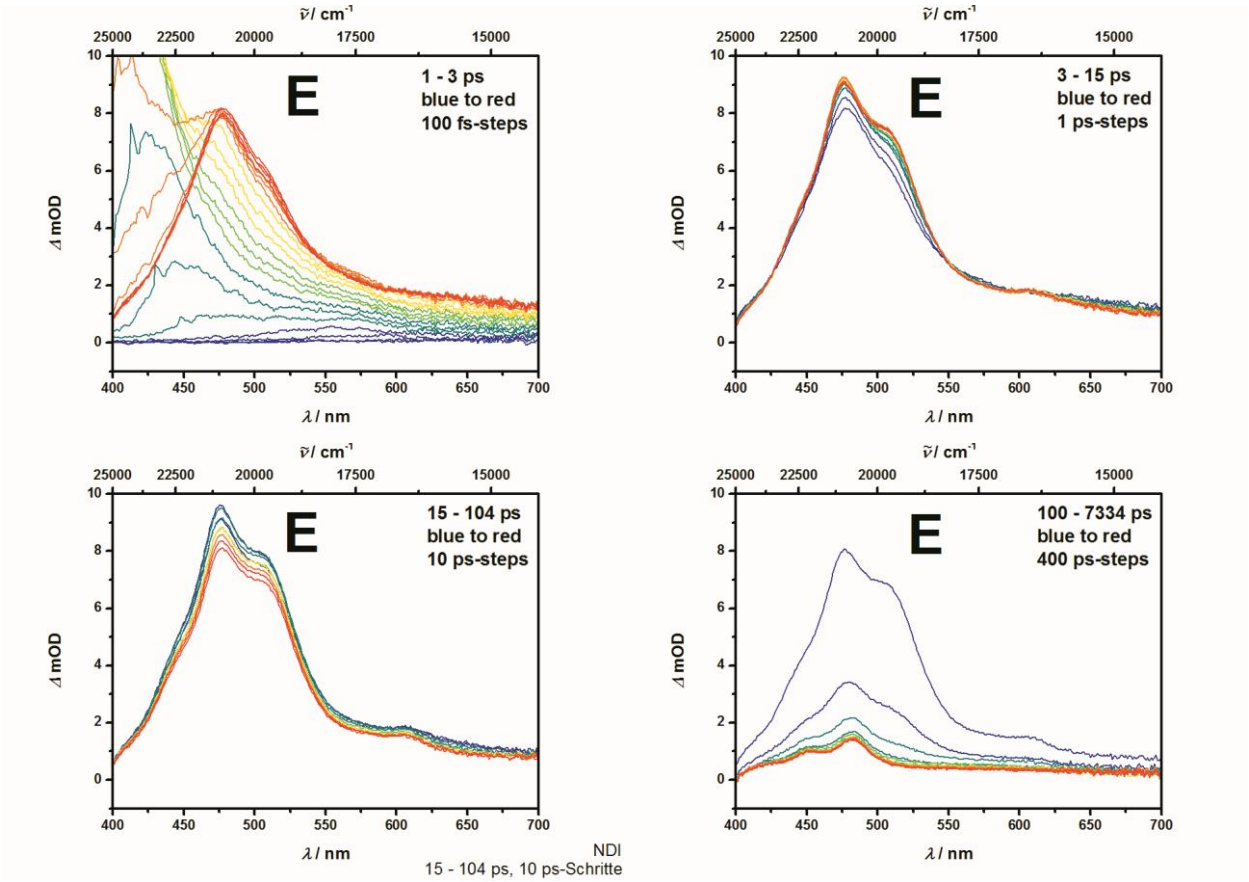


Figure S5. Original raw data of fs-transient absorption data only corrected for chirp and scattered light (excitation at 28200 cm^{-1} [355 nm]) of **E** in toluene.

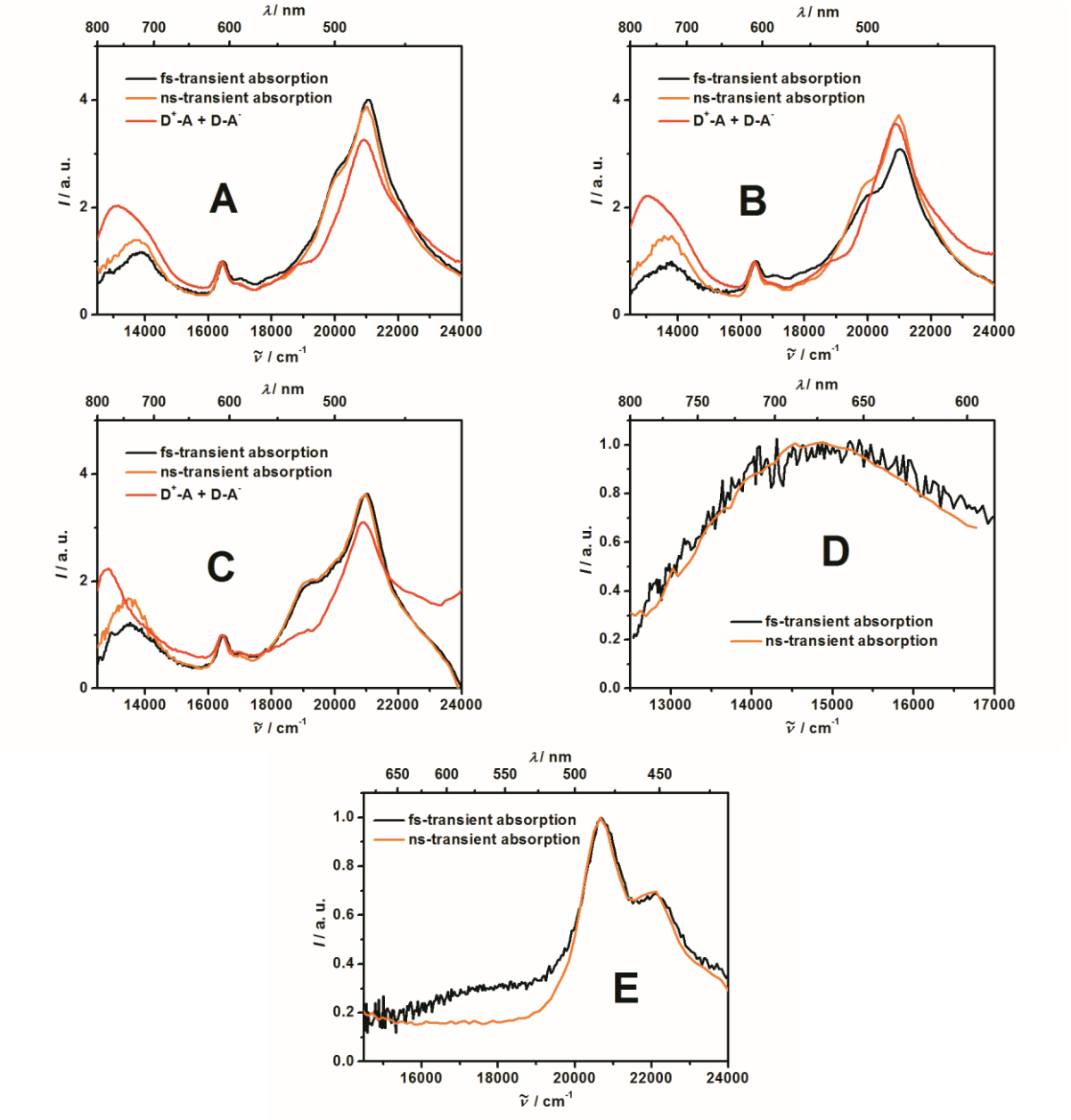


Figure S6. CS state spectra of **A**, **B** and **C** and triplet spectra of **D** and **E**: superposition of the normalized "final" spectra of **A**, **B**, **C, D** and **E** obtained by fs-transient absorption spectroscopy in toluene, ns-transient transient absorption spectroscopy in toluene (excitation at 28 200 cm^{-1} [355 nm]), **A** and **B** averaged over 8 ns and **C** averaged over 2 ns, **D** and **E** averaged over 0.5 μs) and in case of **A**, **B** and **C** the sum of the monoanion and monocation spectra from spectroelectrochemistry in dichloromethane (0.2 M tetrabutylammonium hexafluorophosphate).

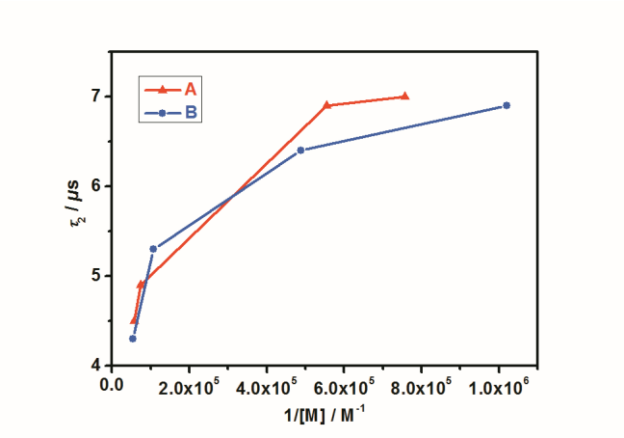


Figure S7. Plot of the long lifetime τ_{long} (from Table S1) vs. 1/concentration of the dyads **A** and **B**.

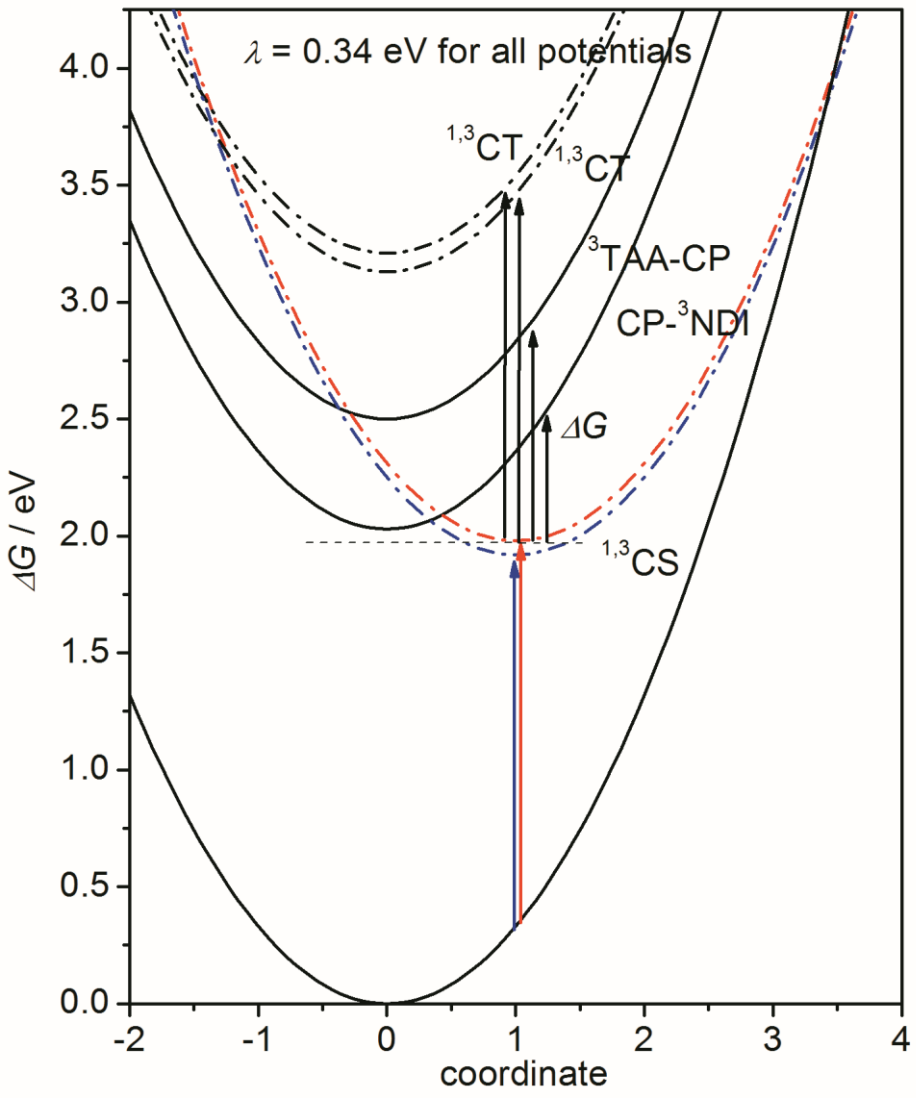


Figure S8. Singlet and triplet CS, CT and local states that are taken into account for second order perturbation interaction to estimate the 2*J* coupling by eq. 3. The red and blue arrows correspond to the TD-DFT calculations of excitation energies at CAM-B3LYP/6-31G* level of theory whose difference yields the 2*J*.[2]

Absolute energy of the first excited state structure of B used for the TD-DFT-calculations in Hartree optimized at CAM-B3LYP/6-31G* level of theory:

E_h=–3313.1310703.

Cartesian Coordinates of the optimized geometry of the excited state of B at CAM-B3LYP/6-31G* level of theory[2]:

C –15.6055 –2.7033 –0.6736

C –14.4544 –2.7656 0.1263

C –13.6401 –1.6641 0.2619

C –13.9532 –0.4693 –0.4042

C –15.1022 –0.4058 –1.1937

C –15.9254 –1.5116 –1.3327

C –15.4098 3.2663 1.0641

C –14.9644 4.4042 0.3732

C –13.9039 4.2920 –0.5315

C –13.3017 3.0605 –0.7357

C –13.7384 1.9304 –0.0419

C –14.8079 2.0460 0.8590

N –13.1241 0.6717 –0.2586

C –11.7471 0.5578 –0.3277

C –11.1485 –0.4530 –1.1145

C –9.7827 –0.5592 –1.1870

C –8.9438 0.3264 –0.4720

C –9.5494 1.3302 0.3188

C –10.9142 1.4492 0.3871

C –7.5483 0.2154 –0.5451

C –6.3354 0.1278 –0.6107

C –4.9274 0.0660 –0.6842

C –4.2786 –0.9130 –1.4773

C –2.9101 –0.7553 –1.6491

C –2.1774 0.0910 –0.8232

C –2.7942 0.8180 0.2034

C –4.1751 0.9191 0.1466

C –4.0482 –2.9268 0.4509

C –4.7566 –2.2530 1.4463

C –4.0982 –1.3726 2.2958

C –2.7300 –1.1386 2.1768

C –1.9838 –2.0349 1.3877

C –2.6590 –2.9203 0.5369

C –4.7311 –3.3790 –0.8193

C –2.0092 1.2277 1.4283

C –2.1482 0.1820 2.6215

C –4.9581 –2.1990 –1.8756

C 2.0376 –1.5342 1.0349

C 2.7657 –2.2273 0.0622

C 4.1216 –1.9941 –0.0967

C 4.7745 –1.0699 0.7136

C 4.0588 –0.3858 1.6916

C 2.7021 –0.6122 1.8507

N 6.1704 –0.8214 0.5427

C 7.0443 –1.9363 0.6267

C 6.5645 0.5203 0.3001

O 5.7137 1.4040 0.2442

C 7.9861 0.7457 0.1303

O 6.5848 –3.0556 0.8317

C 8.4566 –1.6521 0.4607

C 8.4558 2.0495 –0.1157

C 9.8020 2.2895 –0.2726

C 10.7295 1.2368 –0.1900

C 10.2900 –0.0812 0.0532

C 8.8924 –0.3326 0.2169

C 11.1980 –1.1566 0.1391

C 10.7330 –2.4600 0.3829

C 9.3875 –2.7042 0.5409

C 12.1482 1.5190 –0.3524

C 12.6265 –0.9260 –0.0254

N 13.0203 0.4110 –0.2595

O 12.5978 2.6409 –0.5576

O 13.4674 –1.8159 0.0303

C 14.4239 0.6664 –0.4100

C 15.0849 1.5004 0.4838

C 16.4411 1.7424 0.3362

C 17.1840 1.1606 –0.6965

C 16.5012 0.3262 –1.5802

C 15.1386 0.0830 –1.4434

C 18.6847 1.4514 –0.8138

C 19.3267 0.7319 –2.0057

C 19.3993 0.9843 0.4666

C 18.9040 2.9639 –0.9949

O –16.3310 –3.8302 –0.7381

C –17.5165 –3.8428 –1.5180

O –15.6186 5.5434 0.6455

C –15.2173 6.7400 –0.0039

C –0.5646 –1.9030 1.2892

C 0.6292 –1.7433 1.1782

H –14.2363 –3.6929 0.6430

H –12.7646 –1.7117 0.9001

H –15.3436 0.5137 –1.7151

H –16.8037 –1.4410 –1.9609

H –16.2272 3.3789 1.7666

H –13.5541 5.1504 –1.0899

H –12.4952 2.9708 –1.4551

H –15.1465 1.1729 1.4053

H –11.7760 –1.1226 –1.6894

H –9.3307 –1.3187 –1.8139

H –8.9170 2.0007 0.8886

H –11.3620 2.2068 1.0181

H –2.3777 –1.4217 –2.3209

H –1.0938 0.0681 –0.8774

H –4.7069 1.5615 0.8421

H –5.8424 –2.3028 1.4655

H –4.6819 –0.7490 2.9684

H –2.0703 –3.4962 –0.1711

H –4.1337 –4.1563 –1.3033

H –5.7075 –3.8213 –0.5990

H –0.9535 1.3156 1.1634

H –2.3316 2.2076 1.7934

H –1.1592 0.0524 3.0668

H –2.7964 0.6147 3.3891

H –4.5811 –2.5323 –2.8465

H –6.0322 –2.0353 –1.9900

H 2.2605 –2.9493 –0.5707

H 4.6871 –2.5379 –0.8418

H 4.5695 0.3378 2.3132

H 2.1475 –0.0738 2.6122

H 7.7269 2.8487 –0.1751

H 10.1832 3.2859 –0.4611

H 11.4655 –3.2561 0.4416

H 9.0108 –3.7022 0.7299

H 14.5275 1.9689 1.2863

H 16.9286 2.4021 1.0478

H 17.0265 –0.1539 –2.3972

H 14.6304 –0.5785 –2.1350

H 19.2295 –0.3552 –1.9235

H 18.8808 1.0435 –2.9556

H 20.3953 0.9678 –2.0471

H 19.0130 1.4938 1.3539

H 19.2651 –0.0916 0.6165

H 20.4742 1.1900 0.4030

H 18.5052 3.5347 –0.1516

H 19.9738 3.1891 –1.0766

H 18.4084 3.3229 –1.9024

H –17.9293 –4.8449 –1.4134

H –18.2405 –3.1094 –1.1478

H –17.2976 –3.6470 –2.5729

H –15.8733 7.5198 0.3796

H –14.1775 6.9881 0.2335

H –15.3406 6.6608 –1.0891

Fits of decay curves with TENUA

For the fits of the baseline corrected normalized decay curves from ns-transient absorption spectroscopy of the dyads with TENUA[1] the following script (used for **A**) was adapted for each compound. SCS is the concentration of the singlet charge separated state, TCS the concentration of the triplet charge separated state, A1 the overall starting concentration of the CS states and S0 the concentration of the ground state. Starting values for the rate constants where estimated from the reciprocal values of the lifetimes of the long and short component of the biexponential fits ($k(+1)=(1/(\tau_{long}))$ ×3 and $k(+2)=1/\tau_{short}$). A1 and the ratio of the starting concentrations of SCS and TCS were fitted manually.

Script:

SCS<->TCS; SCS<->S0;

k(–1)=A2*k(+1);

k(+1) : 4.3E5;

k(+2) : 2.9E6 A1 : 0.97;

S0 : 0.01;

A2 : 1/3;

TCS : 0.25*(A1);

SCS : 0.75*(A1);

*output

sum(SCS+TCS); sum2=TCS;

*script (“sum”), (“normalizeddecaycurve”);

go varying k(+1), k(+2)

Time Constants:

startTime : 0; endTime: 3.65E–5; timeStep: 1.0E–7; time: 0; epsilon: 1.0E–4

Reference

[1] D. Wachsstock, **2007**.

[2] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. Montgomery, J. A., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.