Electronic Supplementary Information (ESI)

N-Heterotriangulene chromophores with 4-pyridyl anchors for dye-sensitized solar cells

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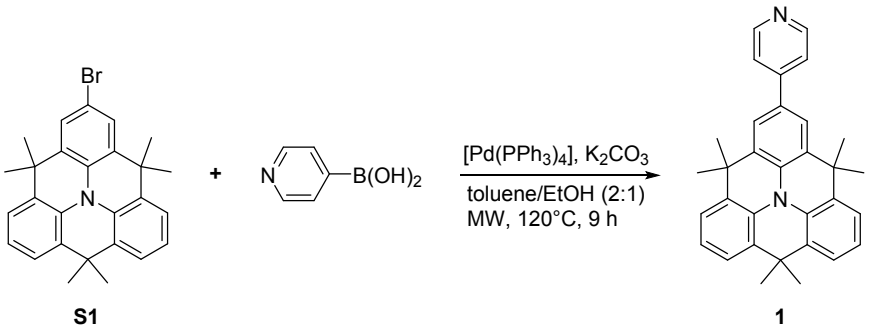
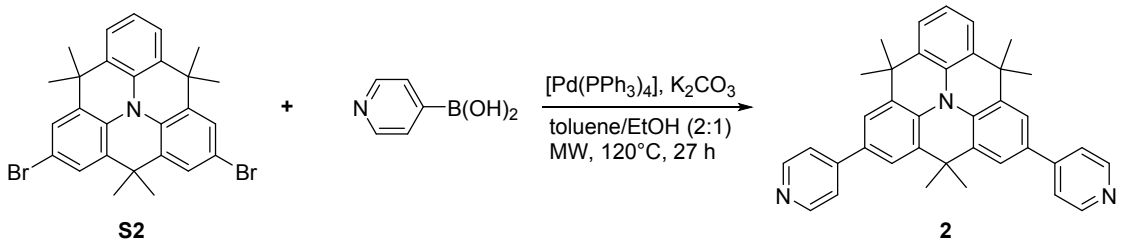
1 Experimental data and compound characterization

General procedures and methods. Reagents were purchased reagent grade from commercial suppliers and used without further purification. Toluene was dried over molecular sieves (4 Å) and distilled over sodium and EtOH was distilled over magnesium. $MgSO_4$ was used as drying agent after aqueous work-up. All microwave reactions were performed in septa capped Biotage® microwave vials (10–20 mL) using Biotage® Initiator+ with stirring and the reaction temperature was controlled by the Biotage® Initiator+ software. ^1H and ^{13}C NMR spectra were recorded on a Bruker Avance 300 spectrometer (300 MHz for ^1H, 75 MHz for ^{13}C). NMR spectra were referenced to the residual solvent signal (^1H: $CDCl_3$ 7.24 ppm; ^{13}C: $CDCl_3$ 77.0 ppm) and recorded at ambient probe temperature. Coupling constants (*J*) are given in Hz and the apparent resonance multiplicity is reported as br (broad), s (singlet), d (doublet), t (triplet), or m (multiplet). $CDCl_3$ (Deutero GmbH, 99.8%) was stored over molecular sieves (4 Å). IR spectra were recorded on a Varian 660-IR spectrometer as solids in ATR-mode and characteristic IR absorptions are reported in cm^{-1} and denoted as strong (s), medium (m), and weak (w) as well as shoulder (sh). UV/vis measurements were performed on a Varian Cary 5000 UV/vis/NIR spectrophotometer at ambient probe temperature. Emission spectra were recorded using a Horiba Jobin Yvon Fluoromax-4 spectrofluorometer. Cyclic voltammetry was performed on a computer-controlled BAS CV-50W instrument at ambient probe temperature in CH_2Cl_2 solutions (1.5 mM) containing 0.1 M *n*-Bu_4NPF_6 as supporting electrolyte at a scan rate of 0.15 V s^{-1}. Pt wire was used as counter electrode, $Ag/AgNO_3$ as reference electrode, and Pt as working electrode. The potential values ($E½$) were calculated using the following equation $E½ = (E_{red} + E_{ox})/2$, where E_{red} and E_{ox} correspond to the cathodic and anodic peak potentials, respectively. Mass spectra were obtained from a Bruker 9.4T Apex-Qe FTICR (MALDI), Bruker micro TOF II (ESI), and Bruker maxis 4G (APPI) instruments. Melting points were determined on a Büchi M-560 melting-point apparatus in open capillaries and are reported uncorrected. "Decomp." refers to decomposition. TLC analyses were carried out on TLC plates from Macherey-Nagel (ALUGRAM® SIL G/UV254) and visualized via UV-light (264/364 nm) or standard coloring reagents. Column chromatography was performed using Merck Silica Gel 60M.



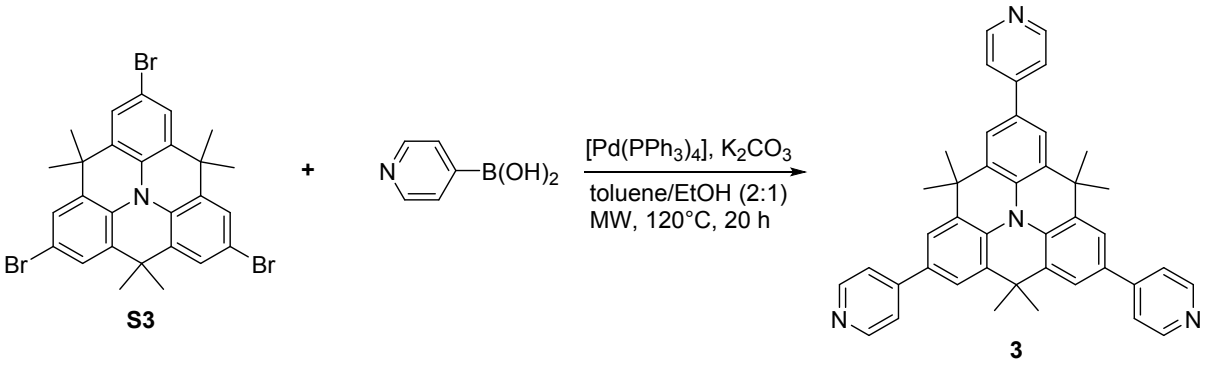
S1 **1**

4,4,8,8,12,12-Hexamethyl-2-pyridin-4-yl-4*H*,8*H*,12*H*-benzo[1,9]quinolizino [3,4,5,6,7-*defg*]acridine (1). Brominated *N*-heterotriangulene **S1** (20.0 mg, 45.0 µmol) and 4-pyridineboronic acid (8.30 mg, 68.0 µmol, 1.4 equiv.) were dissolved in dry toluene/EtOH (2:1, 1.5 mL) under nitrogen in a high pressure reaction vessel. $[Pd(PPh_3)_4]$ (0.50 mg, 0.50 µmol, 1.1 mol%) and degassed aqueous K_2CO_3-solution (2.0 M, 0.15 mL) were added and the vessel was sealed. The reaction was carried out at 120 °C for 9 h under microwave irradiation. After the reaction mixture was cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by column chromatography (SiO_2, acetone/CH_2Cl_2 1:4) to afford **1** (11.0 mg, 55%) as a yellow-orange solid. R_f = 0.52 (SiO_2, acetone/CH_2Cl_2 1:4); Mp 159.0 – 161.0 °C; UV/vis (CH_2Cl_2) λ_{max} (ε) 301 (20200), 318 (sh, 17600), 364 (18700) nm; IR (ATR) $\tilde{\nu}$ 2959 (m), 2921 (m), 2853 (w), 1724 (w), 1593 (m), 1428 (s), 1315 (m), 1293 (m), 821 (m), 795 (m), 743 (m) cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 8.64 (br s, 2H), 7.64 (s, 2H), 7.55 (br s, 2H), 7.39 (d, J = 7.8 Hz, 4H), 7.15 (t, J = 7.7 Hz, 2H), 1.67 (s, 12H), 1.64 (s, 6H) ppm; ^{13}C NMR (75.5 MHz, $CDCl_3$) δ 150.2, 148.1, 133.0, 131.8, 131.4, 130.4, 130.1, 129.7, 123.9, 123.5, 123.3, 121.8, 120.9, 35.7, 35.5, 33.4, 33.0 ppm; MALDI MS (sin) *m/z* 442 ($[M]^+$, 100), 427 ($[M - CH_3]^+$, 60). ESI HRMS (MeOH/MeCN, positive mode) calcd for $C_{32}H_{31}N_2$ $[M + H]^+$ 443.2482, found 443.2487; Anal. calcd for $C_{32}H_{30}N_2 \times 2H_2O$: C, 80.30; H, 7.16; N, 5.85; found: C, 80.34; H, 6.94; N, 5.40.



S2 **2**

4,4,8,8,12,12-Hexamethyl-2,6-dipyridin-4-yl-4*H*,8*H*,12*H*-benzo[1,9]quinolizino [3,4,5,6,7-*defg*]acridine (2). Dibrominated *N*-heterotriangulene **S2** (200 mg, 0.38 mmol) and 4-pyridineboronic acid (280 mg, 2.31 mmol, 6.1 equiv.) were dissolved in toluene/EtOH (2:1, 15 mL) under nitrogen in a high pressure reaction vessel. $[Pd(PPh_3)_4]$ (4.40 mg, 3.80 µmol, 1.0 mol%) and degassed aqueous K_2CO_3-solution (2.0 M, 2.0 mL) were added and the vessel was sealed. The reaction mixture was stirred at 120 °C for 27 h under microwave irradiation. After the reaction mixture was cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by column chromatography (SiO_2, acetone/CH_2Cl_2 1:4 → 1:1) to afford **2** (160 mg, 81%) as an orange solid. R_f = 0.31 (SiO_2, acetone/CH_2Cl_2 1:4); Mp ~248 °C (decomp.); UV/vis (CH_2Cl_2) λ_{max} (ε) 323 (15300), 376 (17300) nm; IR (ATR) $\tilde{\nu}$ 2964 (w), 2924 (w), 2853 (w), 1712 (w), 1596 (m), 1435 (s), 1315 (m), 1289 (m), 820 (m), 766 (w), 737 (w) cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 8.66 (d, J = 5.4 Hz, 4H), 7.67 (s, 4H), 7.55 (dd, J = 4.6, 1.5 Hz, 4H), 7.42 (d, J = 7.8 Hz, 2H), 7.18 (t, J = 7.7 Hz, 1H), 1.74 (s, 6H), 1.70 (s, 12H) ppm; ^{13}C NMR (75.5 MHz, $CDCl_3$) δ 150.2, 147.9, 132.5, 132.4, 131.0, 130.8, 130.4, 129.9, 123.9, 123.8, 122.3, 121.9, 120.9, 35.8, 35.7, 33.3, 33.0 ppm; LDI MS *m/z* 519 ($[M]^+$, 100), 504 ($[M - CH_3]^+$, 30). ESI HRMS (MeCN/toluene/THF, positive mode) calcd for $C_{37}H_{34}N_3$ $[M + H]^+$ 520.2747, found 520.2754; Anal. calcd for $C_{37}H_{33}N_3 \times H_2O$: C, 82.65; H, 6.56; N, 7.81; found: C, 82.82; H, 6.42; N, 7.95.



4,4,8,8,12,12-Hexamethyl-2,6,10-tripyridin-4-yl-4*H*,8*H*,12*H*-benzo[1,9]quinolizino [3,4,5,6,7-*defg*]acridine (3). Tribrominated *N*-heterotriangulene **S3** (80 mg, 0.13 mmol) and 4-pyridineboronic acid (82 mg, 0.67 mmol, 5.2 equiv.) were dissolved in dry toluene/EtOH (2:1, 6 mL) under nitrogen in a high pressure reaction vessel. $[Pd(PPh_3)_4]$ (1.5 mg, 1.3 μmol) and degassed aqueous K_2CO_3-solution (2.0 M, 0.6 mL) was added to the reaction mixture and the vessel was sealed. The reaction mixture was stirred at 120 °C for 20 h under microwave irradiation. After the reaction mixture was cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by column chromatography (SiO_2, EtOAc/MeOH, 9:1) to afford **3** (68 mg, 86%) as a red-orange solid. R_f = 0.04 (SiO_2, EtOAc); Mp ~260 °C (decomp.); UV/vis (CH_2Cl_2) λ_{max} (ε) 330 (12900), 373 (21700) nm; IR (ATR) $\tilde{\nu}$ 2965 (w), 2918 (m), 2851 (w), 1725 (w), 1593 (m), 1438 (s), 1311 (s), 1288 (m), 1260 (m), 893 (m), 820 (s), 795 (s), 764 (m), 727 (m) cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 8.67 (d, J = 5.7 Hz, 6H), 7.69 (s, 6H), 7.56 (d, J = 6.0 Hz, 6H), 1.76 (s, 18H) ppm; ^{13}C NMR (75.5 MHz, $CDCl_3$) δ 150.3, 147.8, 132.9, 132.1, 130.7, 122.3, 121.0, 35.9, 33.3 ppm; LDI MS *m/z* 596 ($[M]^+$, 100), 581 ($[M - CH_3]^+$, 90). ESI HRMS (CH_2Cl_2/MeCN, positive mode) calcd for $C_{42}H_{37}N_4$ $[M + H]^+$ 597.3013, found 597.2995; Anal. calcd for $C_{42}H_{36}N_4 \times 4H_2O$: C, 75.42; H, 6.63; N, 8.38; found: C, 74.93; H, 5.88; N, 8.12.

2 ^{1}H and ^{13}C NMR spectra

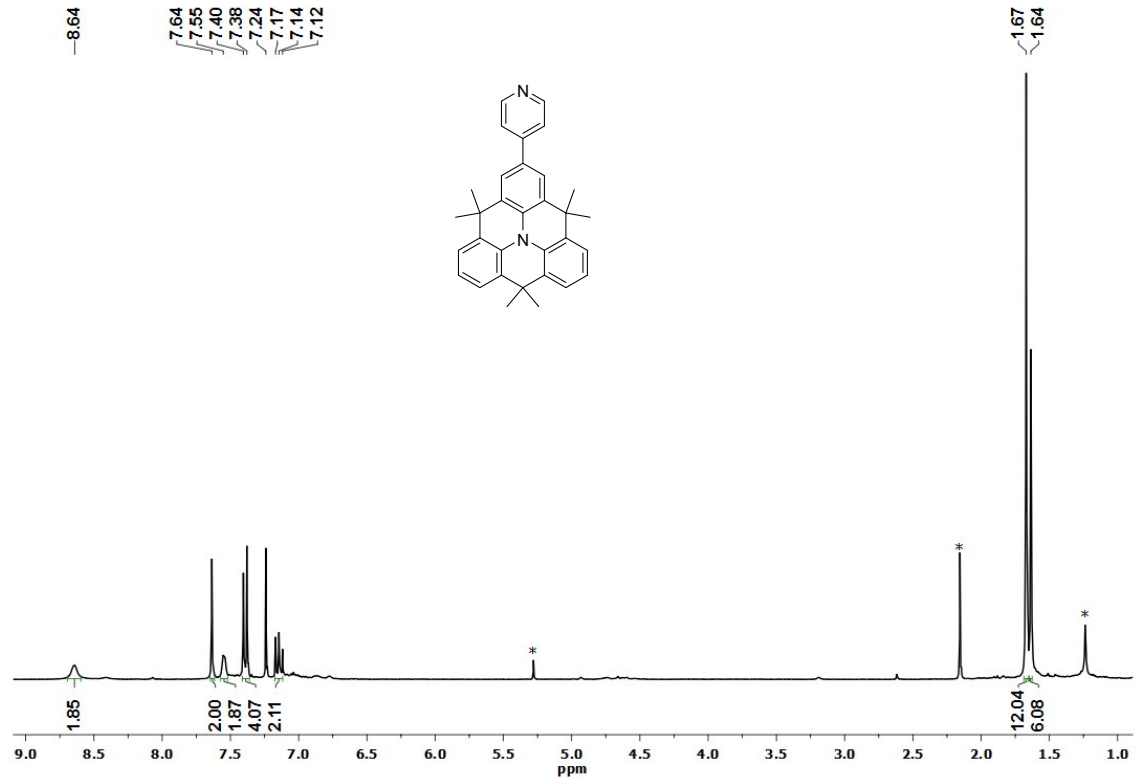


Fig. S1. ^{1}H NMR spectrum of **1** (300 MHz, $CDCl_3$); * residual solvents: CH_2Cl_2, acetone, hexanes.

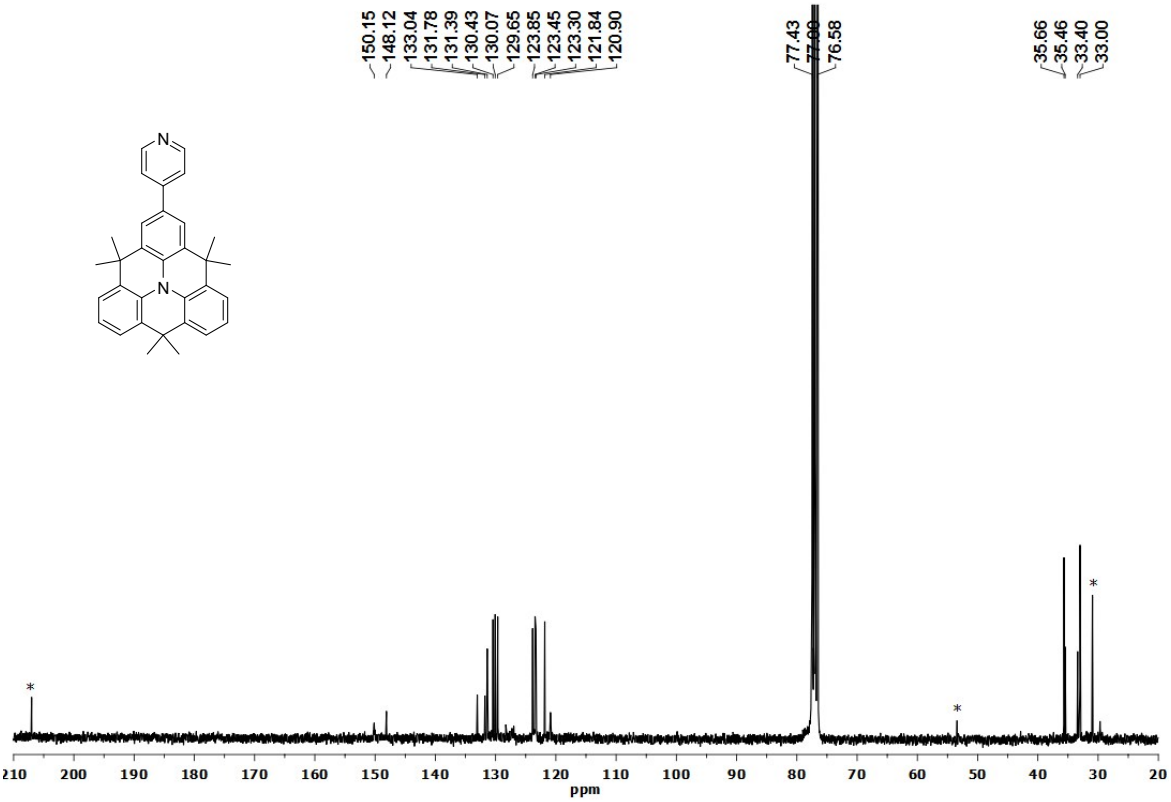


Fig.S2. ^{13}C NMR spectrum of **1** in (75.5 MHz, $CDCl_3$); * residual solvents: CH_2Cl_2, acetone.

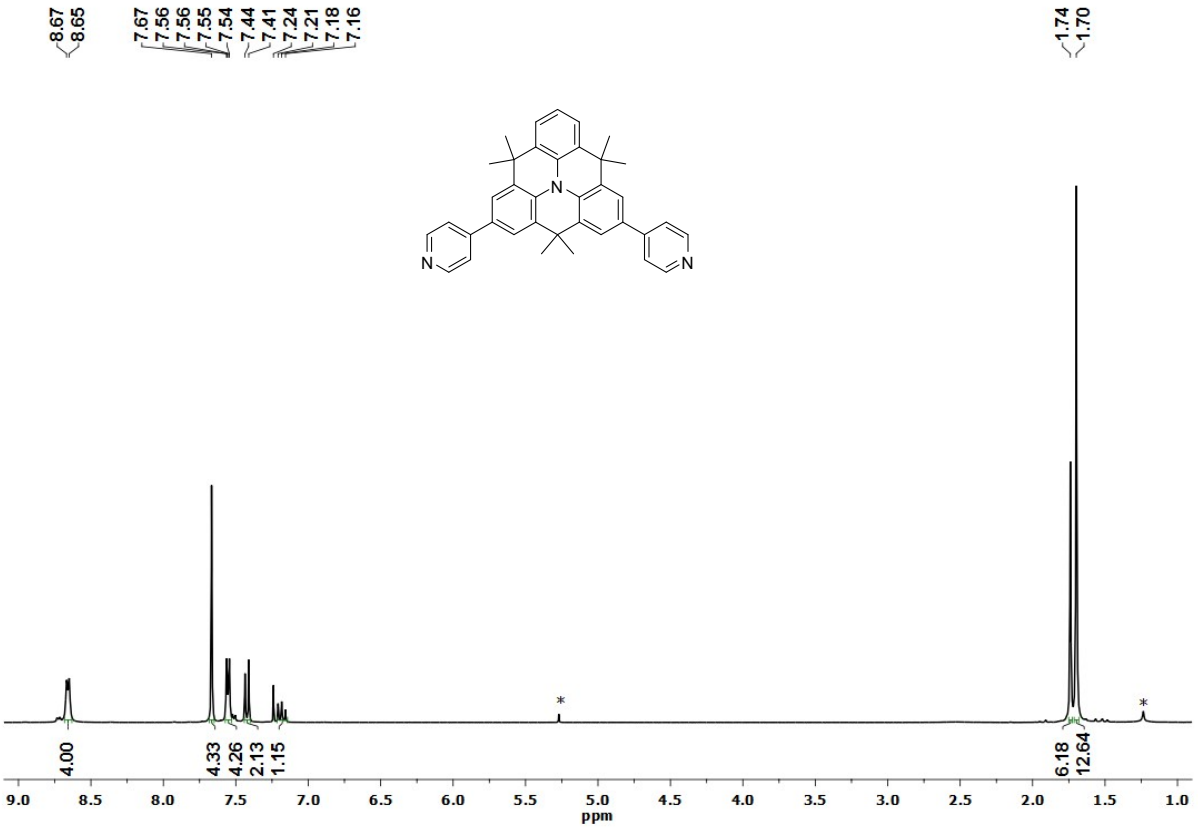


Fig. S3. ^{1}H NMR spectrum of **2** in (300 MHz, $CDCl_3$); * residual solvents: CH_2Cl_2, hexanes.

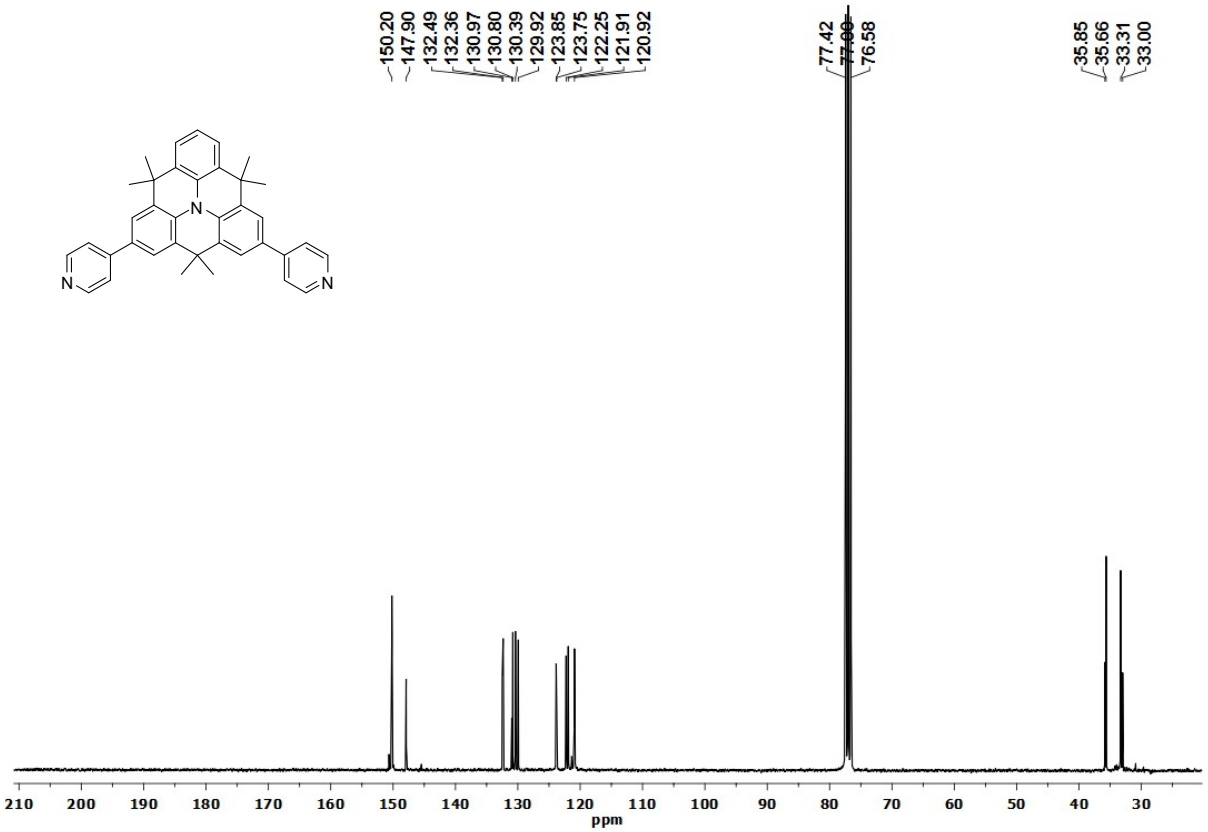


Fig.S4. ^{13}C NMR spectrum of **2** in (75.5 MHz, $CDCl_3$).

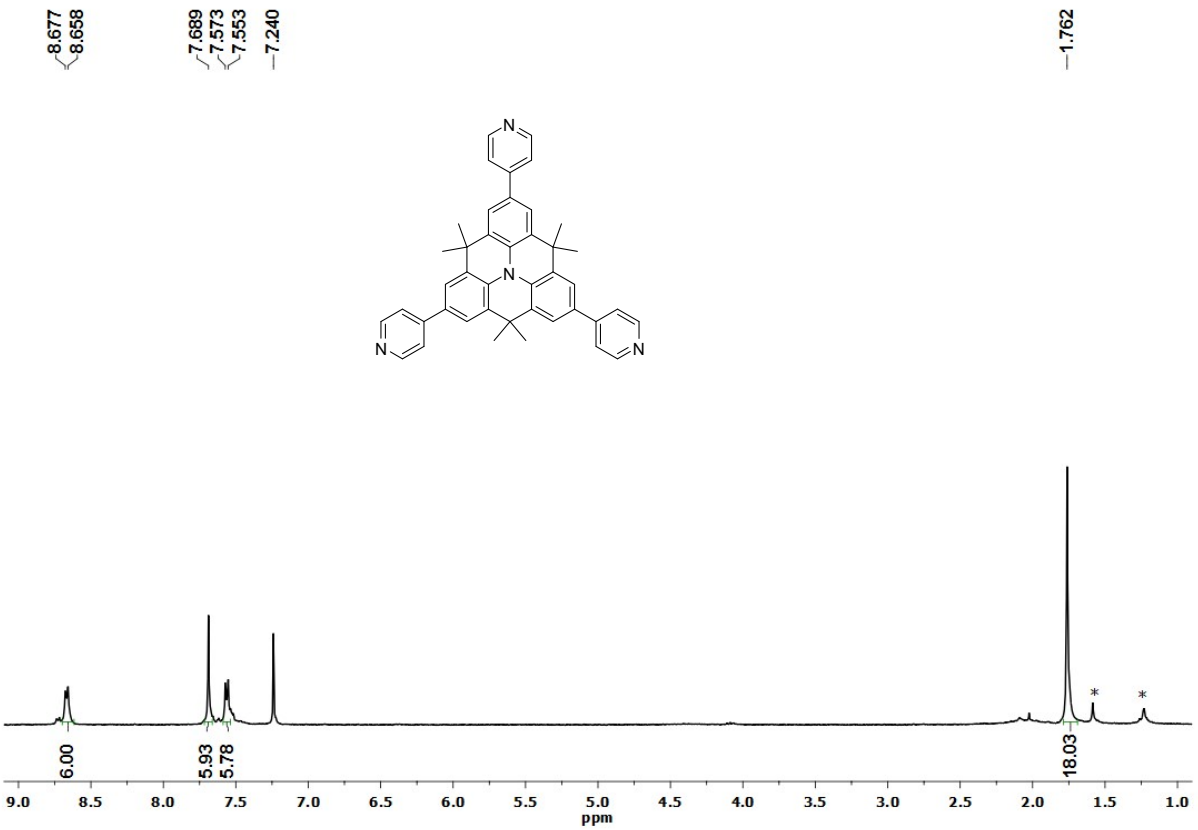


Fig. S5. ^{1}H NMR spectrum of **3** in (300 MHz, $CDCl_3$); * residual solvents: water, hexanes.

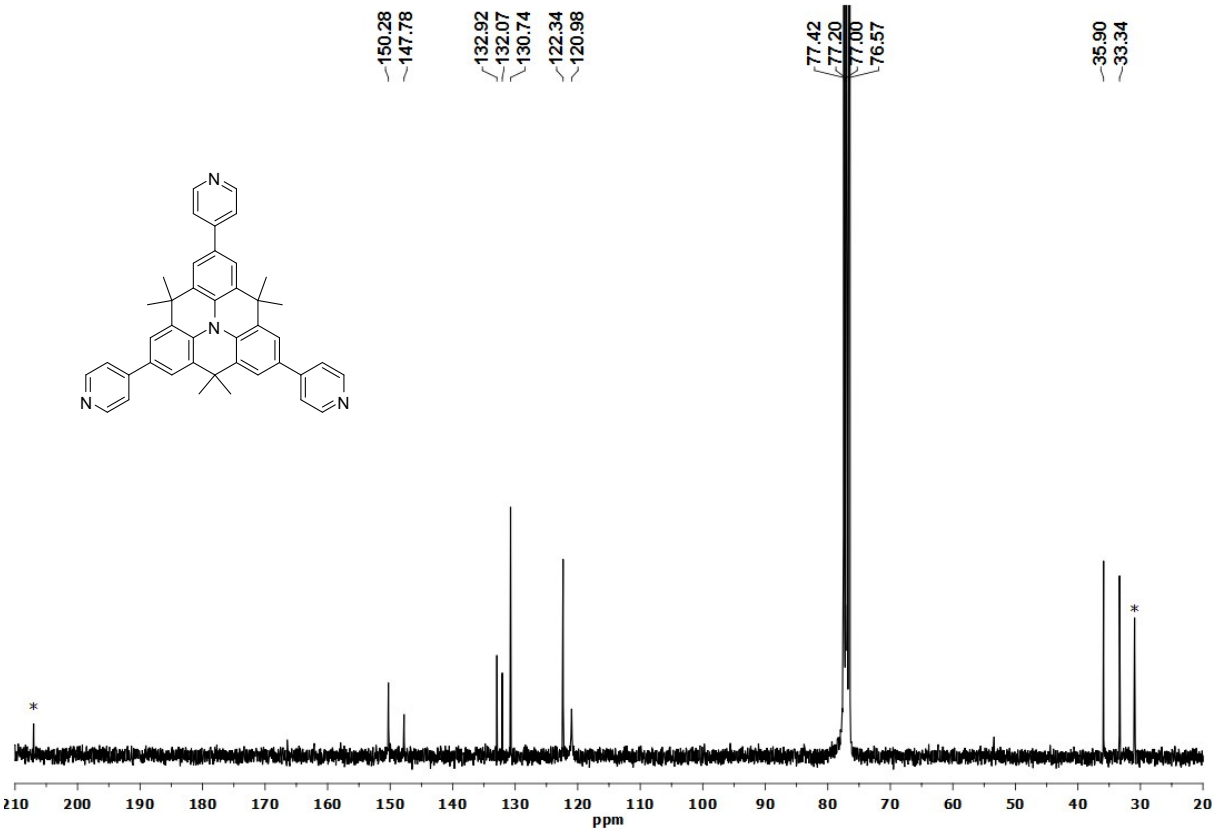


Fig. S6. ^{13}C NMR spectrum of **3** in (75.5 MHz, $CDCl_3$); * residual solvents: acetone.

3 X-Ray structure analysis

General. X-Ray crystallographic data was measured on a Supernova CCD diffractometer (Agilent) at 173 K. A suitable crystal was selected and mounted on a loop on a SuperNova, Dual, Cu at zero, Atlas diffractometer (CuKα, λ = 1.5418 Å). The crystal was kept at 173 K during data collection. Using Olex2,[1] the structure was solved with the ShelXS[2] structure solution program using direct methods and refined with the ShelXL[2] refinement package using least squares minimization. After full-matrix least-square refinement of the non-hydrogen atoms with anisotropic thermal parameters, the hydrogen atoms were placed in calculated positions using a riding model. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre (www.ccdc.cam.ac.uk/data_request/cif).

Single crystals of **2** suitable for X-ray crystallographic analysis were grown by slow evaporation of a solution of **2** in CH_2Cl_2/MeOH (1:2) at room temperature. The compound crystallizes in the monoclinic space group of $P2_1/c$ (no. 14) with one molecule of **2** in the asymmetric unit. $C_{37}H_{33}N_3$, M_w = 519.66; crystal dimensions: 0.21 × 0.16 × 0.04 mm^3; a = 15.0018(6) Å, b = 11.1825(4) Å, c = 16.9177(7) Å; $a = \gamma = 90°$, β = 110.262(4)°; V = 2662.46(17) Å^3, T = 173.00 (10) K, Z = 4, μ(Cu K_α) = 0.581, 7256 reflections measured, 4019 unique (R_{int} = 0.0534) which were used in all calculations. The final wR_2 was 0.1517 (all data) and R_1 was 0.0530 (>2σ(I)). CCDC 1441546

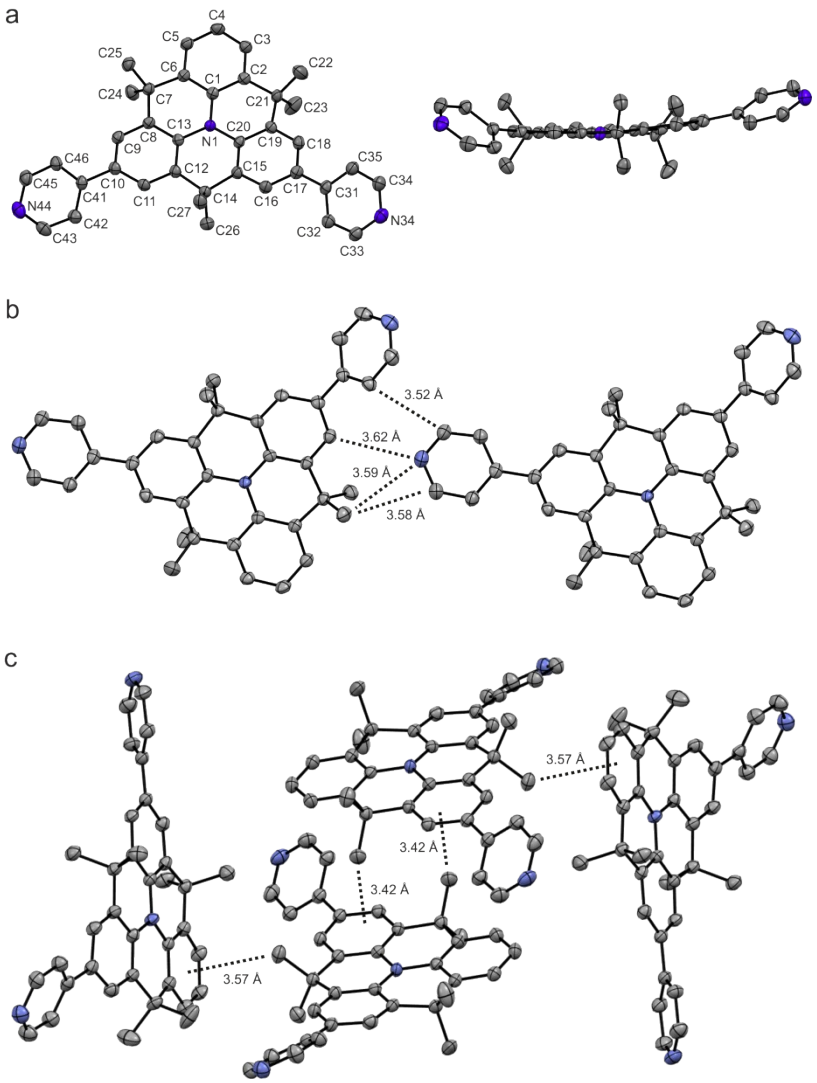


Fig. S7. a) Molecular structure of **2** in the solid state in top view (left) and side view (right) (50% probability level, H-atoms omitted for clarity). Selected bond lengths [Å], bond angles [°], and torsions angles [°]: C1–N1 1.424(3), C13–N1 1.424(3), C20–N1 1.427(3), C1–N1–C13 119.7(2), C1–N1–C20 119.77(19), C13–N1–C20 119.98(19), C18–C17–C31–C36 –40.7(4), C11–C10–C41–C42 27.6(4). b) and c) Illustration of the most important intermolecular interactions in the crystal packing of **2**.

4 UV/vis absorption and emission spectroscopy

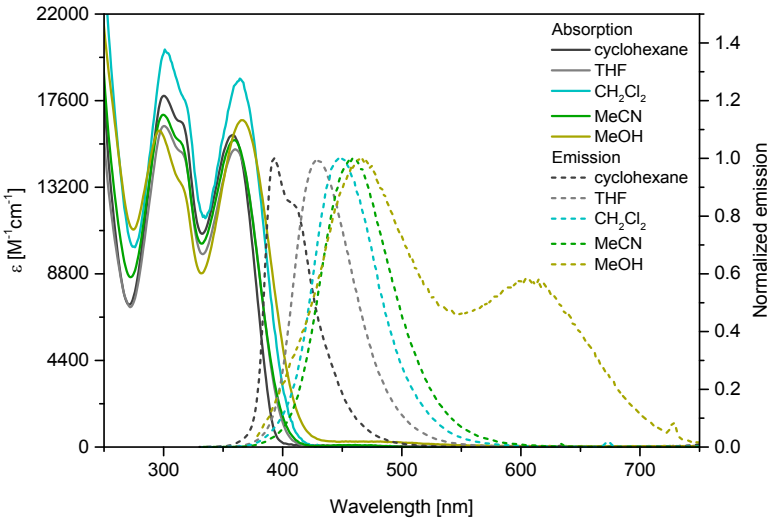


Fig. S8. UV/vis absorption (solid lines) and emission (dashed lines) spectra of **1** in different solvents at room temperature (cyclohexane: λ_{exc} = 315 nm, THF: λ_{exc} = 318 nm, CH_2Cl_2: λ_{exc} = 335 nm, MeCN: λ_{exc} = 316 nm, MeOH: λ_{exc} = 363 nm).

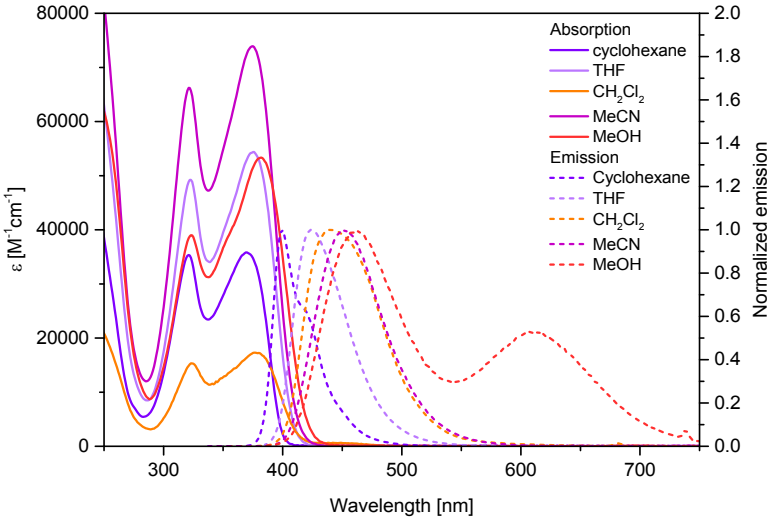


Fig. S9. UV/vis absorption (solid lines) and emission (dashed lines) spectra of **2** in different solvents at room temperature (cyclohexane: λ_{exc} = 321 nm, THF: λ_{exc} = 370 nm, CH_2Cl_2: λ_{exc} = 339 nm, MeCN: λ_{exc} = 323 nm, MeOH: λ_{exc} = 368 nm).

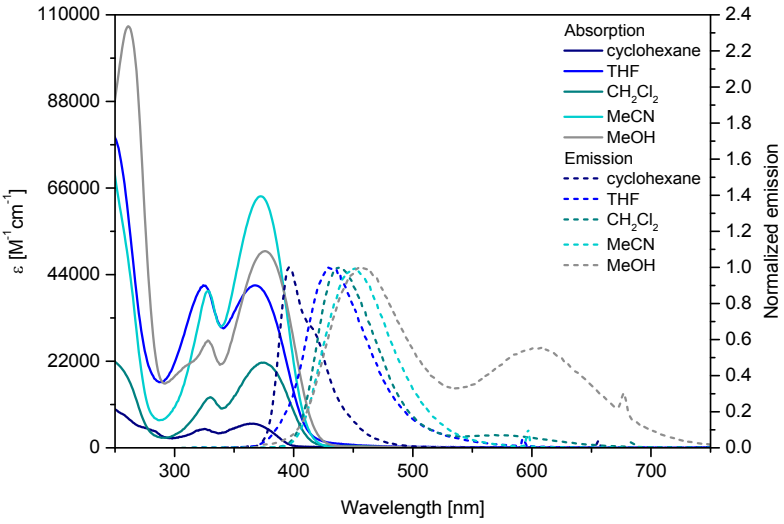


Fig. S10. UV/vis absorption (solid lines) and emission (dashed lines) spectra of **3** in different solvents at room temperature (cyclohexane: λ_{exc} = 327 nm, THF: λ_{exc} = 296 nm, CH_2Cl_2: λ_{exc} = 340 nm, MeCN: λ_{exc} = 298 nm, MeOH: λ_{exc} = 338 nm).

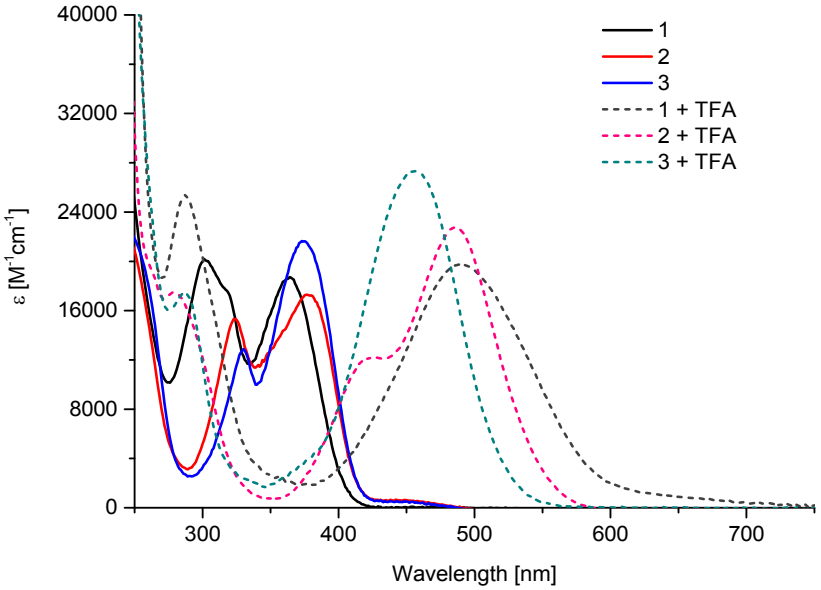


Fig. S11. UV/vis absorption spectra of compounds **1**–**3** in CH_2Cl_2 recorded at room temperature neat (solid lines) and after addition of an excess of trifluoroacetic acid (TFA; dashed lines).

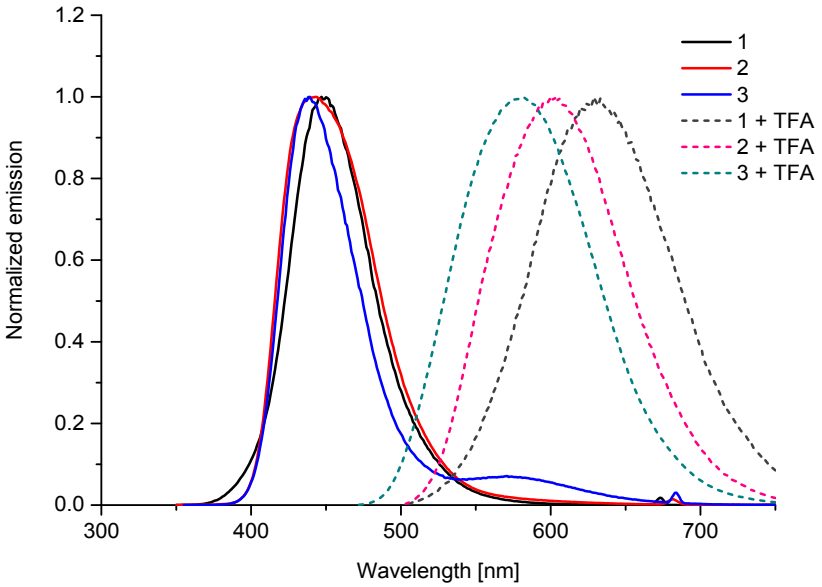


Fig. S12. UV/vis emission spectra of compounds **1**–**3** in CH_2Cl_2 recorded at room temperature neat (solid lines) and after addition of an excess of trifluoroacetic acid (TFA; dashed lines). **1**: λ_{exc} = 335 nm, **2**: λ_{exc} = 339 nm, **3**: λ_{exc} = 340 nm, **1**+TFA: λ_{exc} = 489 nm, **2**+TFA: λ_{exc} = 486 nm, **3**+TFA: λ_{exc} = 455 nm.

5 Dye-sensitized solar cell fabrication and characterization

General. All chemicals were purchased from chemical suppliers and used without further purification. $TiCl_4$ (0.09 M in HCl), guanidinium thiocyanate, 4-*tert*-butylpyridine, 1-butyl-3-methylimidazolium iodide, and H_2Cl_6Pt x H_2O were purchased from Sigma-Aldrich. TiO_2 paste (Ti-Nanoxide T/SP) and the sealing foil (Meltonix 1170-25) were purchased from Solaronix.

Fluorine-doped tin-oxide (FTO) substrates were sonicated for 15 min with a detergent solution, washed with deionized water, and again sonicated in isopropyl alcohol for 15 min. FTOs were immersed into a 40 mM aqueous $TiCl_4$ solution at 70 °C for 30 min and washed with water and EtOH. Treated substrates were sintered at 450 °C for 30 min. The transparent TiO_2 electrodes were prepared on FTO glass plates by using a doctor blade technique. The latter were gradually heated under air flow at 450 °C for 30 min. The thickness of TiO_2-based electrodes was 7 μm. The electrodes were immersed at around 80 °C in solutions of **1**, **2**, or **3** in EtOH for different times.

Fluorine-doped tin-oxide (FTO) substrates were sonicated for 15 min in acetone, subsequently with detergent solution, washed with deionized water, and again sonicated in isopropyl alcohol for 15 min. The ZnO electrodes were prepared on FTO glass plates by using a doctor blade technique and a home-made paste as previously reported.[3] The doctor blading procedure was repeated up to 3 times to reach similar electrode thickness as those in TiO_2 electrodes. The ZnO films were gradually heated under air flow up to 500 °C for 30 min. The electrodes were finally immersed at around 80 °C in an EtOH based dye solution (4×10^{-4} M) for different times. Please notice that, although an extensive family of chemicals were tested to desorb the dyes, *e.g.,* 0.1, 0.5, 1.0 M NaOH in H_2O, 1:1, 2:1 and 1:2 mixtures of 1 M NaOH and EtOH, 16.5% and 37% HCl in H_2O at room temperature as well as at 40 °C, conc. CH_3COOH, conc. CF_3COOH, no dye desorption could be achieved. We also used chenodeoxycholic acid (CDCA) as additive to avoid the formation of aggregates on the electrode surface, but independently of the molar concentrations (1:0.5, 1:1, 1:2, 1:4, 1:10 dye : CDCA) no dye adsorption was observed up to immersion times superior to 100 h.

For preparation of the counter-electrodes two holes (0.1 mm) were drilled into FTOs *via* sandblasting prior to the cleaning procedure (*vide supra*). FTOs were coated with a thin film of chloroplatinic solution (4.88 mM) in isopropyl alcohol. Thereby, always the same amount of chloroplatinic solution (26 μL) was used to assure the same coverage of the FTO. Then, the

slides were annealed to 390 °C for 15 min. For every measurement counter-electrodes were freshly prepared to assure reproducible results.

The photoanodes and the counter-electrodes were assembled into a sealed sandwich-type cell by heating at 130 °C with a controlled pressure using a hot-melt ionomer film (Surlyn). A solution of 0.6 M 1-butyl-3-methylimidazolium iodide 99%, 0.03 M iodine double sublimed, 0.1 M guanidine thiocyanate ≥99.0%, and 0.5 M 4-*tert*-butylpyridine 96% in a solvent mixture of acetonitrile and valeronitrile (85:15 v/v) was employed as electrolyte. The electrolyte was introduced through the aforementioned holes and the final cell was sealed immediately afterwards using another piece of Surlyn and a piece of microscope slide.

The photocurrent measurements were performed using a 150 W lamp (Xenon lamp, calibrated to 1000 W m^{-2} under AM 1.5G conditions with a Si-Reference cell (Oriel SRC-1000-TC-K-KG5-N). Current-voltage measurements were measured by using a potentiostat/galvanostat (PGSTAT30N, Autolab equipped with a frequency response analyzer module – FRA) in the range of -0.9 to 0.2 V. DSSCs were measured by using a shading mask with an aperture size according to the literature.[4] Incident photon-to-current efficiency (IPCE) spectra were measured by using Newport apparatus model 70104. For alpha-step thickness measurements of TiO_2- and ZnO-based electrodes, a Dektak XT profilometer from Bruker was utilized.

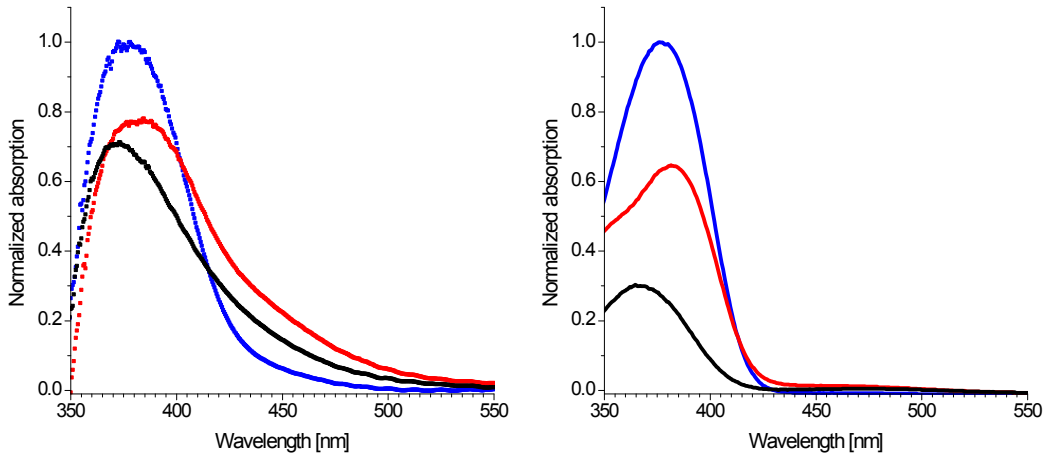


Fig. S13. UV/vis absorption spectra of **1** (black), **2** (red), and **3** (blue) adsorbed on transparent TiO_2 electrodes (left) and in EtOH solution (right).

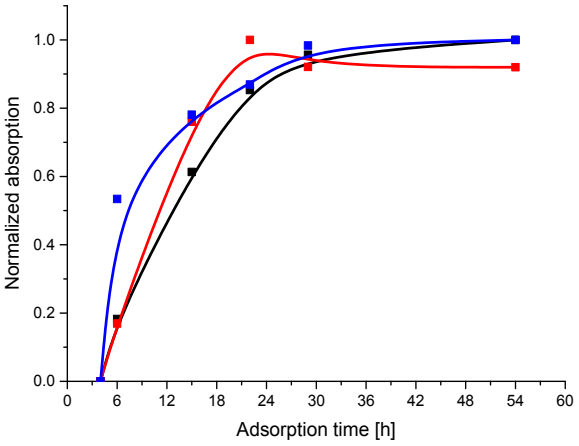


Fig. S14. Adsorption kinetics at 375 nm of **1** (black), **2** (red), and **3** (blue) on transparent TiO_2 electrodes.

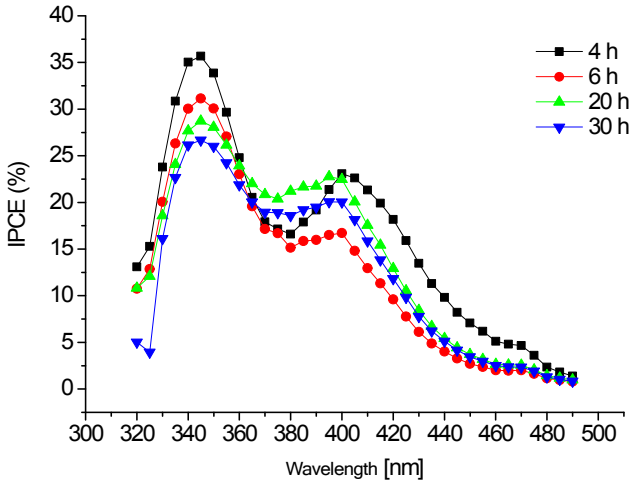


Fig. S15. IPCE spectra of TiO_2-based DSSCs with **1** at different adsorption times.

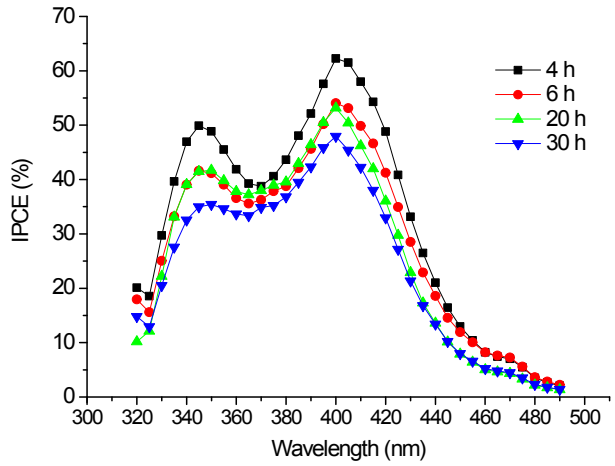


Fig. S16. IPCE spectra of TiO_2-based DSSCs with **3** at different adsorption times

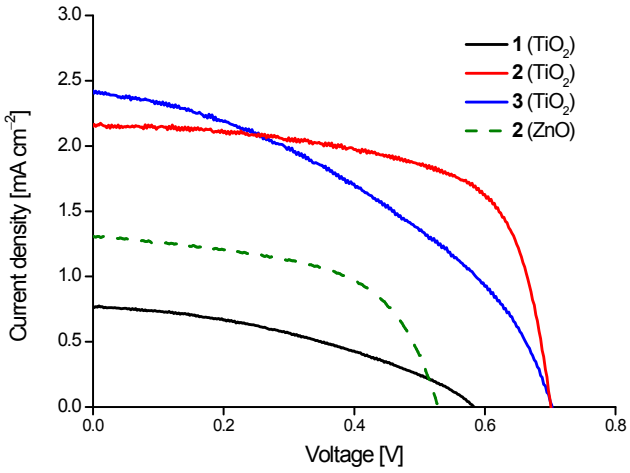


Fig. S17. J-V curves of TiO_2-based DSSCs (solid line) with **1** (22 h immersion time), **2** (30 h), and **3** (4 h) and J-V curve of ZnO-based DSSCs (dotted line) with **2** at 170 h immersion time.

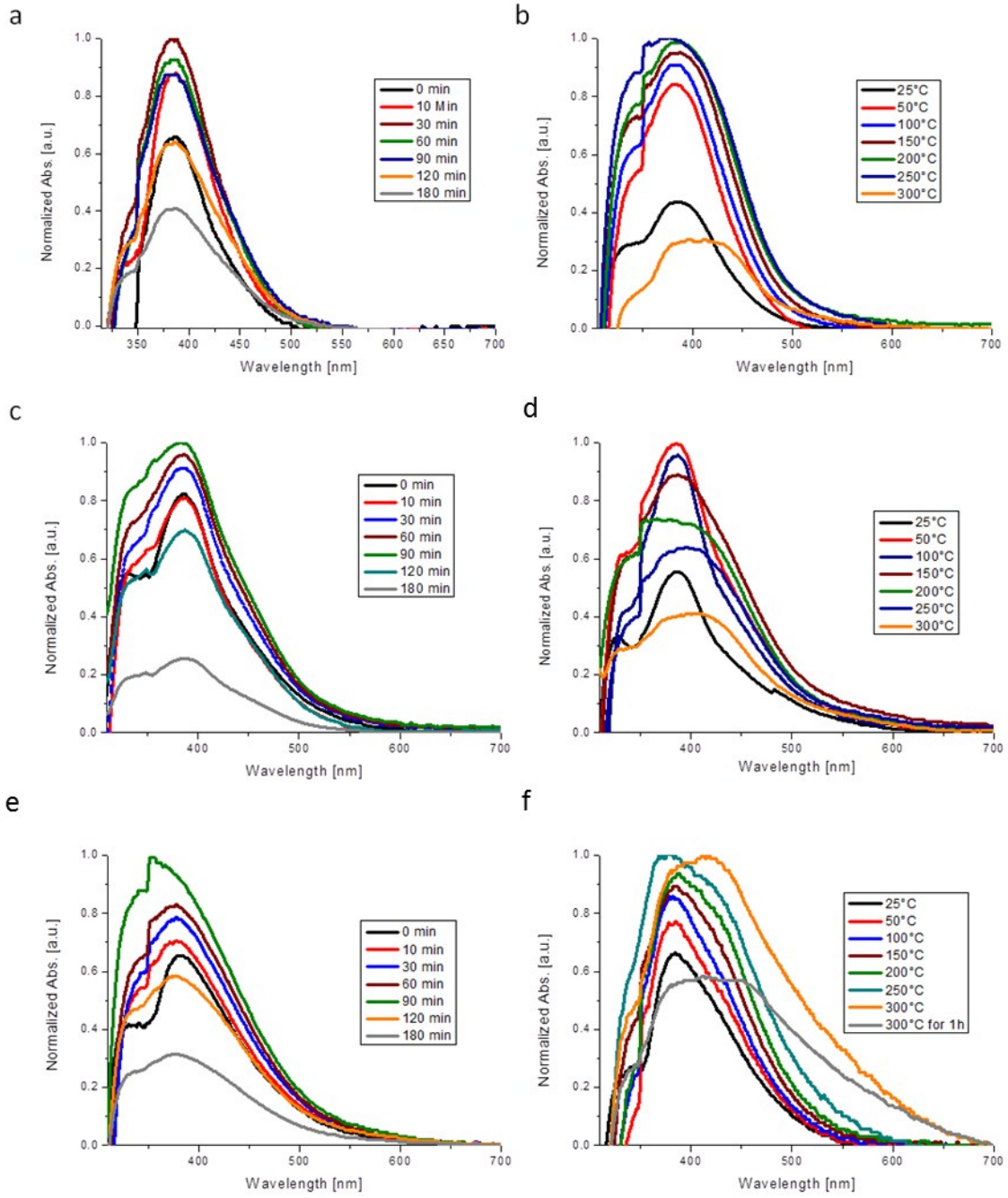


Fig. S18. Irradiation stability (left) under 1 sun illumination and thermal stability (right) of **1** (top, a and b, respectively), **2** (middle, c and d, respectively), and **3** (bottom, e and f, respectively) attached to a TiO_2 electrode measured by UV/vis absorption spectroscopy. For thermal stability studies, the sensitized electrodes were kept at the respective temperature for 30 minutes for each step.

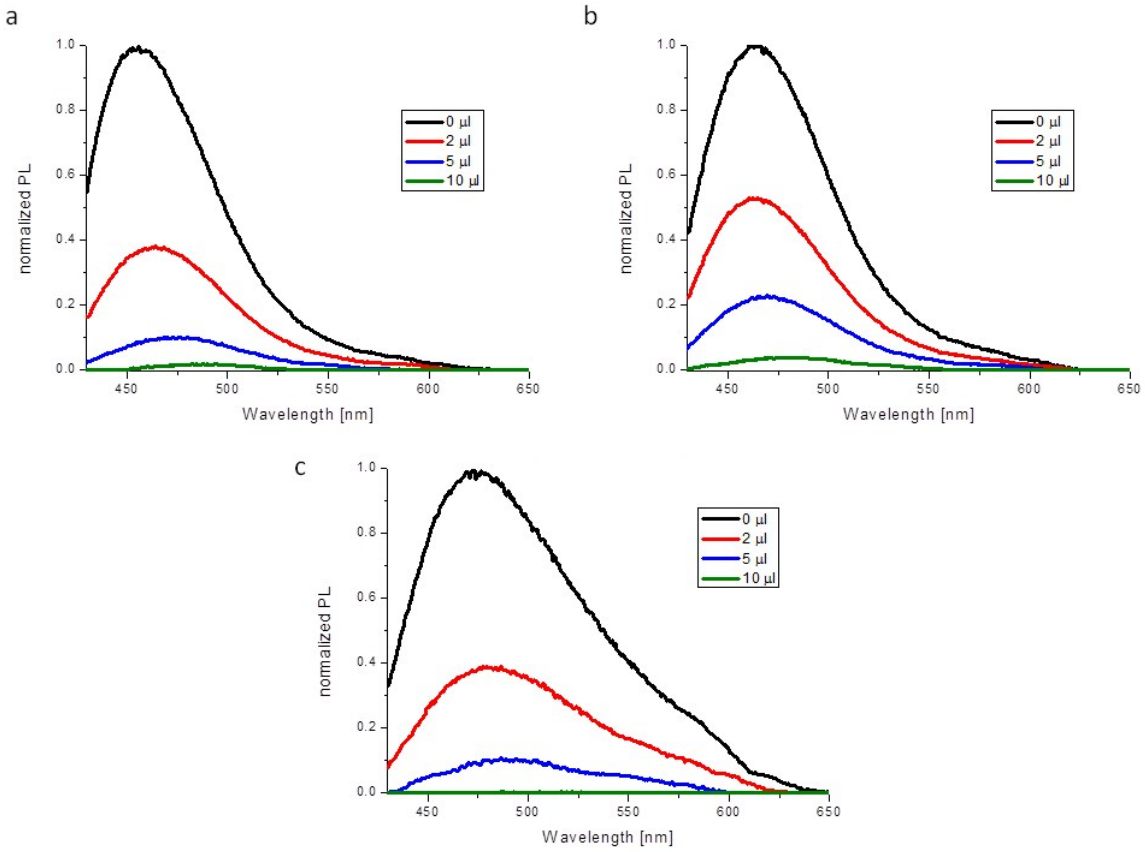


Fig. S19. Emission spectra of **1** (a), **2** (b) and **3** (c) in EtOH solution upon stepwise electrolyte addition.

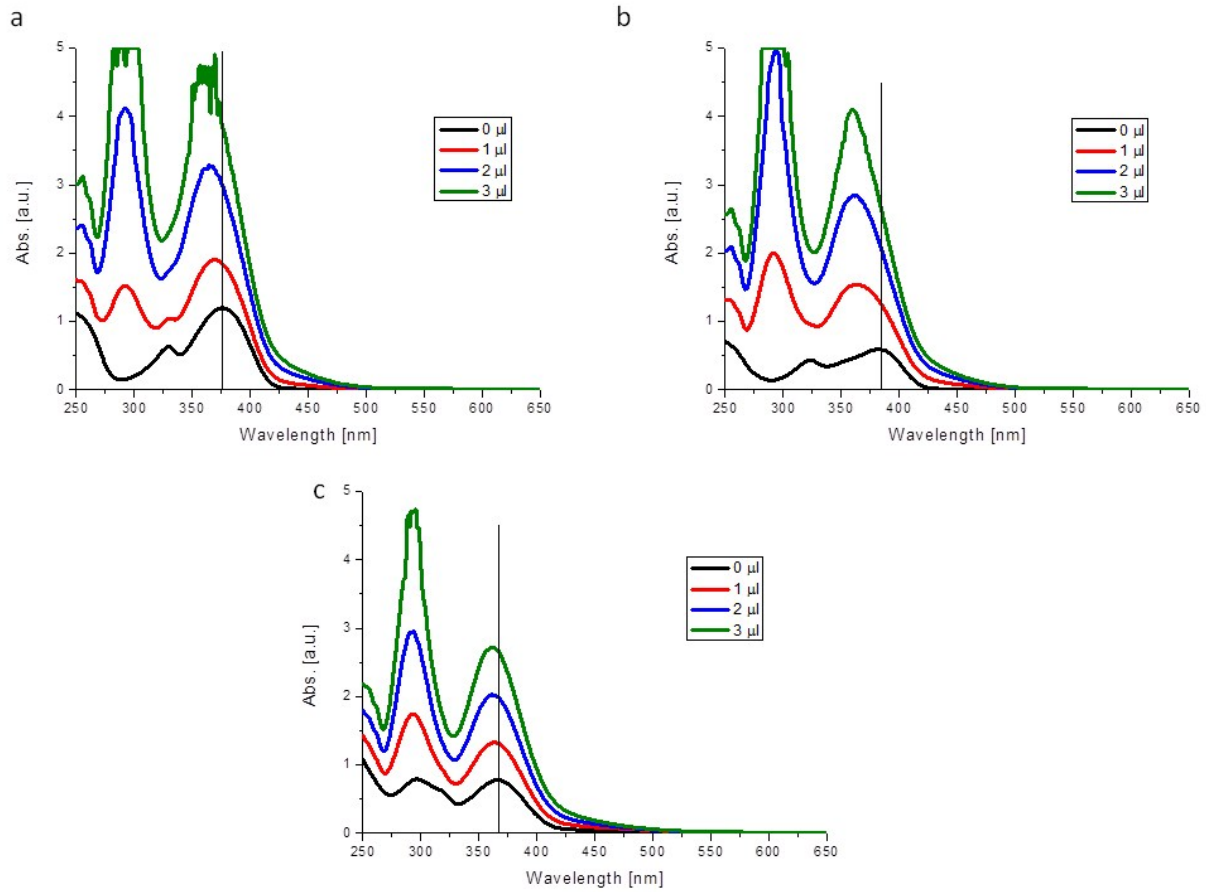


Fig. S20. UV/vis absorption spectra of **1** (a), **2** (b) and **3** (c) in EtOH solution upon stepwise electrolyte addition.

6 Frontier molecular orbital analysis

Calculations were performed with the Gaussian 09 program suite.[5] Full geometry optimizations without symmetry constraints were performed at ωB97XD[6]/6-31G(d).[7-18] Normal vibrational modes within the harmonic approximation were calculated to characterize minima at the same level of theory. Orbital energies were calculated at OLYP[19-22]/6-311+G(d,p)[11-17,23-27] on ωB97XD/6-31G(d) geometries. Structures and orbitals were visualized with Chemcraft 1.7.[28] Cartesian coordinates and archives of the Gaussian 09 calculations are given below.

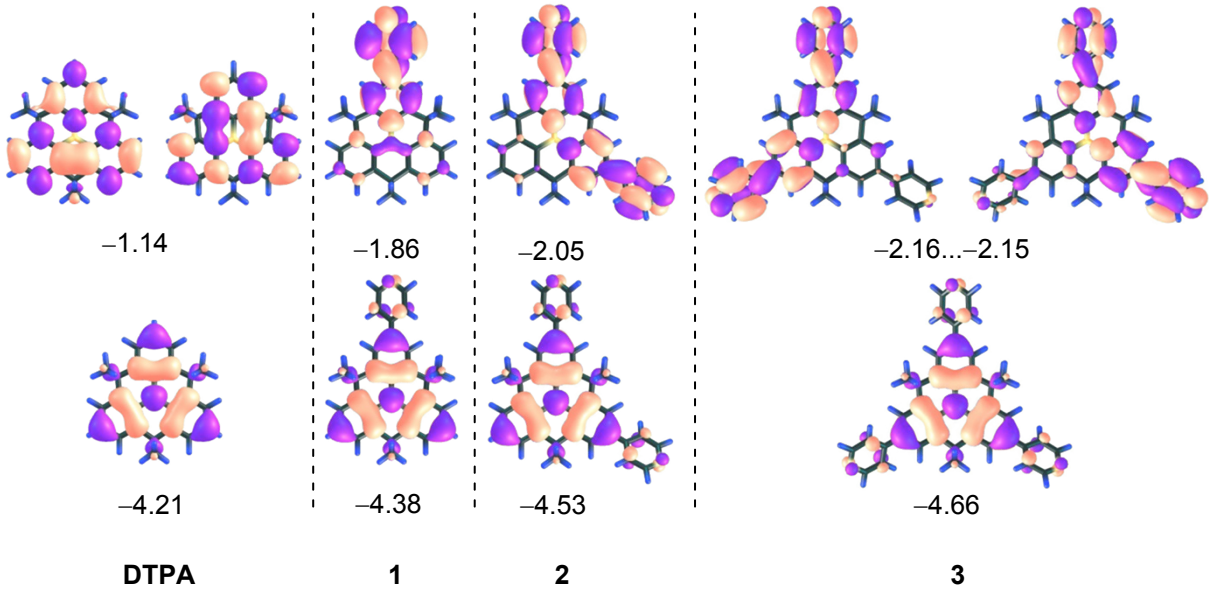


Fig. S21. Frontier molecular orbitals for **DTPA** and **1–3** [eV] calculated at the OLYP/6-311+G(d,p)// ωB97XD/6-31G(d) level of theory. HOMOs in bottom row, LUMOs in top row.

6.1 DTPA

6.1.1 ωB97XD/6–31G(d)

55

C	-2.976850	0.000000	0.007858
C	-2.118243	-1.251143	0.008288
C	-0.709141	-1.229064	0.008458
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C	-0.023693	-2.459941	0.008793
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C	-2.791578	2.471393	0.008448
C	-2.791578	-2.471393	0.008448
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H	-0.201852	-4.593437	0.009533
H	4.080295	-2.121804	0.007478
H	4.080295	2.121804	0.007478
H	1.625622	2.805206	-2.158673
H	1.482409	4.344930	-1.294334
H	3.017374	3.474579	-1.289881
H	3.018218	3.474010	1.306077
H	1.483281	4.344362	1.312025
H	1.627083	2.804225	2.175554
H	1.625622	-2.805206	-2.158673
H	3.017374	-3.474579	-1.289881
H	1.482409	-4.344930	-1.294334
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(Hartree/Particle)
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6.1.2 OLYP/6-311+G(d,p)


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6.2 1

6.2.1 ωB97XD/6–31G(d)

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64

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C       -0.621470     -1.185288     -0.376262
N        0.024702      0.020925      0.006219
C       -0.689910      1.241451     -0.010599
C       -2.046424      1.283644     -0.390340
C        1.389895      0.002735      0.399312
C        2.047998      1.189121      0.778988
C        1.383419      2.553594      0.783663
C       -0.068174      2.452859      0.352888
C        0.077440     -2.408033     -0.382002
C        1.534898     -2.543982      0.018324
C        2.119242     -1.202105      0.418977
C       -0.792195      3.640004      0.321916
C       -2.125283      3.698967     -0.056283
C       -2.724176      2.497517     -0.404682
C       -2.589151     -2.385125     -1.127181
C       -1.906883     -3.585671     -1.141441
C       -0.577682     -3.576562     -0.766965
C        3.455317     -1.194850      0.816010
C        4.103636     -0.035964      1.195058
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C        2.335982     -3.099951     -1.182814
C        1.636190     -3.514589      1.219111
C       -3.421592      0.250829     -2.198820
C       -4.000692     -0.128295      0.240462
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H       -3.775938      2.503886     -0.671565
H       -3.636628     -2.374677     -1.409799
H       -0.026900     -4.511322     -0.769465
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H        3.391987     -3.232539     -0.929617
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H        1.224871     -4.497647      0.972845
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H        1.082044     -3.118433      2.075434
H       -2.610909      0.383601     -2.921715
H       -4.017585     -0.611365     -2.510600
H       -4.071429      1.129357     -2.249062
H       -4.662401      0.743301      0.252413
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 Zero-point correction=                           0.546034
(Hartree/Particle)
 Thermal correction to Energy=                    0.573635
 Thermal correction to Enthalpy=                  0.574579
 Thermal correction to Gibbs Free Energy=         0.489178
 Sum of electronic and zero-point Energies=          -1346.066946
 Sum of electronic and thermal Energies=             -1346.039346
 Sum of electronic and thermal Enthalpies=           -1346.038402
 Sum of electronic and thermal Free Energies=        -1346.123802

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6.2.2 OLYP/6-311+G(d,p)


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6.3 2

6.3.1 ωB97XD/6-31G(d)


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C       -0.935489      0.407965      1.101255
C       -2.312079      0.471350      0.809910
C        1.390525      0.070105      0.403651
C        1.842876      0.299031      1.718247
C        0.919823      0.609742      2.881947
C       -0.529820      0.625287      2.433038
C        0.508472     -0.362268     -2.272562
C        2.004028     -0.476758     -2.040555
C        2.350135     -0.220758     -0.585546
C       -1.482075      0.882297      3.413315
C       -2.841201      0.944367      3.143981
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C	3.203176	0.242654	2.001000
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Zero-point correction=	0.616398
(Hartree/Particle)	
Thermal correction to Energy=	0.648527
Thermal correction to Enthalpy=	0.649471
Thermal correction to Gibbs Free Energy=	0.554135

Sum of electronic and zero-point Energies= -1593.010186
Sum of electronic and thermal Energies= -1592.978056
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0,-1.786493,-0.014433,-1.587175\C,0,-0.420084,-0.080142,-1.252068\N,0,
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.841201,0.944367,3.143981\C,0,-3.222993,0.736406,1.826962\C,0,-2.18370
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6.4 3

6.4.1 ωB97XD/6–31G(d)

82

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N	0.126980	-0.088021	0.071132
C	0.971532	0.993999	0.423315
C	1.364891	1.947158	-0.535677
C	-0.254400	-1.037354	1.051712
C	0.208417	-0.933795	2.377943
C	1.114639	0.181450	2.866873
C	1.441502	1.146464	1.742208
C	-1.186414	-1.281139	-1.630324
C	-1.679553	-2.338540	-0.659781
C	-1.107296	-2.110302	0.727387
C	2.261043	2.223172	2.063592
C	2.655113	3.172927	1.132719
C	2.189868	3.002931	-0.162766
C	-0.434166	0.555638	-3.553157
C	-1.267761	-0.485166	-3.934600
C	-1.626342	-1.388773	-2.945386
C	-1.469094	-3.026225	1.709363
C	-1.016840	-2.943632	3.017876
C	-0.175140	-1.883234	3.319121
C	2.430215	-0.435466	3.397894
C	0.395475	0.954201	3.998254
C	-1.236246	-3.731089	-1.168086
C	-3.222989	-2.268630	-0.580347
C	2.200868	1.780590	-2.877623
C	0.167887	3.196213	-2.336077
H	2.632563	2.312249	3.079227
H	2.463696	3.740229	-0.910177
H	-0.116488	1.266541	-4.308762
H	-2.302213	-2.196752	-3.205836
H	-2.114286	-3.855220	1.437855
H	0.175830	-1.777175	4.340360
H	2.943519	-0.981241	2.600292
H	3.108624	0.336114	3.773367
H	2.238267	-1.132074	4.219282
H	0.148263	0.296166	4.836097
H	1.024143	1.759463	4.389308
H	-0.533532	1.396501	3.625915
H	-0.145473	-3.783641	-1.236713
H	-1.574465	-4.526211	-0.497886
H	-1.651392	-3.941307	-2.157924
H	-3.679726	-2.433748	-1.560516
H	-3.618444	-3.029029	0.099811

H	-3.541786	-1.287030	-0.216571
H	2.747439	0.862764	-2.640254
H	1.941510	1.756800	-3.940065
H	2.874848	2.628343	-2.722868
H	0.783104	4.083870	-2.163807
H	-0.136035	3.208526	-3.386926
H	-0.732005	3.280203	-1.719319
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C	3.400401	4.955896	2.736431
C	5.303815	5.861466	1.035391
C	4.244375	6.018473	3.037170
N	5.187125	6.480300	2.212457
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C	-0.939214	-5.320221	5.949466
C	-3.027409	-5.398743	5.063107
N	-2.171410	-5.831587	5.991578
H	0.511961	-4.035020	5.021502
H	-3.463031	-4.141422	3.375298
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H	-2.464539	-2.908791	-7.730301

Zero-point correction=	0.686556
(Hartree/Particle)	
Thermal correction to Energy=	0.723504
Thermal correction to Enthalpy=	0.724448
Thermal correction to Gibbs Free Energy=	0.617290
Sum of electronic and zero-point Energies=	-1839.953276
Sum of electronic and thermal Energies=	-1839.916328
Sum of electronic and thermal Enthalpies=	-1839.915384
Sum of electronic and thermal Free Energies=	-1840.022542

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6.4.2 OLYP/6-311+G(d,p)

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42H36N4)]\\@

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