Supporting Information for:

Light-Driven Electron Transfer in a Lipid Bilayer with Mixed Valence Molecular Wires

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General Methods

NMR Spectroscopy. ^{1}H-NMR (400 MHz) and ^{13}C-NMR (101 MHz) spectra were recorded on a Bruker Avance III 400 spectrometer or on a Bruker Avance Neo 800 spectrometer in the solvent indicated at room temperature (if not stated otherwise). The spectra were referenced to the residual protonated solvent (^{1}H) or the solvent signal (^{13}C).

ESI Mass Spectrometry. Samples were measured on an MS system from Thermo (Bremen, Germany) consisting of an ITQ 900 ion trap mass spectrometer and a DPC direct injection system using the direct insertion probe (DIP) technique. The sample was placed on a rhenium wire and evaporated using a current slope of 100 mA × sec^{-1} (from 0 to 800 mA). The following MS parameters were used: scan range 50-2000 *m*/*z*. The ion source was set to 200 °C. The damping gas flow was set to 0.3 mL helium. 3 Microscans were used at a maximum ion time of 25 ms.

Cyclic Voltammetry. All voltammetric experiments were performed under argon atmosphere. The voltammograms were recorded using a BASi Epsilon potentiostat and a cell with a platinum electrode (Ø = 1.10 mm, MFC-2012 *BASi*). Prior to each measurement series, the working electrode was freshly polished with diamond pastes with grain sizes of 1 µm and 0.25 µm from *Buehler & Wirtz*. An AgCl and a spiral-shaped Pt wire were used as the reference and counter electrodes. TBA^{+} BAr^{F24-} was used in a concentration of 0.1 mM in CH_2Cl_2 as a supporting electrolyte. All redox potentials were referenced *versus* the FcH/FcH^{+} redox couple after each measurement series by addition of roughly equimolar amounts of ferrocene to the analyte solution. Simulations of cyclic voltammograms were performed using the *DigiSim* program.[1] Therefore, recorded voltammograms at different scan rates (100-2000 mVs^{-1}) were uploaded. Two subsequent one-electron oxidations were used to describe the overall redox process (A → B + e^{-}; B → C + e^{-}). The initial parameters were set as follows: c = 0.8 mM (**1**^{Me}), 1.3 mM (**2**^{Me}), electrode surface area = 0.0256 cm^2, *T* = 298 K, CdI = 8×10^{-7} F, planar electrode geometry, α = 0.5, k_s = 0.01 cms^{-1}, diffusion coefficient = 5.32×10^{-6} cm^{2}s^{-1} (1^{Me}), 2.76×10^{-6} cm^{2}s^{-1} (2^{Me}). The program was then allowed to freely change the chosen parameters iteratively to adequately replicate the experimental voltammograms at any scan rate, until the highest level of convergence was reached.

Computational Details. Ground state electronic structures were calculated based on density functional theory (DFT) employing the Gaussian 16 program package.[2] Geometry optimization was followed by vibrational analysis. Open-shell systems were calculated within the unrestricted Kohn-Sham (UKS) approach. Solvent effects were taken into account using the polarizable continuum model, employing the standard parameter for methylene chloride.[3] The double-ξ basis set of Ahlrichs and co-worker with def2-SVP (split-valence-plus-polarization)[4,5] was employed in combination with Becke´s three-parameter hybrid functional, using Lee-Yang-Parr´s non-local correlation (B3LYP).[6] The B3LYP hybrid functional was artificially mixed with 35% exact Hartree-Fock exchange to compensate for the inherent tendency of the DFT method to delocalize charges in extended π-conjugated systems.[7–10] The GaussSum[11], Avogadro[12], GNU Parallel[13] and vmd program packages were used in combination with POV-Ray for data processing, and graphical representations.

UV-Vis/NIR/IR Spectroscopy. UV-Vis/NIR spectra were acquired using a TIDAS fiber optic diode array spectrometer, combining an MCS UV/NIR and a PGS NIR instrument from *j&m Analytic AG* or using a JASCO V760 spectrometer. Extinction coefficients were determined from solutions of the analyte in a quartz cell with an optical path length of 0.2 cm, purchased from *Hellma Analytics*. IR spectra were recorded on a *Tensor II* instrument by *Bruker* equipped with a halogen NIR lamp and an MCT detector.

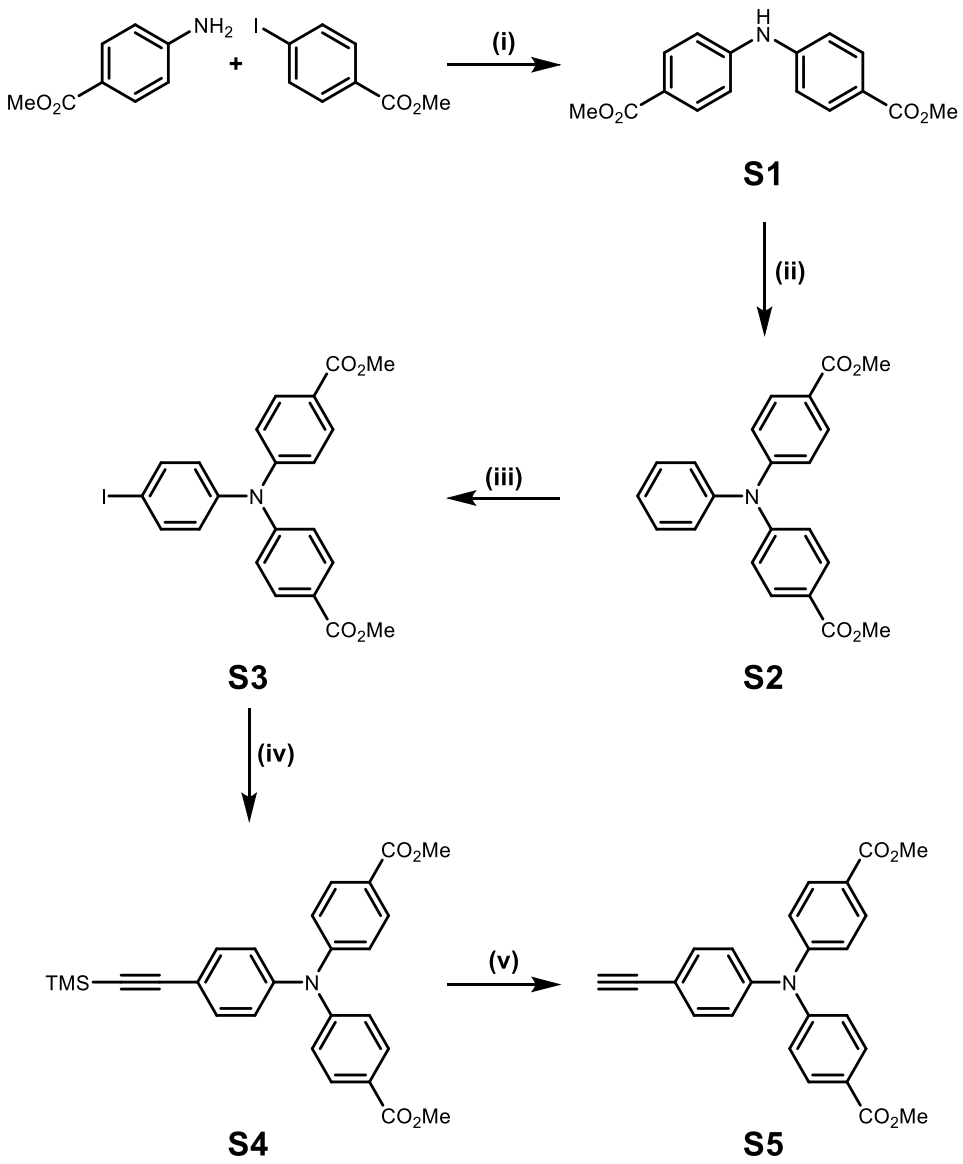
A Wenking Pos 2 potentiostat from *intelligent controls GmbH* was used for spectroelectrochemical measurements. According to HARTL's design, a custom-made optically transparent electrochemical thin-layer cell (OTTLE) was used,[14] consisting of a working and counter electrode made of Pt grid and a thin silver wire as a *pseudo* reference electrode. The electrodes are sandwiched in between two optically transparent CaF_2 windows. CH_2Cl_2 was used as the solvent. A 0.1 M solution in $TBA^+ BAr^{F24-}$ in methylene chloride was used for the spectroelectrochemical studies.

Fluorescence spectroscopy. Luminescence spectra were recorded on an FP-8500 Spectrofluorometer. Starna fluorescence quartz cuvettes with a path length of 1 cm and screw caps with an air-tight silicon seal were used

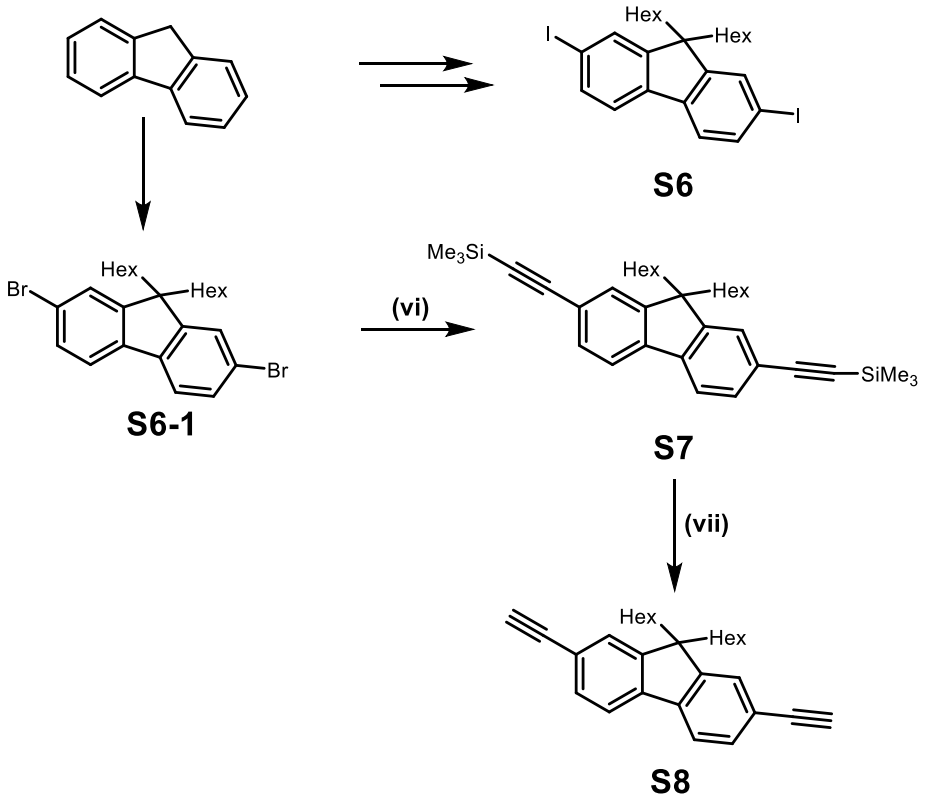
Confocal microscopy. The images were acquired on a Leica TCS SP8 confocal microscope equipped with a 488 nm laser as an excitation source and detected within a range of 500-600 nm. Sample wells (m-Slide 8 Well ibiTreat) characterized giant vesicles. Confocal microscopy images were processed with the LasX software.

Fluorescence lifetimes. Fluorescence lifetimes were determined with a DeltaPro from Horiba Scientific using a 372 nm pulsed Laser source (Class 3B Laser Product, <0.5 W peak in pulsed and CW mode). The Delta Pro instrumentation consists of a DeltaDiode (Picosecond diode controller), DeltaHub (High throughput TCSPC controller), DPS-1 (Detector Power supply), and a PPD (Picosecond photon detection module). The IRF (Instrument response function) was measured with LUDOX silica nanoparticles. Fits were done with the software EzTime.

S1 Synthesis and Characterization



Scheme S1 | Schematic route for the synthesis of intermediates **S1**-**S5**. (i) $Pd(OAC)_2$, *rac*-BINAP, Cs_2CO_3, toluene, 100 °C, overnight; (ii) bromobenzene, $Pd(OAC)_2$, P^tBu_3, Cs_2CO_3, toluene, 100 °C, overnight; (iii) ICl, $Zn(OAc)_2$, 1,4-dioxane, r.t., 2 h; (iv) TMSA, CuI, $PdCl_2(PPh_3)_2$, NEt_3, THF, 70 °C, overnight; (v) K_2CO_3, MeOH/THF (1:1), r.t., 3 h.

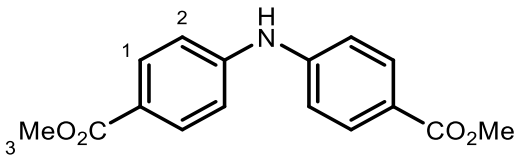


Scheme 2 | Schematic route for the synthesis of intermediates **S6**-**S8**. (vi) TMSA, CuI, $PdCl_2(PPh_3)_2$, NEt_3, THF, 60 °C, overnight; (v) K_2CO_3, MeOH/THF (1:1), r.t., 3 h.

General remarks on the experimental procedures

If not stated otherwise, all syntheses were performed under inert gas conditions using standard SCHLENK techniques. Solvents used under inert atmosphere were predried over common desiccants and subsequently stored in Schlenk flasks over molecular sieves of appropriate pore sizes.[15] Dry toluene was obtained from an *MB-SPS-7* solvent purifier by *M. Braun Inertgas-Systeme GmbH*. All other solvents used were used as purchased in technical grade. Commercially available starting materials used in the syntheses were purchased from commercial suppliers and were used without further purification.

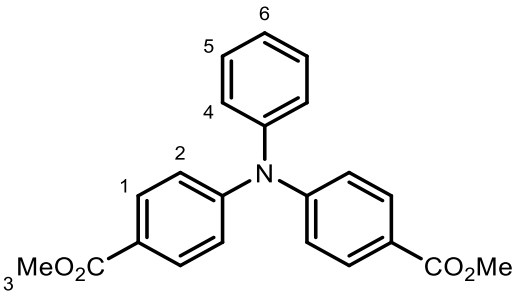
***N*-(Methyl-4-benzoate)-4-carbomethoxyaniline (S1)**



Methyl 4-aminobenzoate (907 mg, 6.00 mmol, 1.20 eq.), methyl 4-iodobenzoate (1.31 g, 5.00 mmol, 1.00 eq.), Cs_2CO_3 (2.28 g, 7.00 mmol, 1.40 eq.), $Pd(OAc)_2$ (56.1 mg, 0.25 mmol, 0.05 eq.), and *rac*-BINAP (249 mg, 0.40 mmol, 0.08 eq.) were dissolved in dry, degassed toluene (50 mL). The resulting mixture was stirred at 100 °C overnight. After allowing the mixture to cool to ambient temperature, it was filtered and the residue was washed with toluene (3 × 15 mL). The organic phases were combined and the solvent was removed under reduced pressure. The crude product was purified *via* column chromatography on silica (hexanes/ethyl acetate; 3:2) to give compound **S1** in 82% yield (1.17 g, 4.10 mmol).

^{1}H-NMR ($CDCl_3$, 400 MHz, 298 K) δ [ppm] = 7.98 (d, $^3J_{HH}$ = 8.7 Hz, 4H, H-1/2), 7.13 (d, $^3J_{HH}$ = 8.7 Hz, 4H, H-1/2), 6.31 (s, 1H, *N*-H), 3.90 (s, 6H, H-3).

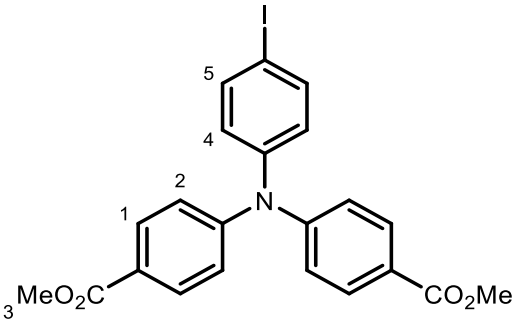
***N*,*N*-Di(methyl-4-benzoate)aniline (S2)**



Compound **S1** (600 mg, 2.10 mmol, 1.00 eq.), Cs_2CO_3 (1.03 g, 3.15 mmol, 1.50 eq.), $Pd(OAc)_2$ (29.2 mg, 0.13 mmol, 0.05 eq.), bromobenzene (0.44 mL, 659 mg, 4.20 mmol, 2.00 eq.), and P^{t}Bu$_3$ (10%wt in hexane, 0.77 mL, 52.6 mg, 0.26 mmol, 0.10 eq.) were dissolved in dry, degassed toluene (50 mL). The resulting mixture was stirred at 100 °C overnight. The reaction was quenched by the addition of water (30 mL) and the phases were separated. The aqueous phase was further extracted with methylene chloride (3 × 30 mL) and the combined organic phases were dried over $MgSO_4$. The solvent was removed under reduced pressure. The crude product was used without further purification. Compound **S2** was obtained in quantitative yield (759 mg, 2.10 mmol).

^{1}H-NMR ($CDCl_3$, 400 MHz, 298 K) δ [ppm] = 7.91 (d, $^3J_{HH}$ = 8.7 Hz, 4H, H-1/2), 7.37-7.11 (m, 5H, H-4/5/6), 7.09 (d, $^3J_{HH}$ = 8.7 Hz, 4H, H-1/2), 3.89 (s, 6H, H-3).

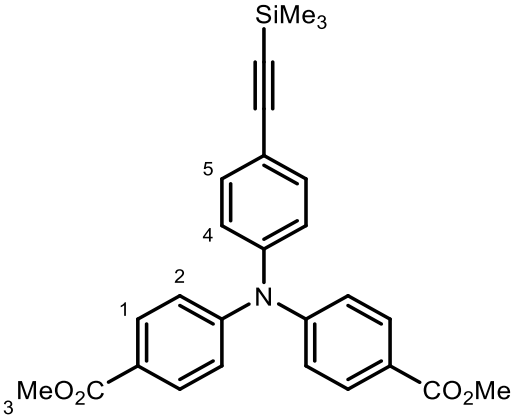
***N*,*N*-Di(methyl-4-benzoate)-4-iodoaniline (S3)**



Compound **S2** (820 mg, 2.27 mmol, 1.00 eq.) was dissolved in dry, degassed 1,4-dioxane (5 mL) and subsequently added dropwise to a mixture of $Zn(OAc)_2$ (417 mg, 2.27 mmol, 1.00 eq.) and ICl (0.23 mL, 738 mg, 4.55 mmol, 2.16 eq.) in 1,4-dioxane (5 mL). The mixture was stirred at ambient temperature for two hours. Then, the reaction was quenched by the addition of a saturated aqueous solution of $Na_2S_2O_3$. The product was extracted with CH_2Cl_2 (3 × 30 mL) and the combined extracts were dried over $MgSO_4$. The solution was concentrated under reduced pressure and subsequently filtered over silica. Compound **S3** was obtained as tan solid in 90% yield (995 mg, 2.04 mmol). Recrystallization from EtOH gave colorless crystals.

^{1}H-NMR ($CDCl_3$, 400 MHz, 298 K) δ [ppm] = 7.92 (d, $^3J_{HH}$ = 8.7 Hz, 4H, H-1/2), 7.63 (d, $^3J_{HH}$ = 7.6 Hz, 4H, H-5/4), 7.08 (d, $^3J_{HH}$ = 8.7 Hz, 4H, H-1/2), 6.89 (d, $^3J_{HH}$ = 7.6 Hz, 4H, H-5/4), 3.90 (s, 6H, H-3).

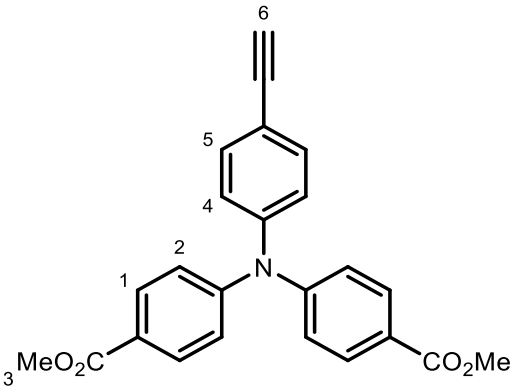
***N*,*N*-Di(methyl-4-benzoate)-4-trimethylsilylaniline (S4)**



To a solution of compound **S3** (600 mg, 1.23 mmol, 1.00 eq.) in THF/NEt_3 (30 mL, 1:1), CuI (11.8 mg, 0.06 mmol, 0.05 eq.) and $PdCl_2(PPh_3)_2$ (43.5 mg, 0.06 mmol, 0.05 eq.) were added, followed by the addition of ethynyltrimethylsilane (0.26 mL, 182 mg, 1.85 mmol, 1.50 eq.). The mixture was stirred at 70 °C overnight. Then, the reaction was quenched by the addition of a saturated aqeous solution of NH_4Cl. The product was extracted with CH_2Cl_2 (3 × 30 mL) and the combined extracts were dried over $MgSO_4$. The solvent was removed under reduced pressure and the crude product was purified *via* column chromatography on silica (hexanes/ethyl acetate; 9:1) to give compound **S4** in 82% yield (456 mg, 1.00 mmol).

^{1}H-NMR ($CDCl_3$, 400 MHz, 298 K) δ [ppm] = 7.92 (d, $^3J_{HH}$ = 8.7 Hz, 4H, H-1/2), 7.41 (d, $^3J_{HH}$ = 8.5 Hz, 4H, H-5/4), 7.08 (d, $^3J_{HH}$ = 8.7 Hz, 4H, H-1/2), 7.04 (d, $^3J_{HH}$ = 8.5 Hz, 4H, H-5/4), 3.90 (s, 6H, H-3), 0.25 (s, 9H, TMS-H).

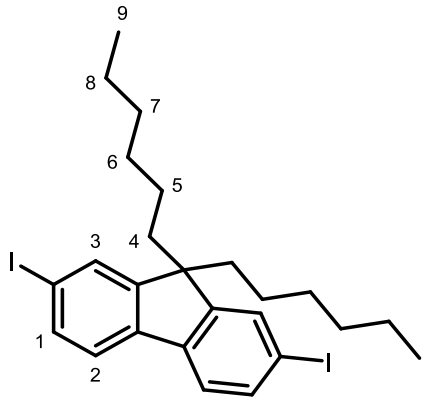
***N*,*N*-Di(methyl-4-benzoate)-4-ethynylaniline (S5)**



Compound **S4** (456 mg, 1.00 mmol, 1.00 eq.) was dissolved in MeOH/THF (30 mL, 1:1) and K_2CO_3 (275 mg, 2.00 mmol, 2.00 eq.) was added. The mixture was stirred for three hours at ambient temperature. Subsequently, the reaction was quenched with water (20 mL) and the product was extracted with methylene chloride (3 × 30 mL). The combined extracts were dried over $MgSO_4$ and the solvent was removed under reduced pressure. The crude product was further purified *via* column chromatography on silica (hexanes/ethyl acetate; 9:1) to give 294 mg (0.76 mmol) of compound **S5** in 76% yield.

^{1}H-NMR ($CDCl_3$, 400 MHz, 298 K) δ [ppm] = 7.93 (d, $^3J_{HH}$ = 8.8 Hz, 4H, H-1/2), 7.43 (d, $^3J_{HH}$ = 8.7 Hz, 4H, H-5/4), 7.09 (d, $^3J_{HH}$ = 8.8 Hz, 4H, H-1/2), 7.06 (d, $^3J_{HH}$ = 8.7 Hz, 4H, H-5/4), 3.90 (s, 6H, H-3), 3.09 (s, 9H, H-6).

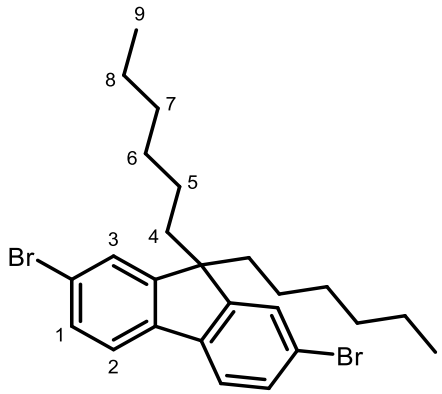
9,9-Dihexyl-2,7-diiodo-9H-fluorene (S6)



Compound **S6** was prepared according to literature procedures in a two-step protocol starting from fluorene.[16]

^{1}H-NMR ($CDCl_3$, 400 MHz, 298 K) δ [ppm] = 7.64 (dd, $^3J_{HH}$ = 8.7 Hz, $^4J_{HH}$ = 1.6 Hz, 2H, H-1), 7.64 (s, 2H, H-3), 7.64 (d, $^3J_{HH}$ = 8.7 Hz, 2H, H-2), 1.92-1.84 (m, 4H, H-4), 1.16-1.08 (m, 4H, H-5), 1.08-0.98 (m, 8H, H-8/7), 0.78 (t, $^3J_{HH}$ = 7.2 Hz, 6H, H-9), 0.62-0.51 (m, 4H, H-6).

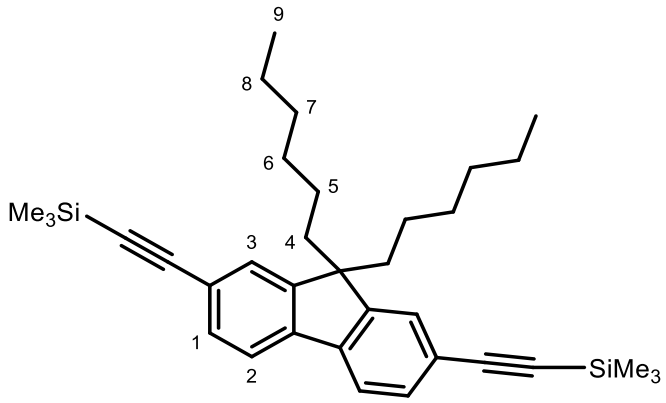
9,9-dihexyl-2,7-dibromo-9H-fluorene (S6-1)



Compound **S6-1** was prepared by stirring a solution of 2,7-dibromo-9H-fluorene (10.0 g, 30.8 mmol, 1.00 eq.), benzyl triethylammonium chloride (355 mg, 1.56 mmol, 0.05 eq.), 1-Bromohexane (11 mL 78.6 mmol, 2.55 eq.) in DMSO (50 mL) and aqueous NaOH (18.24 g, 456 mmol, 40 eq.) solution was added dropwise until the solution turned to blue. The reaction mixture was stirred at room temperature for 3 h. The mixture was extracted once with petroleum ether and the organic phase was washed once with 1 M HCl and three times with water. The organic layer was dried over anhydrous $MgSO_4$. The solvent was removed under reduced pressure. The residual powder was washed with ice-cold ethanol to purify the compound to give the desired product (**S6-1**, 15.2 g, 98%).

^{1}H-NMR ($CDCl_3$, 400 MHz, 298 K) δ [ppm] = 7.52 (d, *J* = 8.0 Hz, 2H), 7.47 – 7.42 (m, 4H), 1.91 (dd, *J* = 8.0, 4.2 Hz, 4H), 1.12 (h, *J* = 7.1 Hz, 12H), 0.78 (t, *J* = 7.3 Hz, 6H), 0.58 (p, *J* = 7.0 Hz, 4H).

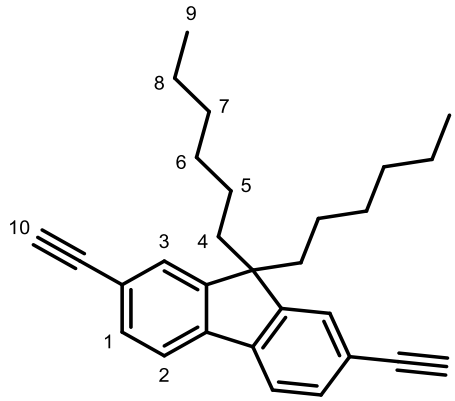
2,7-Di(trimethylsilyl)-9,9-dihexylfluorene (S7)



2,7-Dibromo-9,9-dihexylfluorene (492 mg, 1.00 mmol, 1.00 eq.) was dissolved in THF/NEt_3 (10 mL, 7:3). Then, ethynyl(trimethyl)silane (0.43 mL, 295 mg, 3.00 mmol, 3.00 eq.), CuI (19.0 mg, 0.10 mmol, 0.10 eq.) and $PdCl_2(PPh_3)_2$ (70.2 mg, 0.10 mmol, 0.10 eq.) were added. The mixture was stirred at 60 °C overnight. After cooling to room temperature, the reaction was quenched by the addition of ethyl acetate and sat. $NH_4Cl_{(aq.)}$. The phases were separated and the aqueous phase was further extracted with ethyl acetate (2 × 20 mL). The combined organic extracts were dried over $MgSO_4$. The solvent was removed under reduced pressure and the crude product was purified *via* column chromatography on silica (hexanes) to give compound **S7** in 87% yield (456 mg, 0.87 mmol).

^{1}H-NMR ($CDCl_3$, 400 MHz, 298 K) δ [ppm] = 7.59 (d, $^3J_{HH}$ = 7.7 Hz, 2H, H-2), 7.45 (dd, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.5 Hz, 2H, H-1), 7.42 (d, $^4J_{HH}$ = 1.5 Hz, 2H, H-3), 1.98-1.88 (m, 4H, H-4), 1.15-1.06 (m, 4H, H-5), 1.06-0.94 (m, 8H, H-8/7), 0.77 (t, $^3J_{HH}$ = 7.2 Hz, 6H, H-9), 0.58-0.47 (m, 4H, H-6), 0.29 (s, 18H, TMS-H).

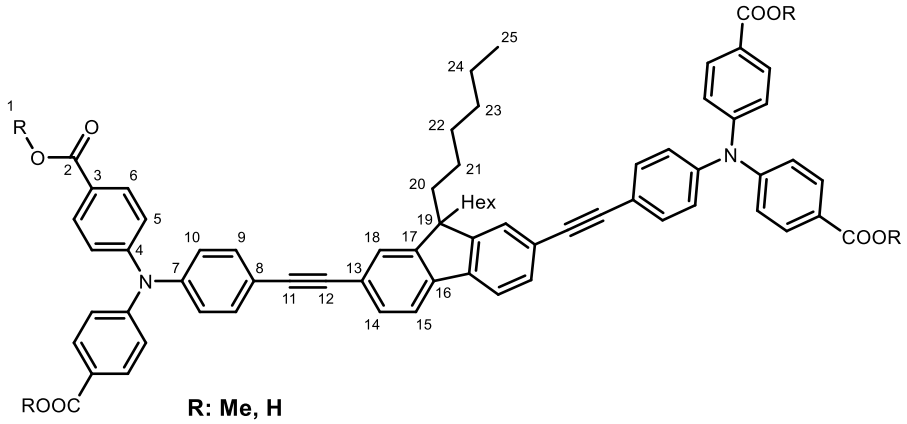
2,7-Di(ethynyl)-9,9-dihexylfluorene (S8)



Compound **S7** (457 mg, 0.87 mmol, 1.00 eq.) was dissolved in CH_2Cl_2/MeOH (14 mL, 1:1) and K_2CO_3 (480 mg, 3.47 mmol, 4.00 eq.) was added. The mixture was stirred for three hours at ambient temperature. Subsequently, the reaction was quenched with water (50 mL) and the product was extracted with ethyl acetate (3 × 30 mL). The combined organic phases were dried over $MgSO_4$ and the solvent was removed under reduced pressure. The crude product was further purified *via* column chromatography on silica (hexanes) to give compound **S8** in 80% yield (265 mg, 0.80 mmol).

^{1}H-NMR ($CDCl_3$, 400 MHz, 298 K) δ [ppm] = 7.63 (d, $^3J_{HH}$ = 7.9 Hz, 2H, H-2), 7.48 (dd, $^3J_{HH}$ = 7.9 Hz, $^4J_{HH}$ = 1.4 Hz, 2H, H-1), 7.46 (d, $^4J_{HH}$ = 1.4 Hz, 2H, H-3), 3.15 (s, 2H, H-10), 1.97-1.88 (m, 4H, H-4), 1.16-1.05 (m, 4H, H-5), 1.05-0.95 (m, 8H, H-8/7), 0.77 (t, $^3J_{HH}$ = 7.2 Hz, 6H, H-9), 0.61-0.48 (m, 4H, H-6).

2,7-Bis(N,N-di(methyl-4-benzoate)-4-ethynylaniline]-9,9-dihexylfluorene ($1^{Me/H}$)



Precursors **S5** (388 mg, 1.01 mmol, 2.20 eq.) and **S6** (270 mg, 0.46 mmol, 1.00 eq.) were dissolved in THF/NEt_3 (8 mL; 1:1). CuI (8.80 mg, 0.46 mmol, 0.10 eq.) and $PdCl_2(PPh_3)_2$ (32.3 mg, 0.46 mmol, 0.10 eq.) were added. The reaction mixture was stirred at 70 °C overnight. Subsequently, the saturated aqueous solution of NH_4Cl. The crude product was extracted with ethyl acetate (3 × 20 mL) and the combined extracts were subsequently dried over $MgSO_4$. The solvent was removed under reduced pressure and the crude product was purified *via* column chromatography on silica (hexanes/ethyl acetate; 4:1). Compound $\mathbf{1^{Me}}$ was obtained in 49% (250 mg, 0.23 mmol).

To deprotect the carboxylic acid functionalities, compound $\mathbf{1^{Me}}$ was dissolved in THF/H_2O (3 mL, 2:1) and LiOH (110 mg, 4.60 mmol, 20.0 eq.) was added. The resulting mixture was stirred at room temperature overnight, then, water was added and the product was extracted with ethyl acetate. The organic phase was dried over $MgSO_4$ and the solvent was removed under reduced pressure. The crude product was washed with methylene chloride and pentane to give compound $\mathbf{1^{H}}$ in quantitative yield (236 mg, 0.23 mmol).

^{1}H-NMR ($CDCl_3$, 800 MHz, 298 K) δ [ppm] = 7.94 (d, c$^3J_{HH}$ = 8.7 Hz, 8H, H-6), 7.66 (d, $^3J_{HH}$ = 8.0 Hz, 2H, H-15), 7.51 (d, $^3J_{HH}$ = 8.7 Hz, 6H, H-9/14), 7.49 (s, 2H, H-18), 7.15-7.09 (m, 12H, H-5/10), 3.91 (s, 12H, H-1), 2.02-1.93 (m, 4H, H-20), 1.15-0.99 (m, 12H, H-21/22/23), 0.77 (t, $^3J_{HH}$ = 8.3 Hz, 6H, H-25), 0.65-0.56 (m, 4H, H-24).

^{13}C{^{1}H}-NMR ($CDCl_3$, 201 MHz, 298 K) δ [ppm] = 166.6, 151.1, 150.6, 146.0, 140.7, 133.0, 131.1, 130.7, 125.9, 125.4, 124.8, 123.1, 121.9, 120.0, 119.6, 90.9, 89.3, 55.3, 52.0, 40.4, 31.6, 29.7, 23.7, 22.6, 14.0.

ESI-MS *calc.* for m/z = 1100.50 (M^-); *found* m/z = 1100.05.

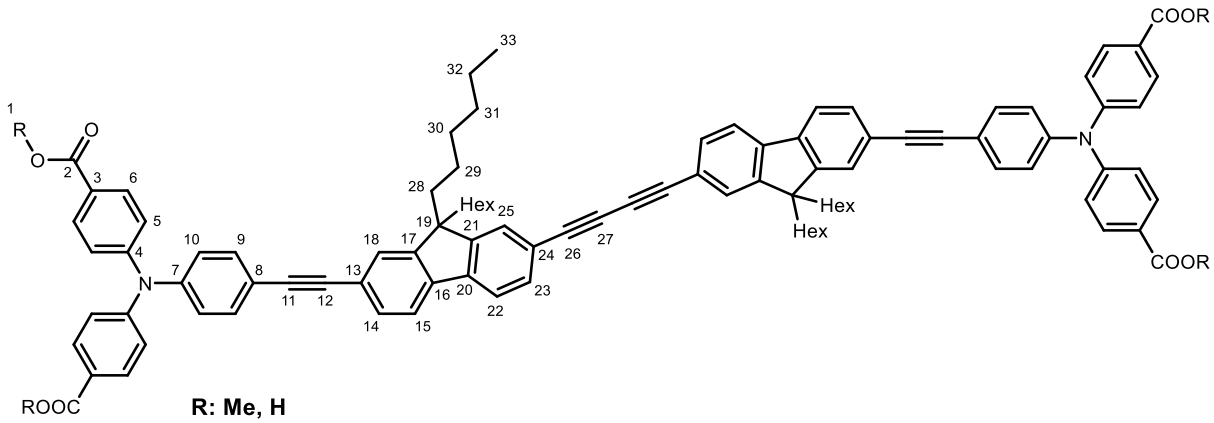
UV-Vis Absorption (CH_2Cl_2) λ_{max} = 366 nm; ε_{max} = 112×10^3 $M^{-1}cm^{-1}$.

^{1}H-NMR (DMSO-d_6, 400 MHz, 298 K) δ [ppm] = 12.77 (s, 4H, H-1), 7.97-7.79 (m, 10H, H-6/15), 7.63 (s, 2H, H-18), 7.59-7.47 (m, 6H, H-9/14), 7.21-7.09 (m, 12H, H-5/10), 2.02 (bs, 4H, H-20), 1.12-0.84 (m, 12H, H-21/22/23), 0.70 (t, $^3J_{HH}$ = 7.6 Hz, 6H, H-25), 0.45 (bs, 4H, H-24).

^{13}C{^{1}H}-NMR (DMSO-d_6, 101 MHz, 298 K) δ [ppm] = 167.2, 151.3, 150.4, 146.5, 140.8, 133.4, 131.6, 131.1, 126.1, 125.9, 125.6, 123.6, 121.8, 121.1, 118.7, 91.0, 90.1, 55.5, 31.4, 29.4, 23.9, 22.4, 14.3.

ESI-MS *calc.* for m/z = 1044.43 (M^-); *found* m/z = 1044.46.

1,4-Bis(7-[N,N-di(methyl-4-benzoate)-4-ethynylaniline]-9,9-dihexylfluoren-2-yl)buta-1,3-diyne ($2^{Me/H}$)



Compounds **S3** (560 mg, 1.15 mmol, 2.20 eq) and **S8** (200 mg, 0.52 mmol, 1.00 eq.) were dissolved in THF/NEt_3 (25 mL; 3:2). CuI (9.90 mg, 0.05 mmol, 0.10 eq.) and $PdCl_2(PPh_3)_2$ (36.5 mg, 0.05 mmol, 0.10 eq.) were added. The reaction mixture was stirred at 70 °C overnight and another portion of the catalyst was added. After additional 24saturated aqueous soluztion of NH_4Cl. The crude product was extracted with ethyl acetate (3 × 30 mL) and the combined extracts were subsequently dried over $MgSO_4$. The solvent was removed under reduced pressure and the crude product was purified *via* column chromatography on silica (hexanes/ethyl acetate; 4:1). Compound $\mathbf{2^{Me}}$ was obtained in 23% yield (90.0 mg, 0.06 mmol).

$\mathbf{2^{Me}}$ was then subjected to an ester-cleavage reaction. Therefore, compound $\mathbf{2^{Me}}$ was dissolved in THF/H_2O (3 mL, 2:1) and LiOH (20.0 eq.) was added. The resulting mixture was stirred at room temperature overnight, then, water was added and the product was extracted with ethyl acetate. The organic phase was dried over $MgSO_4$ and the solvent was removed under reduced pressure. The crude product was washed with methylene chloride and pentane to give compound $\mathbf{2^{H}}$ in quantitative yield (86 mg, 0.06 mmol).

^{1}H-NMR ($CDCl_3$, 800 MHz, 298 K) δ [ppm] = 7.94 (d, $^3J_{HH}$ = 8.7 Hz, 8H, H-6), 7.68-7.64 (m, 4H, H-15/22), 7.54-7.47 (m, 12H, H-9/14/18/23/25), 7.14-7.09 (m, 12H, H-5/10), 3.91 (s, 12H, H-1), 2.01-1.92 (m, 8H, H-28), 1.15-0.98 (m, 24H, H-29/30/31), 0.81-0.74 (m, 12H, H-33), 0.65-0.56 (m, 8H, H-32).

^{13}C{^{1}H}-NMR ($CDCl_3$, 201 MHz, 298 K) δ [ppm] = 166.3, 151.4, 151.2, 150.6, 146.1, 141.7, 140.7, 140.4, 132.9, 131.7, 130.9, 130.6, 127.0, 125.9, 125.5, 125.5, 124.9, 124.9, 123.1, 123.1, 121.9, 120.0, 119.4, 90.6, 89.3, 40.3, 31.6, 31.5, 29.7, 29.7, 23.8, 22.6, 13.8.

ESI-MS *calc.* for m/z = 1481.75 (M^-); *found* m/z = 1481.34.

UV-Vis Absorption (CH_2Cl_2) λ_{max} = 375 nm; ε_{max} = 140×10^3 M^{-1}cm^{-1}.

^{1}H-NMR (Acetone-d_6, 400 MHz, 298 K) δ [ppm] = 11.12 (s, 4H, H-1), 8.00 (d, $^3J_{HH}$ = 8.7 Hz, 8H, H-6), 7.94-7.87 (m, 4H), 7.74-7.64 (m, 4H), 7.64-7.53 (m, 8H), 7.25-7.15 (m, 12H, H-5/10), 2.18-2.09 (m, 8H, H-28), 1.18-0.97 (m, 24H, H-29/30/31), 0.81-0.71 (m, 12H, H-33), 0.68-0.55 (m, 8H, H-32).

^{13}C{^{1}H}-NMR (Acetone-d_6, 101 MHz, 298 K) δ [ppm] = 209.1, 166.2, 151.2, 150.7, 146.4, 140.8, 140.5, 133.0, 133.0, 131.3, 130.8, 126.93 125.9, 125.5, 125.5, 125.2, 125.2, 123.2, 123.2, 122.2, 120.3, 119.3, 90.5, 89.4, 55.4, 55.3, 39.9, 39.8, 31.4, 31.4, 23.7, 22.3, 13.4.

ESI-MS *calc.* for m/z = 1425.69 (M^-); *found* m/z = 1425.45.

NMR Spectroscopy

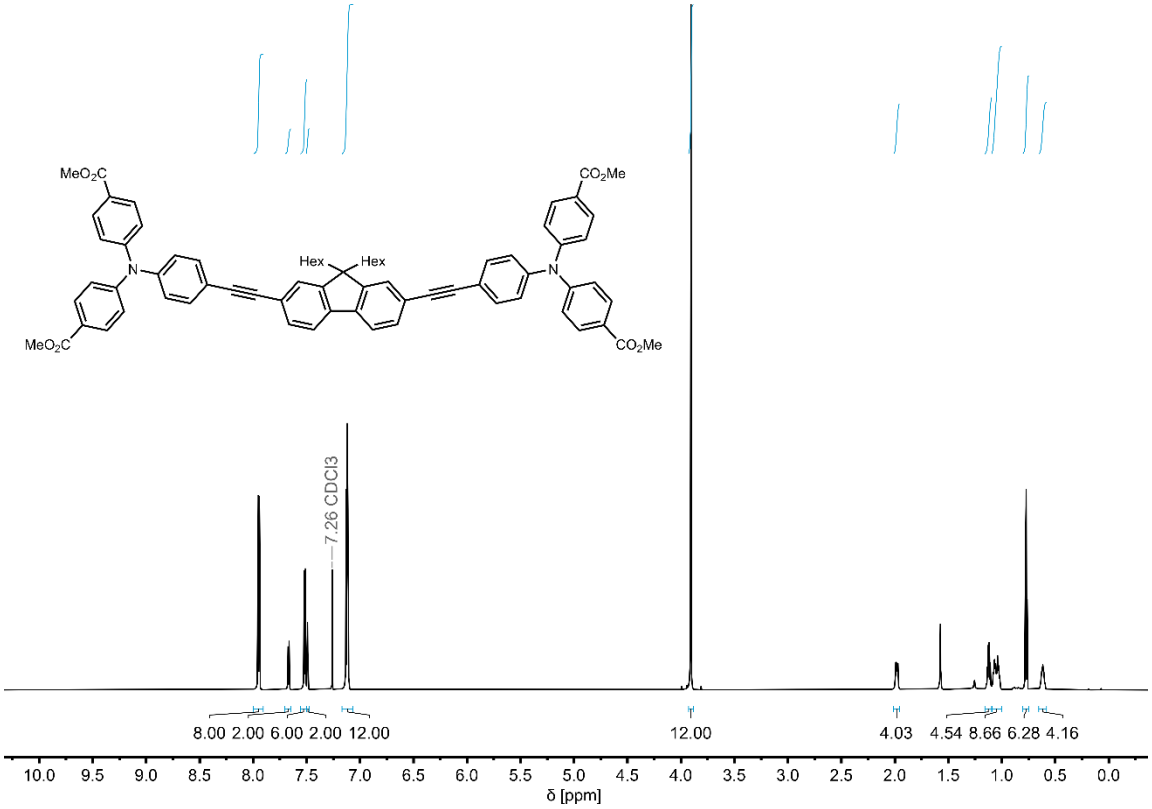


Figure S1. ^{1}H-NMR (800 MHz, 298 K) spectrum of compound **1^{Me}**, measured in $CDCl_3$.

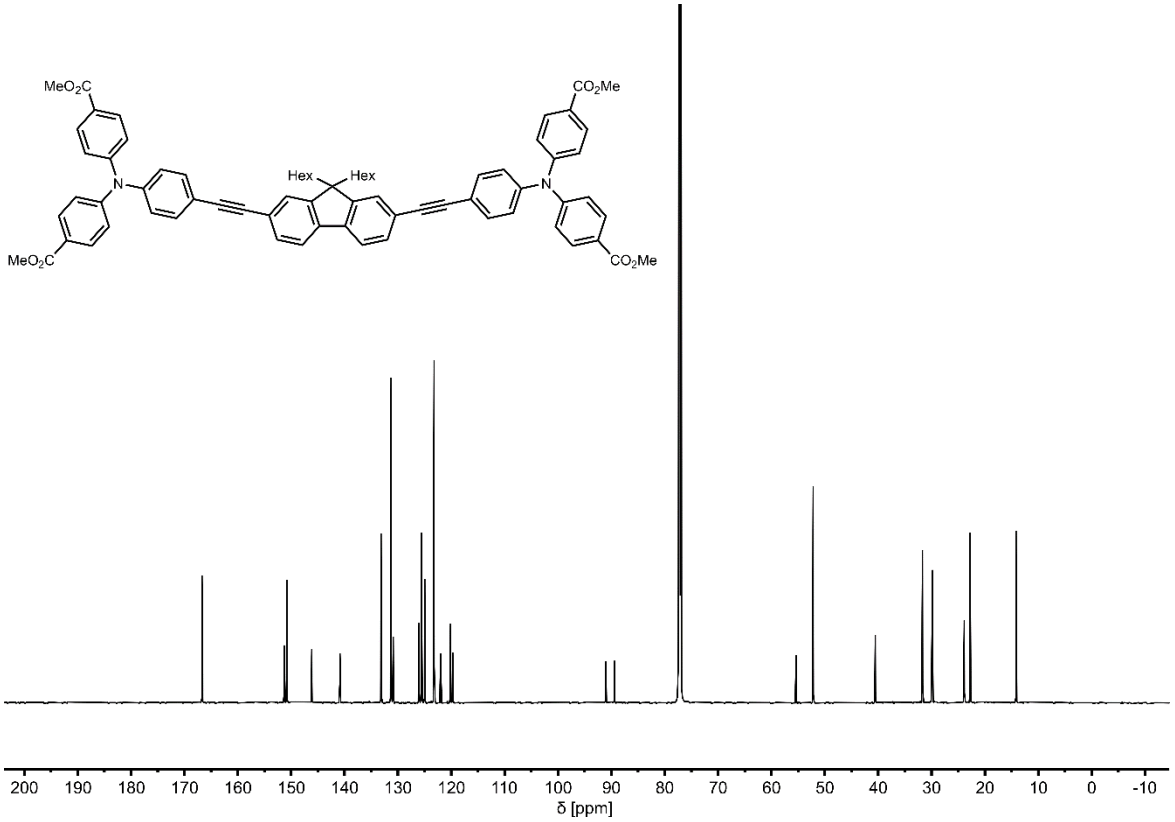


Figure S2. ^{13}C-NMR (202 MHz, 298 K) spectrum of compound **1^{Me}**, measured in $CDCl_3$.

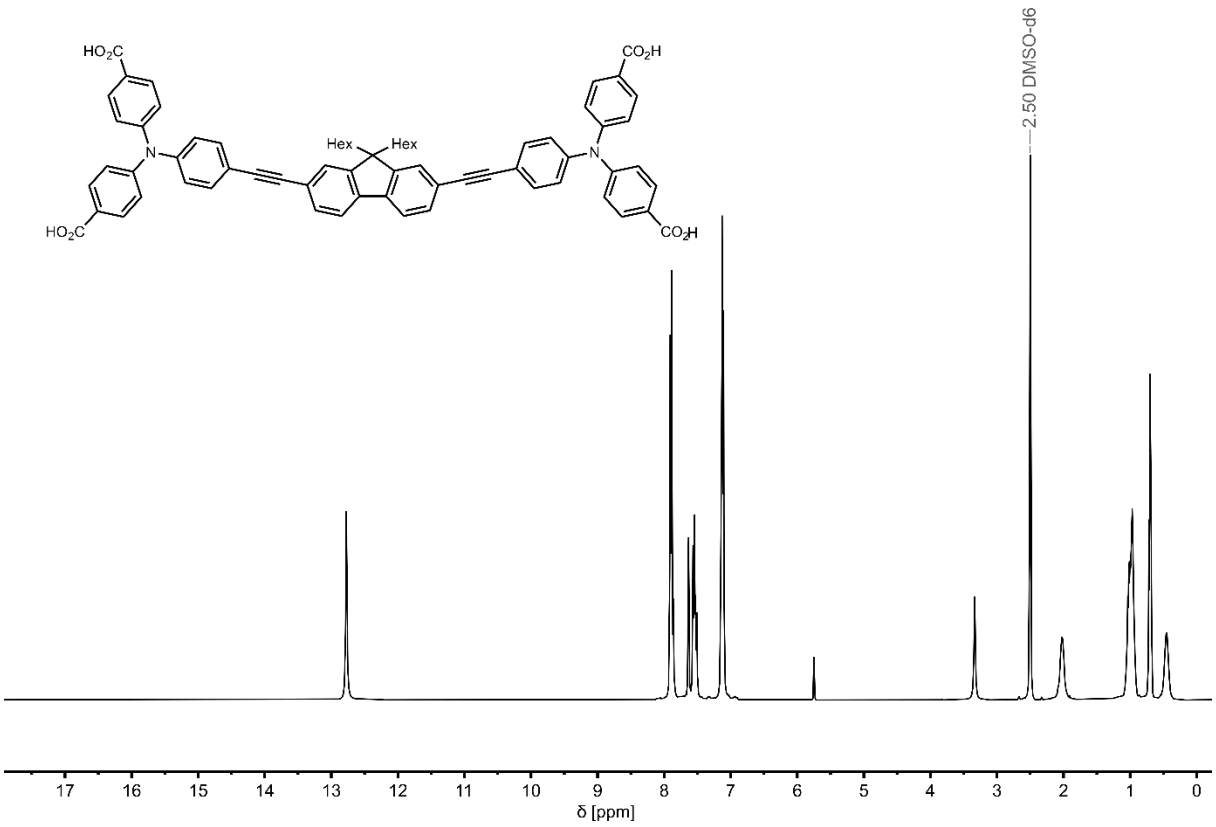


Figure S3. ^{1}H-NMR (400 MHz, 298 K) spectrum of compound **1^{H}**, measured in DMSO-d_6.

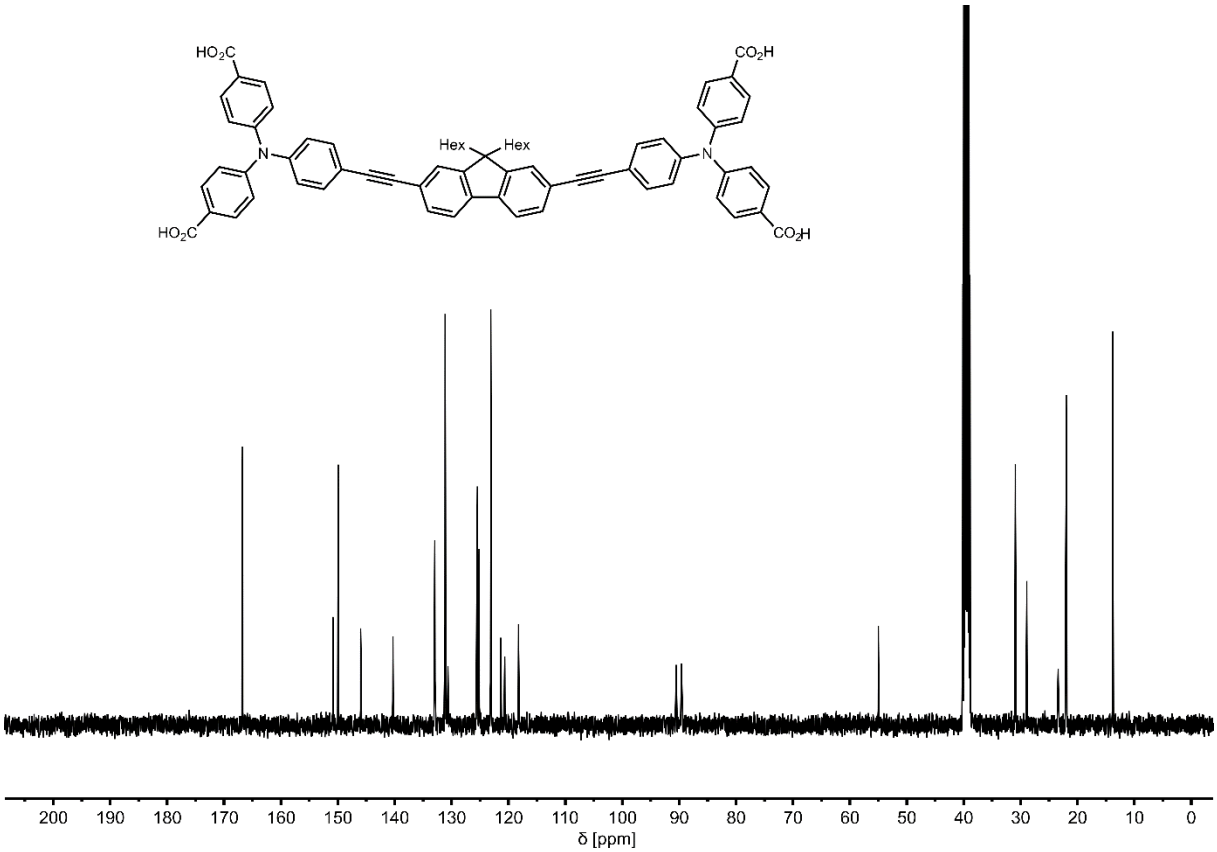


Figure S4. ^{13}C-NMR (400 MHz, 298 K) spectrum of compound **1^{H}**, measured in DMSO-d_6.

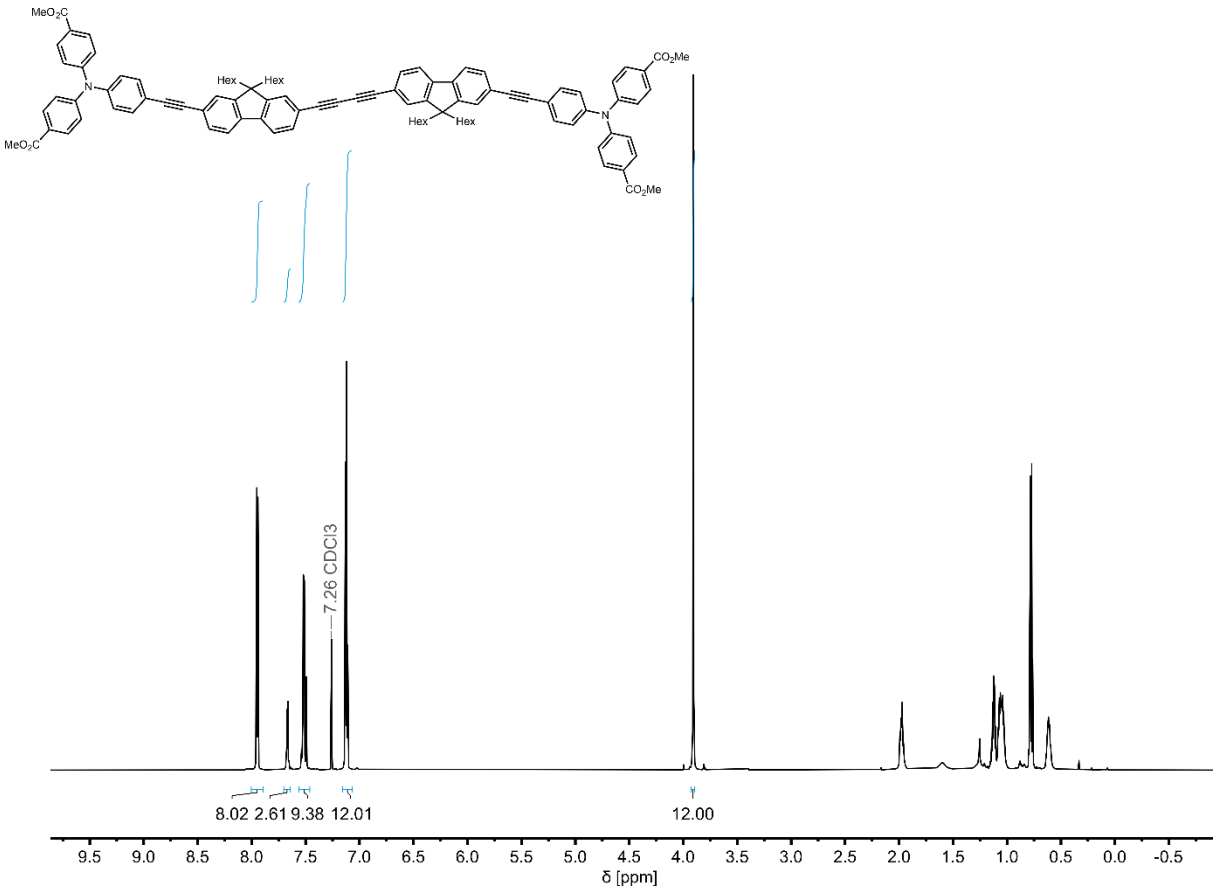


Figure S5. ^{1}H-NMR (800 MHz, 298 K) spectrum of compound **2^{Me}**, measured in $CDCl_3$.

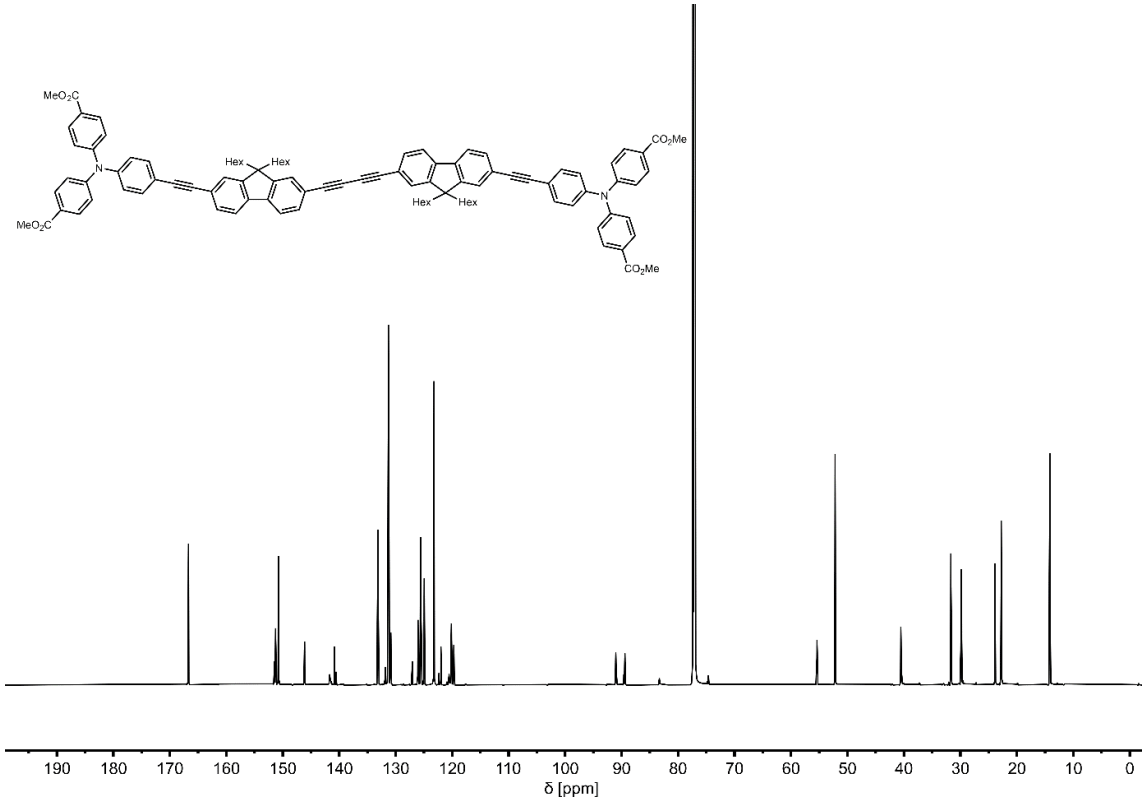


Figure S6. ^{13}C-NMR (800 MHz, 298 K) spectrum of compound **2^{Me}**, measured in $CDCl_3$.

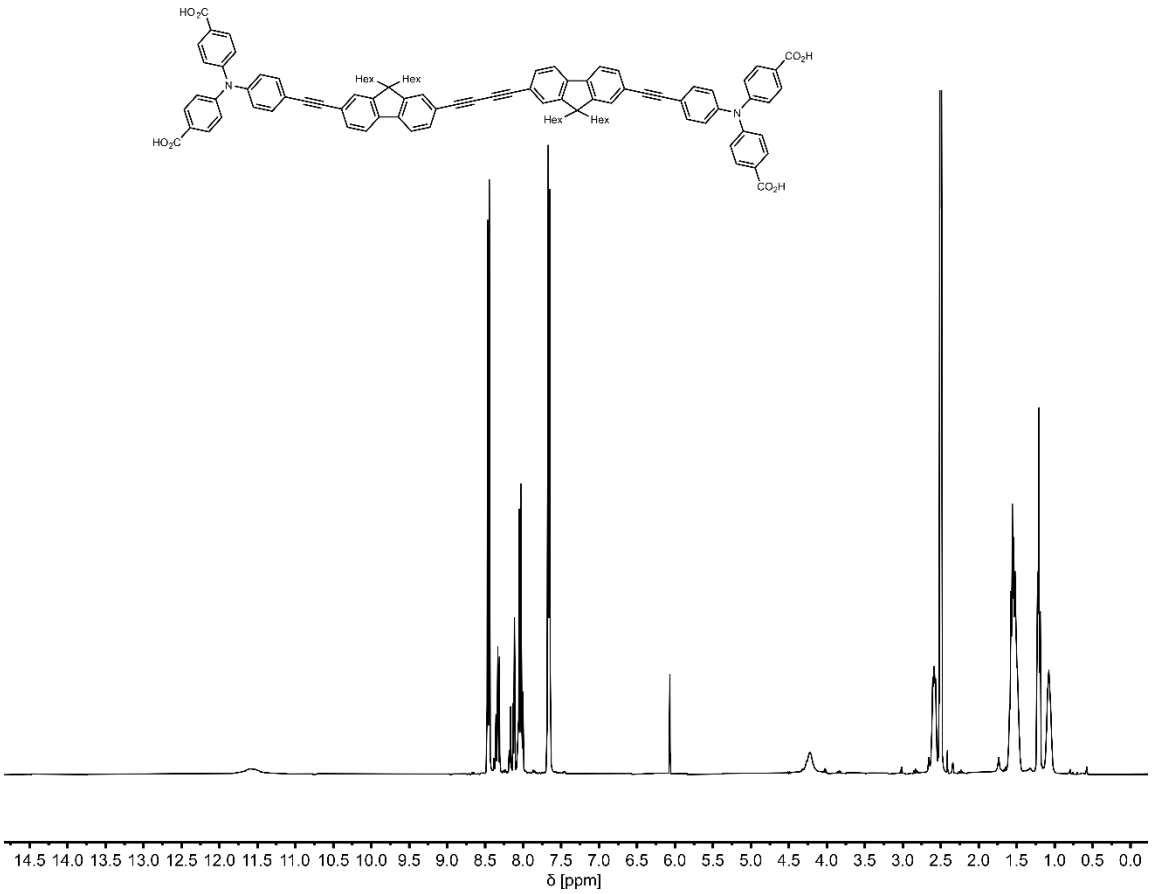


Figure S7. ^{1}H-NMR (400 MHz, 298 K) spectrum of compound **2^{H}**, measured in acetone-d_6.

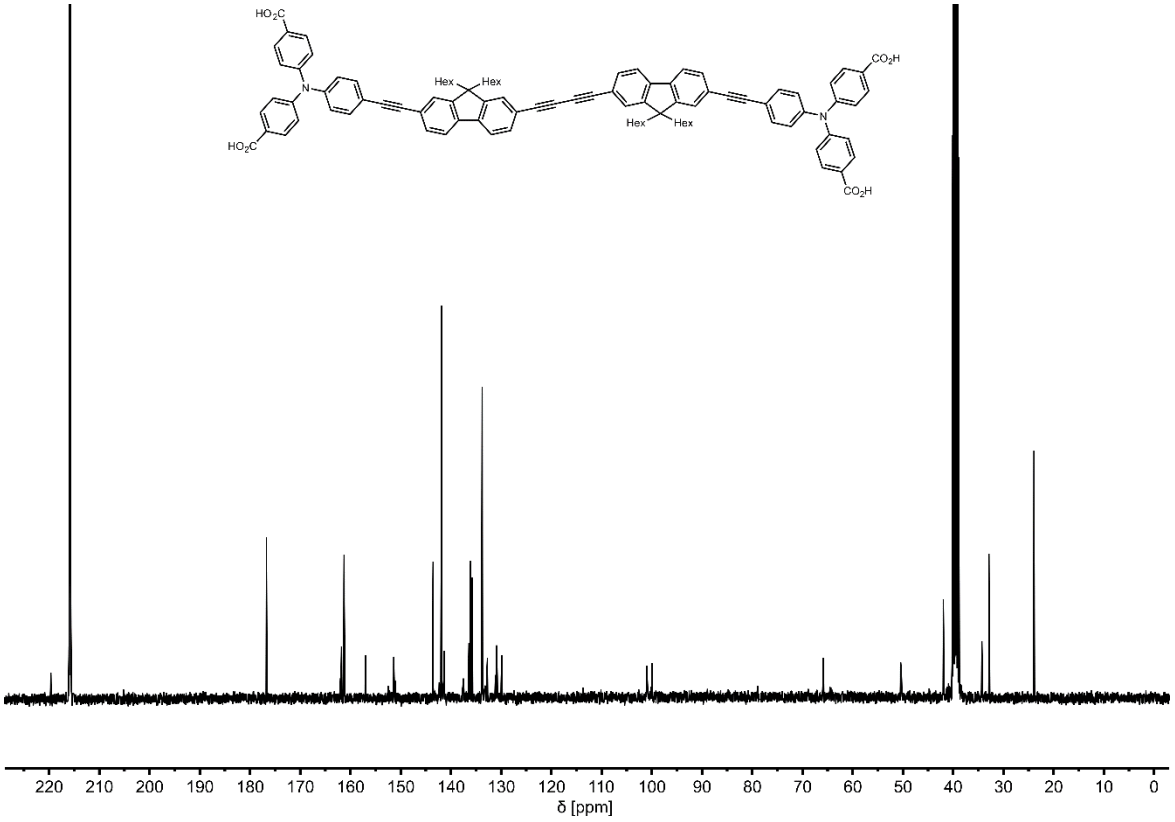


Figure S8. ^{13}C-NMR (400 MHz, 298 K) spectrum of compound **2^{H}**, measured in acetone-d_6.

Mass Spectrometry

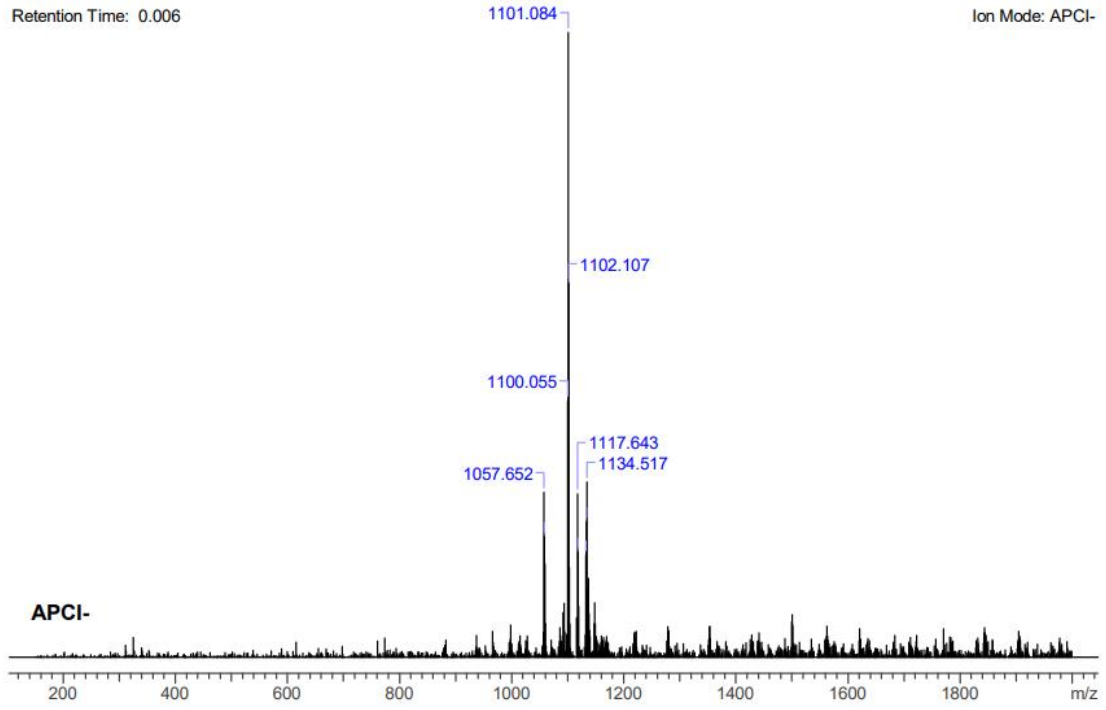


Figure S9. ESI mass spectrum of **1**^{Me}, recorded in negative ion mode.

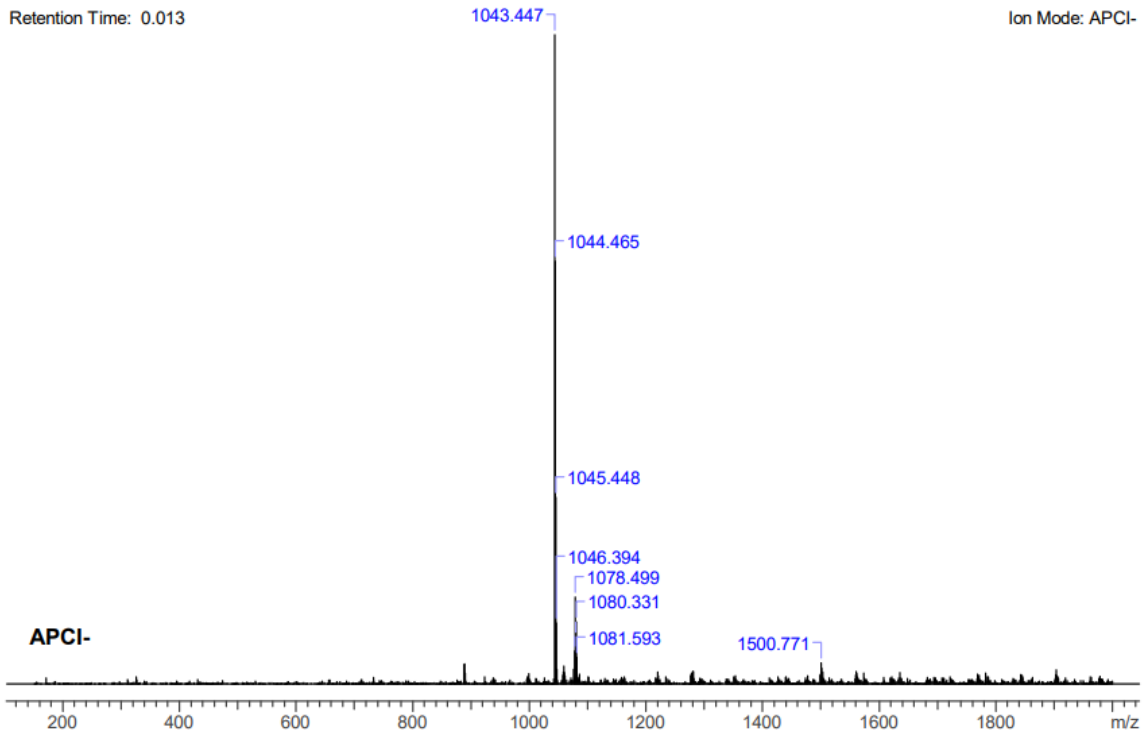


Figure S10. ESI mass spectrum of **1**^{H}, recorded in negative ion mode.

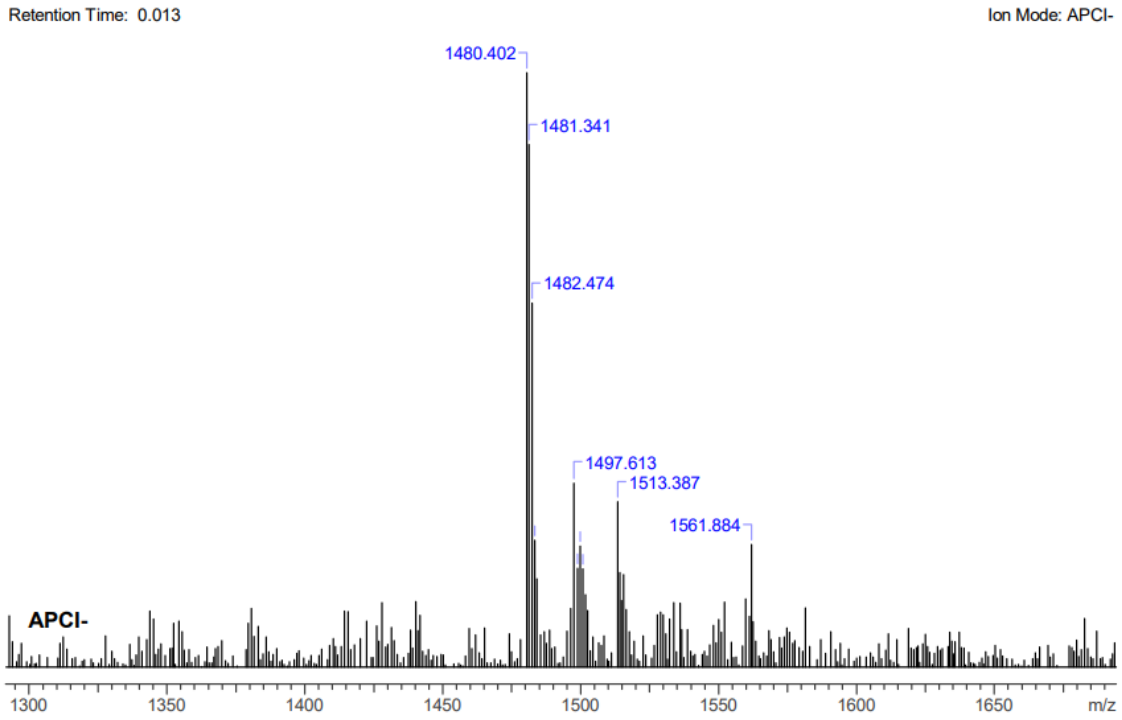


Figure S11. ESI mass spectrum of **2**^{Me}, recorded in negative ion mode.

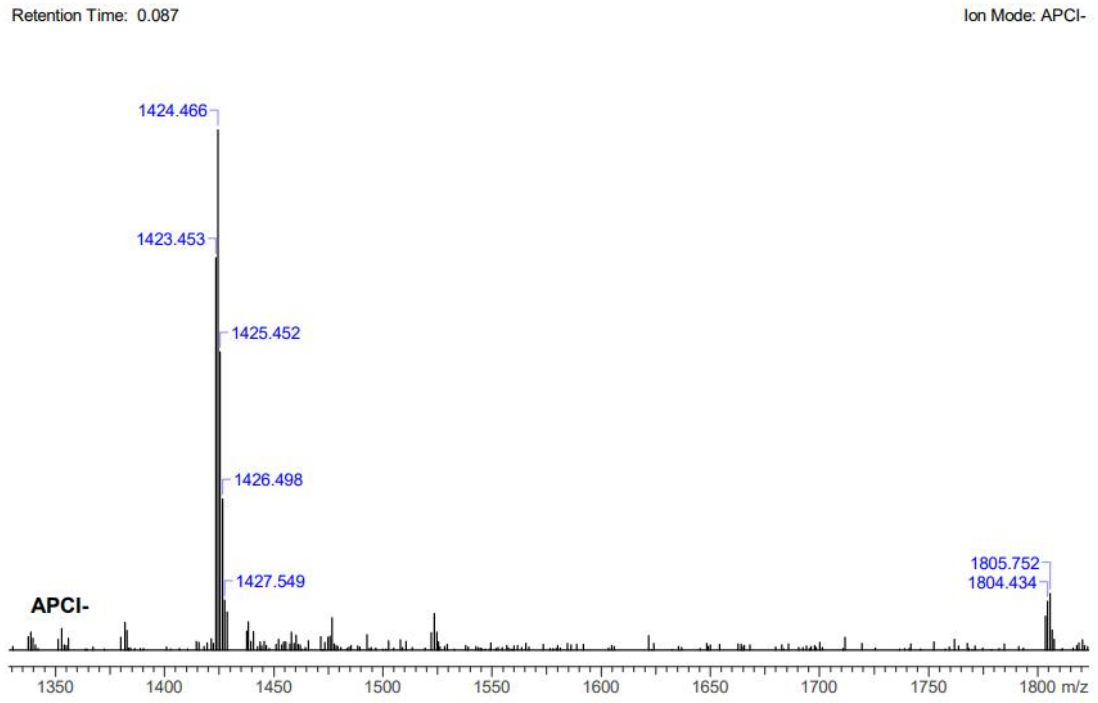


Figure S12. ESI mass spectrum of **2**^{H}, recorded in negative ion mode.

S2 Cyclic Voltammetry

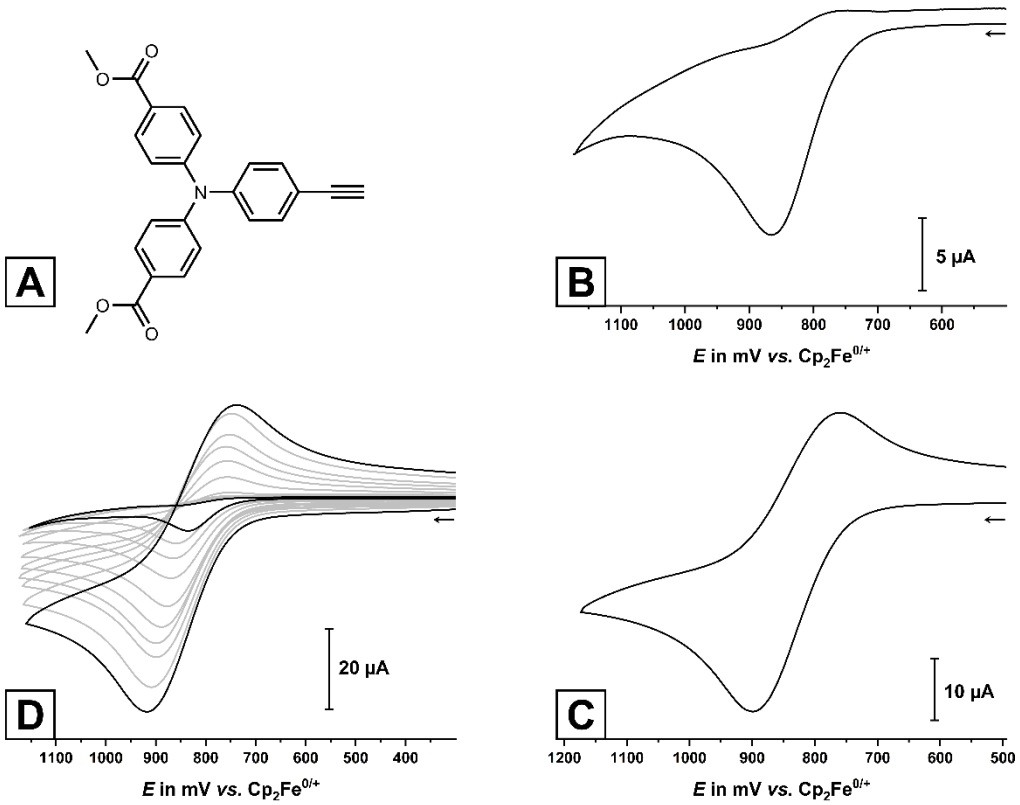


Figure 13. A: Molecular structure of compound **S5**. B. Cyclic voltammogram of S5 at a scan rate of 100 mV/s in 0.1 mM TBA^+ $BAr^{F_{24}-}$ CH_2Cl_2 at r. t. C: Cyclic voltammogram of **S5** at a scan rate of 800 mV/s in 0.1 mM TBA^+ $BAr^{F_{24}-}$ CH_2Cl_2 at r. t. D: Cyclic voltammograms of **S5** (in 0.1 mM TBA^+ $BAr^{F_{24}-}$ CH_2Cl_2 at r. t) at different scan rates ranging from 25 mV/s to 2000 mV/s.

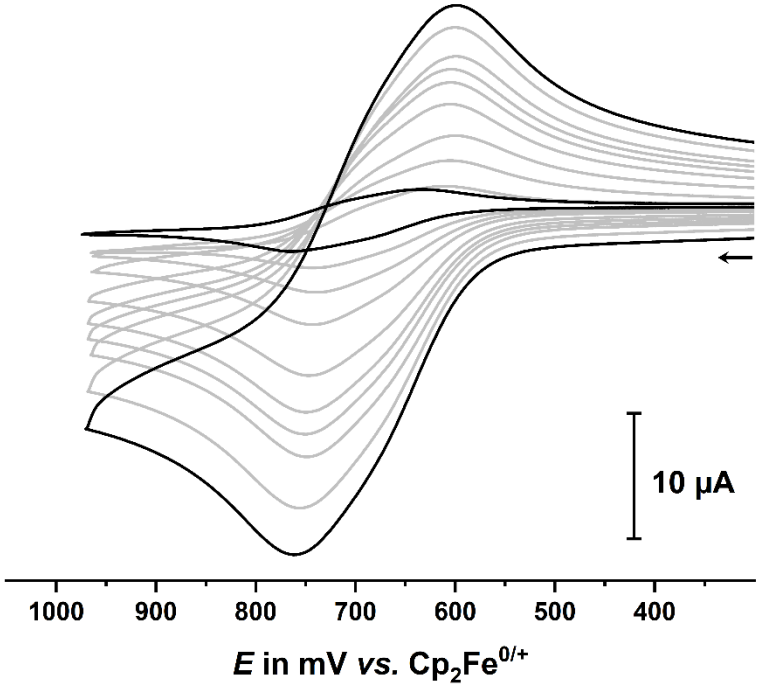


Figure 14. Cyclic voltammograms of $\mathbf{1^{Me}}$ (in 0.1 mM TBA^+ $BAr^{F_{24}-}$ CH_2Cl_2 at r. t.) at different scan rates ranging from 25 mV/s to 2000 mV/s.

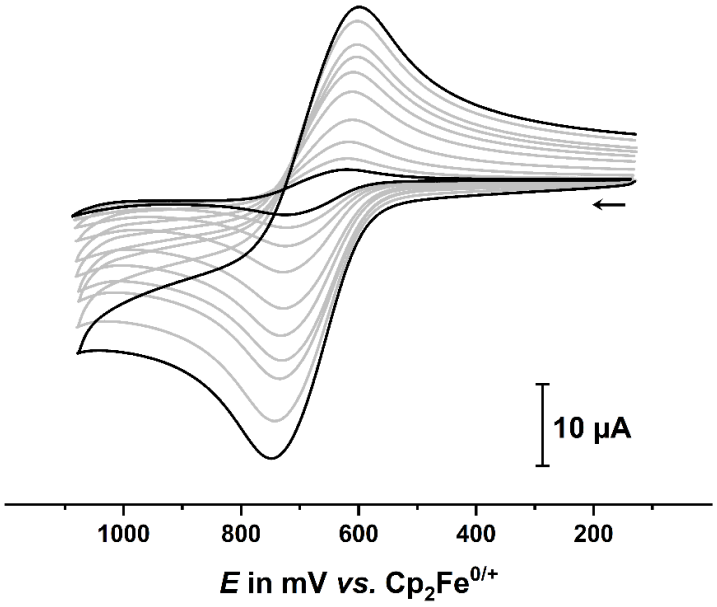


Figure 15. Cyclic voltammograms of $\mathbf{2^{Me}}$ (in 0.1 mM TBA^+ $BAr^{F_{24}-}$ CH_2Cl_2 at r. t.) at different scan rates ranging from 25 mV/s to 2000 mV/s.

Table S1. Electrochemical data of compound **S5** (0.1 mM TBA^+ $BAr^{F}{}_{24}^-$ CH_2Cl_2 at r. t).

Scan rate [mVs^{-1}]	$E_{1/2}^{0/n+}$ **[mV]**	**Δ E_p [mV]**
25	790	90
50	810	95
100	815	95
200	810	115
400	815	120
600	825	130
800	830	140
1000	825	140
1500	830	160
2000	830	175

Table S2. Electrochemical data of ester $\mathbf{1}^{Me}$ (0.1 mM TBA^+ $BAr^{F}{}_{24}^-$ CH_2Cl_2 at r. t).

Scan rate [mVs^{-1}]	$E_{1/2}^{0/n+}$ **[mV]**	**Δ E_p [mV]**
25	685	110
50	675	130
100	670	130
200	675	140
400	675	140
600	675	145
800	680	145
1000	675	150
1500	680	155
2000	680	160

Table S3. Electrochemical data of ester **2**$^{\mathbf{Me}}$ (0.1 mM TBA^+ $BAr^{F_{24}-}$ CH_2Cl_2 at r. t).

Scan rate [mVs^{-1}]	$E_{1/2}^{0/n+}$ **[mV]**	**Δ E_p [mV]**
25	675	105
50	670	105
100	670	105
200	670	120
400	670	120
600	670	125
800	670	130
1000	670	135
1500	670	140
2000	675	150

Table S4. Electrochemical data obtained from the digital simulation of the cyclic voltammograms of **1**$^{\mathbf{Me}}$ and **2**$^{\mathbf{Me}}$ in CH_2Cl_2/NBu_4^+ $[BAr^{F_{24}}]^-$ (0.1 M, T = 293 K (±3 K) *v* = 600 mV/s).

	1$^{\mathbf{Me}}$	**2**$^{\mathbf{Me}}$
$E_{1/2}^{0/+}$ [mV]	635	640
$E_{1/2}^{+/2+}$ [mV]	715	685
Δ*E*	80	45
K_c	23	6
$\alpha^{0/+}$ [eV]	0.41	0.55
$\alpha^{+/2+}$ [eV]	0.79	0.55
$k_s^{0/+}$ [cm/s]	0.009	0.005
$k_s^{+/2+}$ [cm/s]	0.011	0.012
D [cm^2/s]	5.32×10^{-6}	2.76×10^{-6}

S3 UV-Vis/NIR Spectroscopy

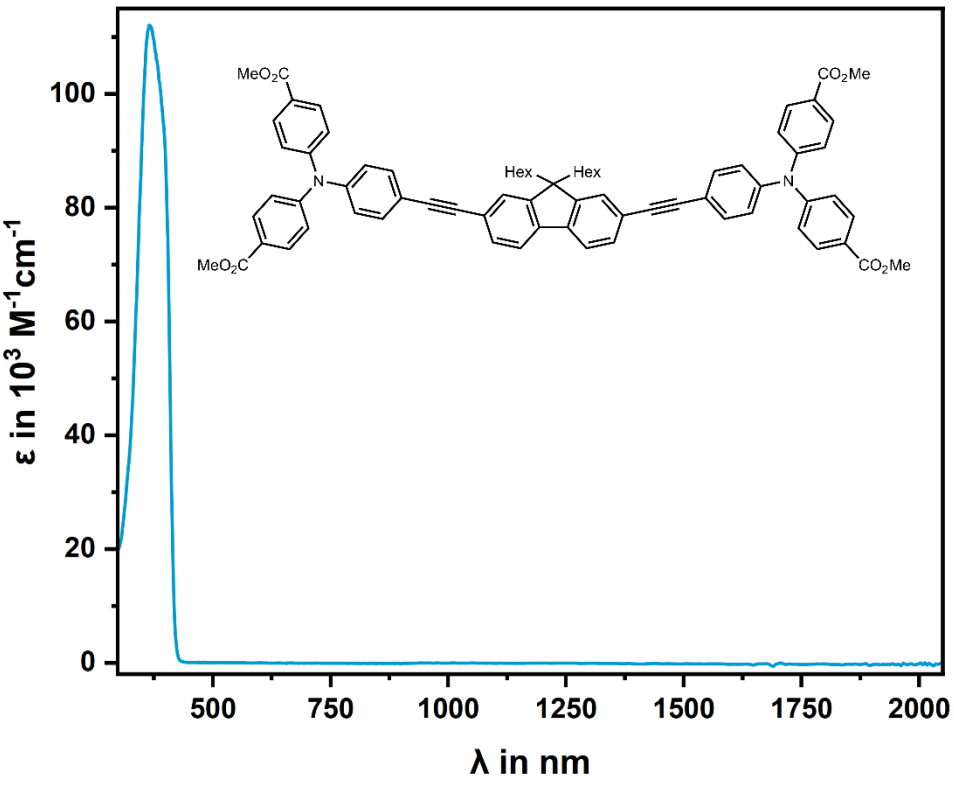


Figure S16. Experimentally determined UV-Vis/NIR spectrum of $\mathbf{1^{Me}}$ in CH_2Cl_2 λ_{max} = 366 nm; ε_{max} = 112×10^3 $M^{-1}cm^{-1}$.

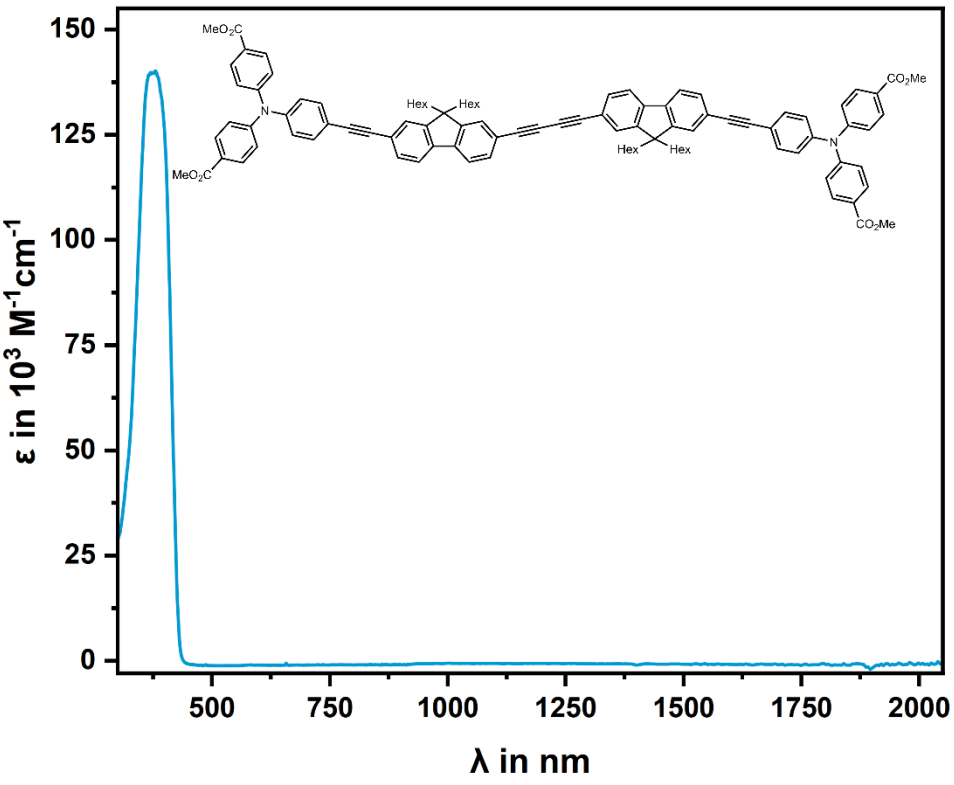


Figure S17. Experimentally determined UV-Vis/NIR spectrum of **2^{Me}** in CH_2Cl_2 λ_{max} = 375 nm; ε_{max} = 140×10^3 $M^{-1}cm^{-1}$.

Table S5. Relevant data obtained from UV-Vis/NIR spectroelectrochemistry of compounds **1**^{Me} and **2**^{Me} in their corresponding oxidation states as well as the TD-DFT calculated wavelengths, oscillator strengths, and corresponding transitions.

Compound		λ_{max} [nm] (ε [10^3 $M^{-1}cm^{-1}$])	TD-DFT calculated transitions	
			λ [nm] (*f*)	**contribution**
1^{Me}	0	366 (112)	397 (3.47)	H→L (85%)
	1+	360 (77), 547 (13), 712 (13), 1405 (11)	334 (0.57), 465 (0.69), 558 (0.27), 672 (0.03), 1037 (0.28), 1674 (1.08)	βH→βL+4 (45%), αH→αL+3 (45%) αH-1→αL (25%) αH-1→αL (10%), αH→αL (17%), αH→αL+2 (10%) βH-2→βL (72%), βH-1→βL (11%) βH-2→βL (11%), βH-1→βL (73%), βH→βL (15%) βH-1→βL (13%), βH→βL (85%)
	2+	353 (51), 528 (19), 688 (25), 1250 (22)	348 (0.08), 515 (0.30), 517 (0.60), 598 (0.10), 1183 (1.82)	βH-13→βL+1 (15%) αH→αL (15%), βH-3→βL (25%), βH-2→βL+1 (29%) αH→αL (37%), βH-3→βL (18%), βH-2→βL+1 (11%) βH-4→βL (15%), βH-3→βL (15%), βH-1→βL+1 (48%) βH-1→βL+1 (11%), βH→βL (86%)
2^{Me}	0	379 (140)	421 (5.07)	H→L (73%), H-2→L (11%)
	1+	362 (102), 550 (15), 708 (18), 1400 (11)	356 (0.52), 539 (0.19), 865 (0.08), 1213 (0.46), 1549 (0.84)	βH→βL+1 (49%), βH→βL+2 (12%) αH-1→αL (10%) βH-3→βL (19%), βH-2→βL (43%), βH-1→βL (32%) βH-2→βL (19%), βH-1→βL (45%), βH→βL (30%) βH-1→βL (21%), βH→βL (70%)
	2+	355 (70), 533 (22), 690 (42), 1250 (19)	395 (0.71), 586 (0.25), 618 (0.24), 1345 (2.39)	αH→αL (10%), βH-1→βL+3 (12%), βH→βL+2 (26%) αH→αL (19%), βH-2→βL (21%), βH-1→βL+1 (13%), βH→βL+2 (10%) αH→αL (16%), βH-2→βL (19%), βH-1→βL+1 (18%), βH→βL+2 (11%) βH-1→βL+1 (18%), βH→βL (76%)

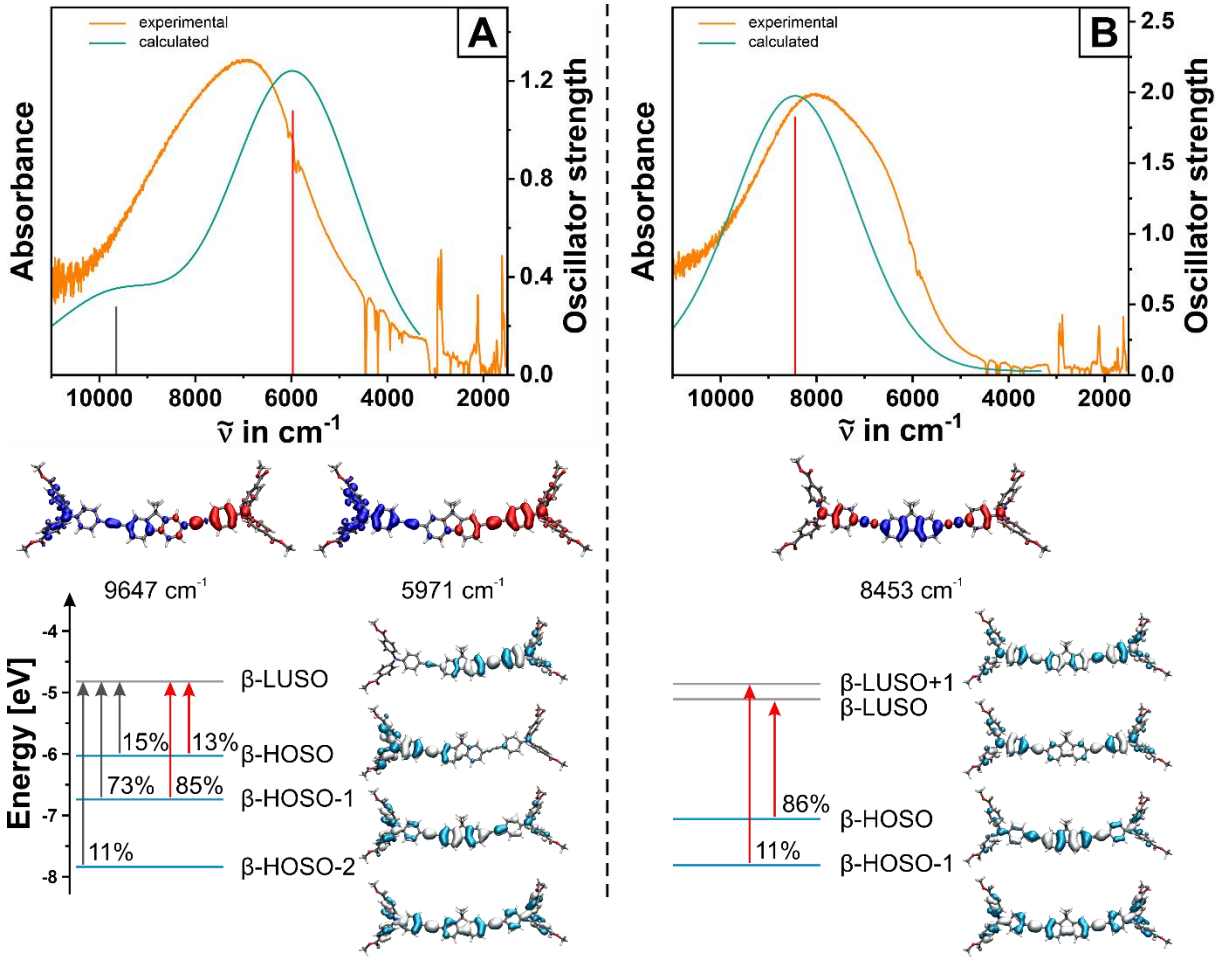


Figure S18. Top: Comparison between experimental NIR spectra of $\mathbf{1}^{Me\,\bullet+}$ (orange line in panel A) and $\mathbf{1Me}^{2+}$ (green line in panel B) in 1,2-CH_4Cl_2 (0.1 M NBu_4^+ $[BAr^{F_{24}}]^-$ as the supporting electrolyte) and TD-DFT calculated electronic spectra of model compound $\mathbf{1}^{Me'\,\bullet+}$ (panel A, turquoise line) and $\mathbf{1}^{Me'\,\bullet2+}$ (panel B, violet). Computed transitions are provided as red and grey vertical bars. Bottom: Contour diagrams of the acceptor and donor MOs involved in the NIR transitions together with their contributions to the respective transition, and corresponding electron density difference maps (EDDMs). Blue colour indicates electron density loss, red colour an increase in electron density. Isosurface values for the MO plots are set as ±0.02.

S4 Molecular Dynamics Simulation

To explore the incorporation of **1**^{H} or **2**^{H} in the lipid bilayer membrane, MD simulations with the AMBER forcefield were performed using the YASARA v21.6.2 software. The assisted model building was utilized based on the macro for running a molecular dynamics simulation of a membrane protein. This macro sets up and runs a simulation of a membrane protein; in our case, the protein is the chromophore (**1**^{H} or **2**^{H}). It scans the chromophore for secondary structure elements with hydrophobic surface residues, orients it accordingly, and embeds it in a membrane of adjustable lipid composition. Finally, 250 ps restrained equilibration simulations were run, which ensures that the membrane can adapt to the newly embedded chromophore.[17,18] Then, the real simulation starts. The macro can be found at yasara.org/md_runmembrane.mcr.

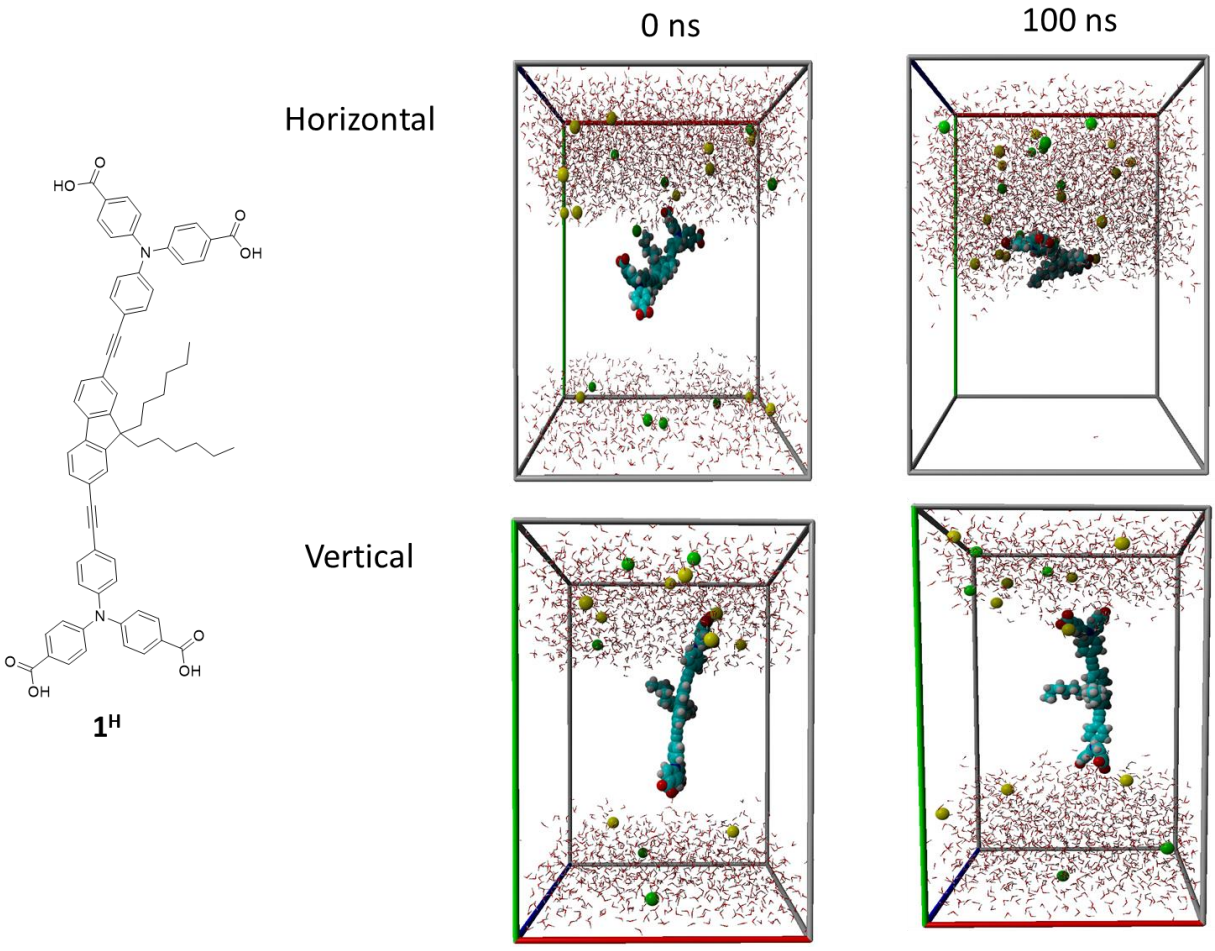


Figure S19. The final point of trajectories shows how **1**^{H} orients in the membrane. Top, the simulation started with parallel alignment for 0 ns (left) and after 100 ns (right). Bottom, the simulation started with transmembrane alignment for 0 ns (left) and after 100 ns (right). Red spheres represent water molecules; the membrane was omitted for a clearer view.

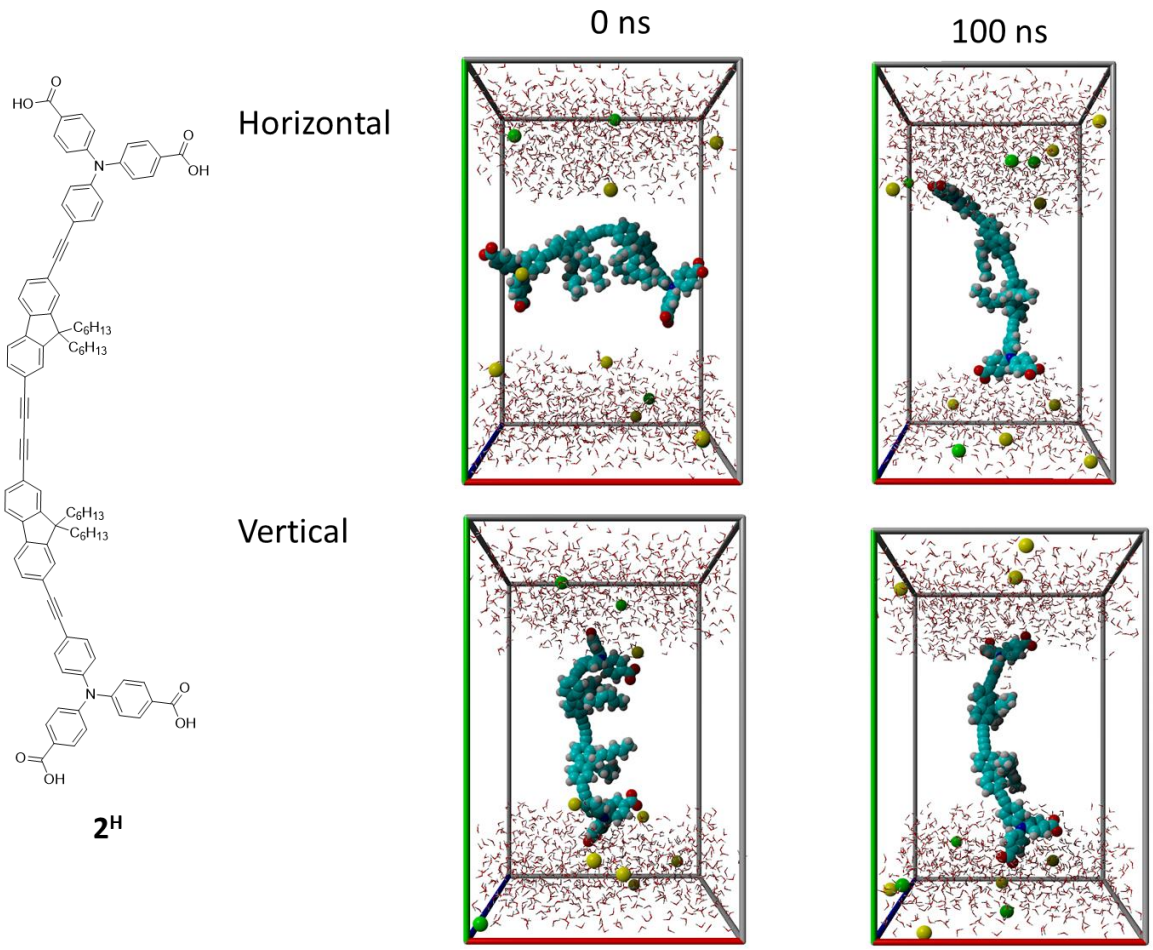


Figure S20. The final point of trajectories shows how $\mathbf{2^H}$ orients in the membrane. Top, the simulation started with parallel alignment for 0 ns (left) and after 100 ns (right). Bottom, the simulation started with transmembrane alignment for 0 ns (left) and after 100 ns (right). Red spheres represent water molecules; the membrane was omitted for a clearer view.

S5 Calceine-Luminescence Leakage Test

We conducted a calceine test to check the impermeability of the membrane, which is a standard procedure used to assess the potential for membrane disruption during encapsulation.[18,19] We examined the DPPC liposome with and without integration of $\mathbf{1^H}$ and $\mathbf{2^H}$ and monitored the solution for 3 days.

The calceine test preparation is as follows: in a 5 mL round bottom flask, 1 mL of a stock solution of DPPC (5.0 mM), 1 mL 14:0 PEG2000 PE (0.05 mM) and 1 mL of $\mathbf{1^H}$ or $\mathbf{2^H}$ (0.05 mM) in acetonitrile were combined. The organic solvents were evaporated under vacuum for at least one hour. Calceine (43.58 mg, 0.07 mmol) was added to the flask and hydrated with 1 mL phosphate buffer (K_2HPO_4/KH_2PO_4, pH 7.7) to yield a calceine concentration of 70 mM. The dispersed lipid film was freeze-thawed three times, using liquid N_2 and a water bath at 52 °C. The dispersion was extruded at 52 °C through 200 nm cellulose membrane filters 11 times with an Avanti Polar Lipids mini-extruder. The obtained solutions of liposomes were separated from excess calceine using an SEC with phosphate buffer pH 7.7 as eluent. Luminescence measurements were carried out with 10 µl of liposome solution diluted with 990 µl of phosphate buffer pH 7.7. After the measurements, Triton X-100 (1 mM, 50 µl) was added to

the liposome sample. The liposomes are disturbed by the addition of Triton X-100 and release the encapsulated calceine. To check the stability of encapsulation in liposomes, other samples were measured after 2 h irradiation with a 470 nm LED stick. All luminescence spectra were recorded from 495 – 700 nm with excitation at λ_{ex} = 485 nm. Experiments were carried out for 3 days to investigate the stability of the membrane.

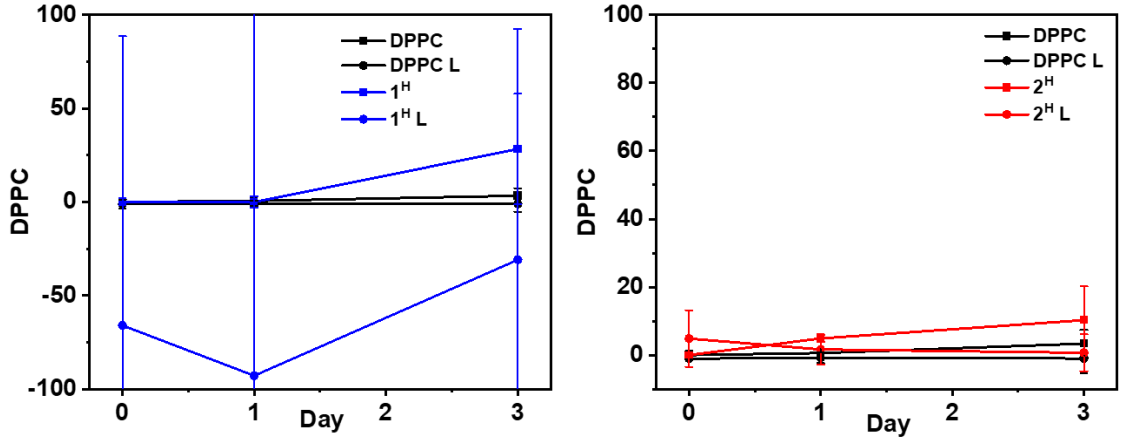


Figure S21. (left) Leakage test with and without **1**^{H}, (right) Leakage test with and without **2**^{H}. The percentage of calcein leakage is measured by comparing the luminescence before and after the addition of Triton X-100. The L symbol means, that the measurements were carried out after 2h irradiation with 470 nm LED.

S6 Liposome preparation

Stock Solutions.

The lipids 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) and 1,2-dimyristoyl-sn-glycero-3-phosphoethanolamine-N-[methoxy(polyethylene glycol)-2000] (ammonium salt) (14:0 PEG2000 PE) were prepared as stock solutions in $CHCl_3$ with the concentration of 5 mM and 0.05 mM respectively. The chromophores **1**^{H} or **2**^{H} were prepared with a concentration of 0.05 mM in methanol and $CHCl_3$ (1:1) mixture and for bis(2,2'-bipyridine)-(4,4'-dinonyl-2,2'-bipyridine)-ruthenium(II) hexafluorophosphate (RuC_9) was diluted with the same concentration (0.05 mM) in acetonitrile. Phosphate buffer pH 7.0 was prepared with the mixture of KH_2PO_4 (626 mg, 4.6 mmol), $K_2HPO_4{\cdot}3H_2O$ (1.186 g, 5.2 mmol), and K_2SO_4 (1.70 g, 9.74 mmol) in Milli-Q water (1 L) to reach a final pH of 7.0. The tetrazolium dye XTT (sodium 4-methoxy-5-[3-(2-methoxy-4-nitro-5 sulfonatophenyl)-5-(phenylcarbamoyl)tetrazol-3-ium-2-yl]-2 nitrobenzenesulfonate) was prepared with a concentration of 1 mM in phosphate buffer pH 7.0.

Preparation and characterization of giant vesicles and liposomes.

Giant vesicles and liposomes were prepared as follows. To prepare a lipid film, 1 mL stock solution of DPPC (5.0 mM), 1 mL 14:0 PEG2000 PE (0.05 mM), and 1 mL **1**^{H} or **2**^{H} (0.05 mM) were combined in a 5 mL round bottom flask. The organic solvents were evaporated under vacuum leading to deposition of lipid film on the flask wall. The lipid film was dried under a high vacuum for at least one hour and

hydrated with phosphate buffer pH of 7.0 and 15 mg of NADH or XTT. The dispersed lipid film was repeatedly subjected to freeze-thawing, using liquid N_2 and a water bath at 52 °C, yielding giant vesicles.

Before microscopy, and if applicable, giant vesicles were subjected to a Sephadex G-25 size exclusion chromatography (SEC) column (6 cm length, 2 cm diameter) using phosphate buffer at pH 7.0 as eluent. To prepare the sample for confocal microscopy measurements, a 50-100 μL amount of the giant vesicle sample was loaded into a well of the sample holder. Next, 200 μL of a freshly prepared, air-cooled agarose solution (1 weight-% in water) were added to the well and mixed with the sample. The mixed solution was then allowed to settle at room temperature before confocal microscopy measurements were taken with an excitation laser at λ_{ex}=405 nm and detected emission from 420-650 nm.

To obtain liposomes of uniform size, the dispersion was extruded at 52 °C through 200 nm cellulose membrane filters 11 times with an Avanti Polar Lipids mini-extruder. The mixture of liposomes was treated with an SEC column, with phosphate buffer pH 7.0 as eluent, to separate the unencapsulated NADH. The liposome solution was collected and measured using dynamic light scattering (DLS). The results showed a Z_{Avg}-diameter ranging from 130-150 nm with a polydispersity index of about 0.1.

The procedure of photoirradiation

The typical reactions were carried out within quartz cuvettes where 300 μl of liposome solution, 10 μl of 1 mM XTT or 1 mM NADH, and 190 μl phosphate buffer pH 7.0 were added. The mixtures were illuminated within a custom-made reactor equipped with four ventilators to exclude heating of the samples and an LED stick (λ = 460 $\pm$ 22 nm and λ = 370 $\pm$ 24 nm).[21] The samples were monitored via UV-Vis spectroscopy after 0, 5, 15, 30, 60, 120, and 180 minutes.

Transmembrane electron transfer experiments

To evaluate the photoinduced electron transfer, the number of formazan (n_{fz}) (Fz) was calculated by measuring the increasing absorbance at 470 nm; the increasing absorbance value was converted to the amount of Fz formed with the reported extinction coefficient of Fz at 470 nm (21.600 M^{-1} cm^{-1}).[22]

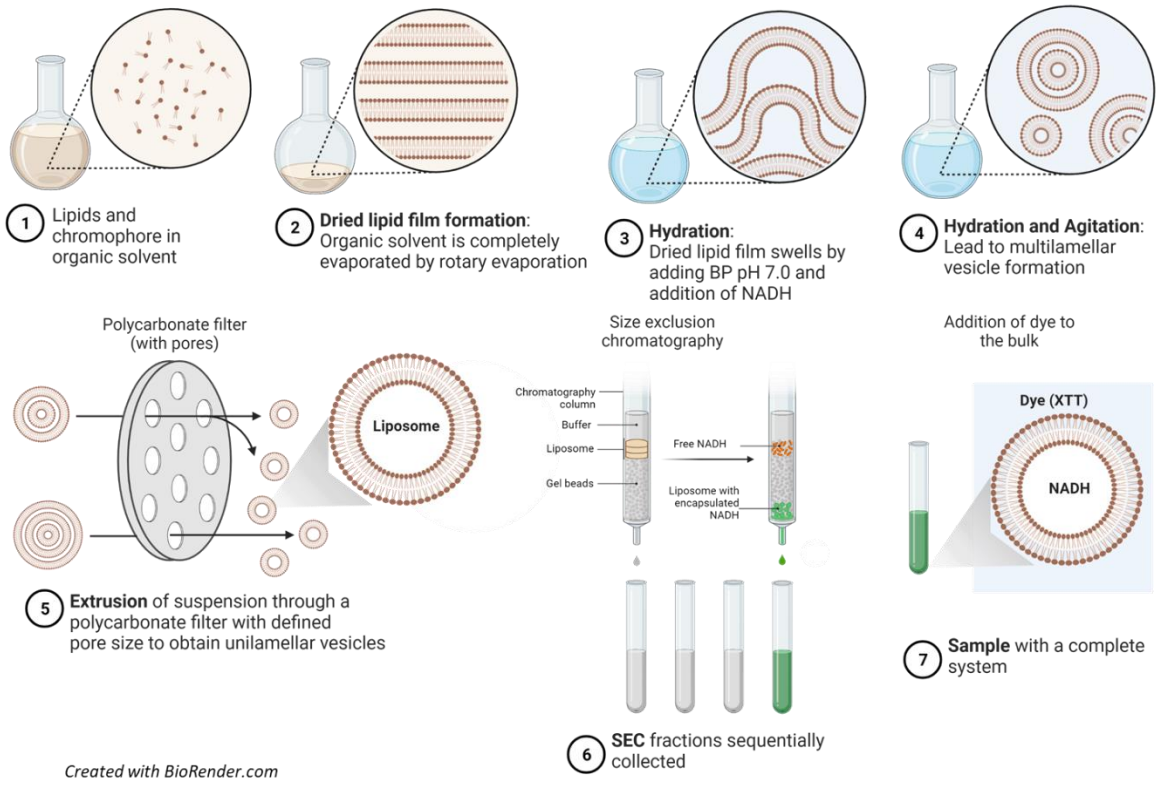


Figure S22. Liposome preparation via thin film hydration with NADH encapsulated in the inner part of liposomes. Created with Biorender.com.

S7 The Typical Hydrodynamic Diameter of DPPC Liposome

The size distribution of the hydrodynamic diameter (Z_{Avg}) was measured at 20 °C with a Zetasizer Pro from Malvern operating at 633 nm with a scattering angle of 173°.

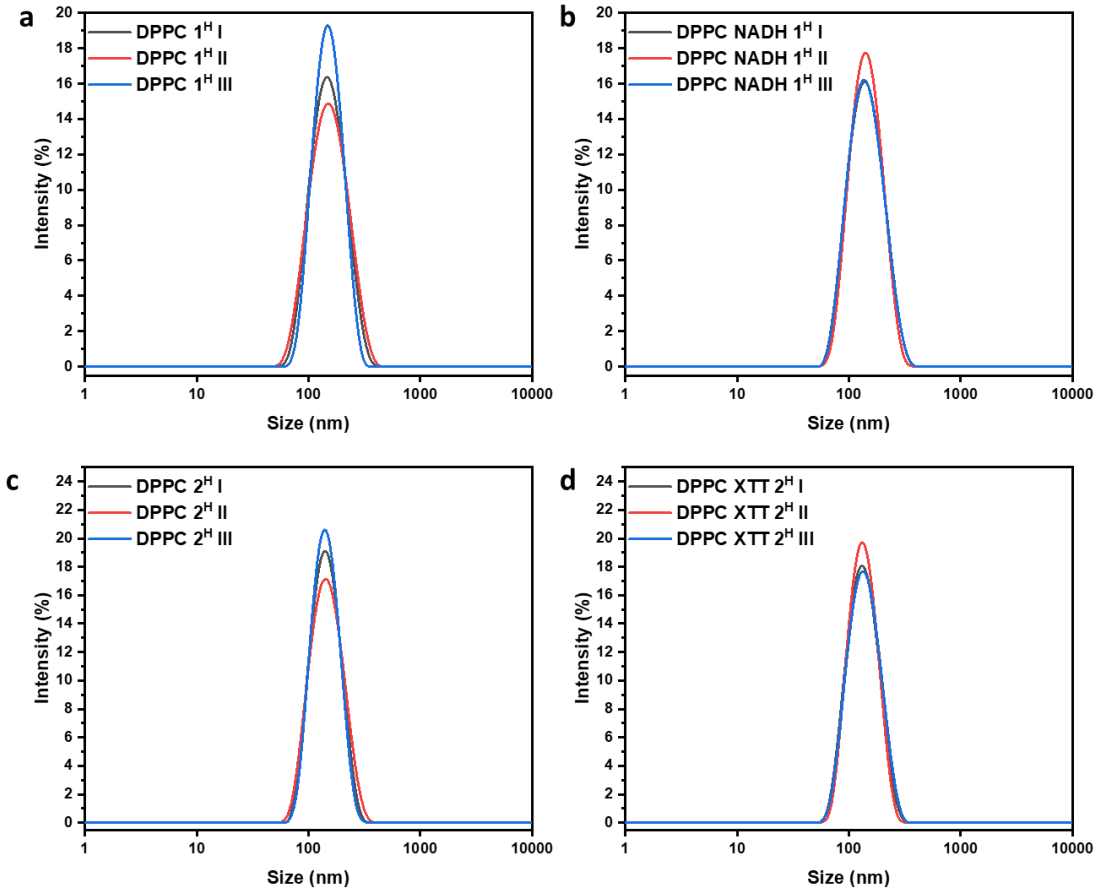


Figure S23. Typical DLS measurements of DPPC:(14:0 PEG2000 PE):$[1]^{2+}$= 100:1:1 liposomes, a) 1 mol% of $\mathbf{1}^{H}$, b) 1 mol% of $\mathbf{1}^{H}$ with encapsulated NADH, c) 1 mol% of $\mathbf{2}^{H}$, and d) 1 mol% of $\mathbf{2}^{H}$ with encapsulated XTT.

S8 Spectra of LEDs and DPPC with integrated $\mathbf{1^H}$ or $\mathbf{2^H}$

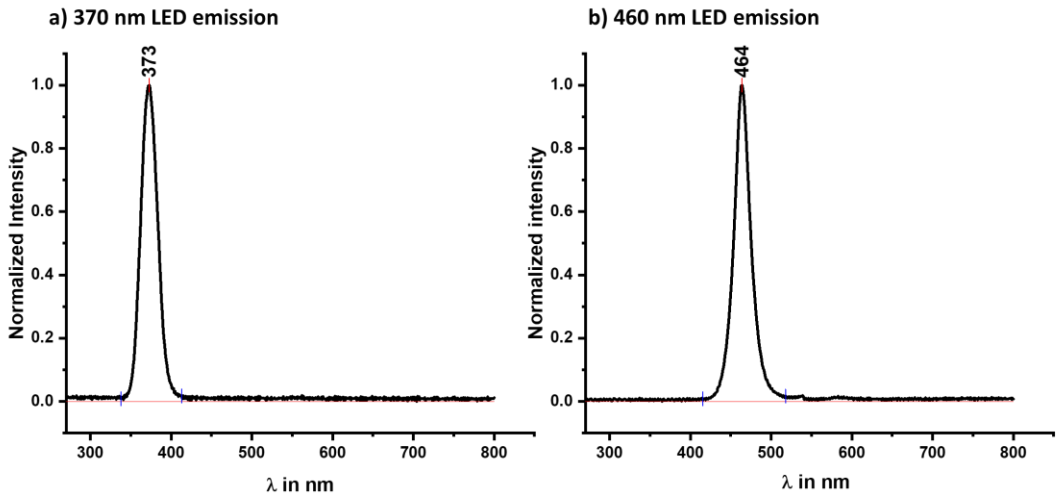


Figure S24. Emission spectra of a) 370 nm LED and b) 460 nm LED.

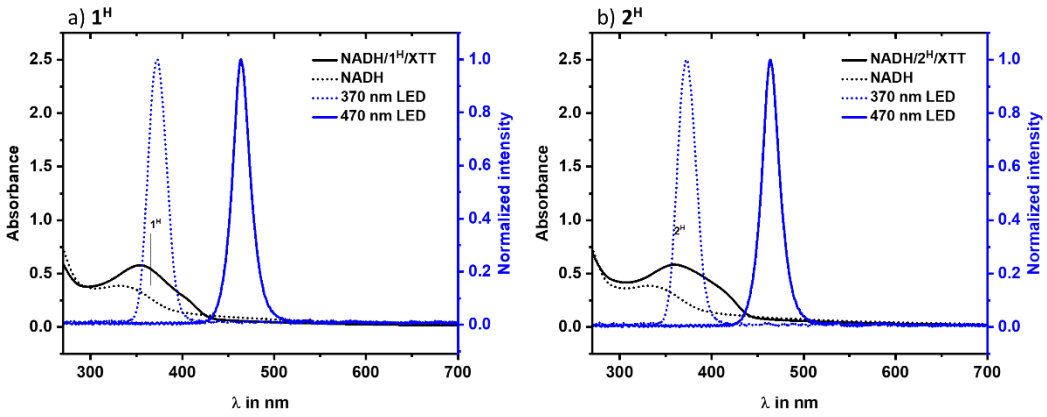


Figure S25. Overlap spectra of a) NADH/$\mathbf{2^H}$/XTT (solid black line) and encapsulated NADH in DPPC liposome (dotted black line) and b) NADH/$\mathbf{1^H}$/XTT (solid black line) and encapsulated NADH in DPPC liposome (dotted black line) before irradiation with the emission spectra of 370 nm (dotted blue line) and 470 nm LEDs (solid blue line).

S9 Photoinduced electron transfer reactions in the membrane

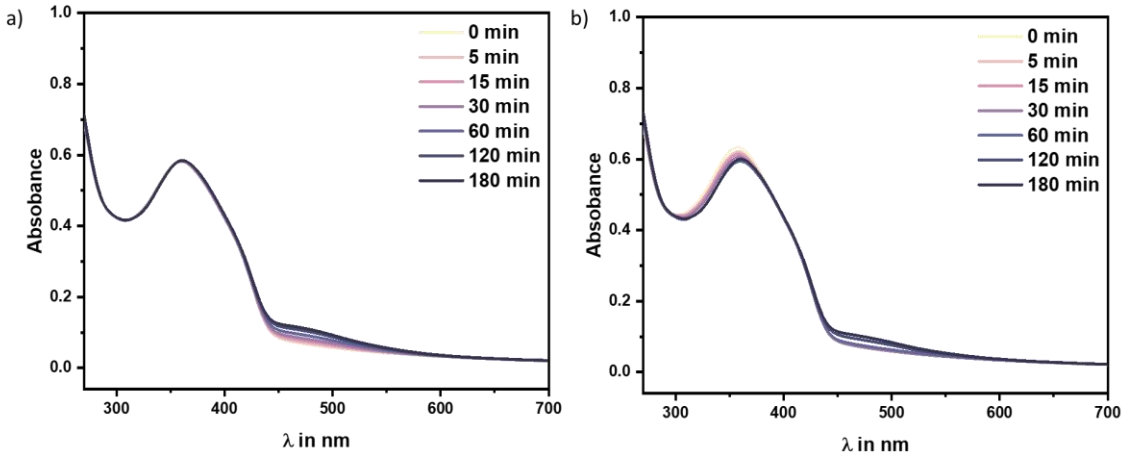


Figure S26. Temporal UV-vis spectra of NADH/**2**^{H}/XTT in phosphate buffer pH 7.0, irradiated with a) 470 nm LED; b) 370 nm LED.

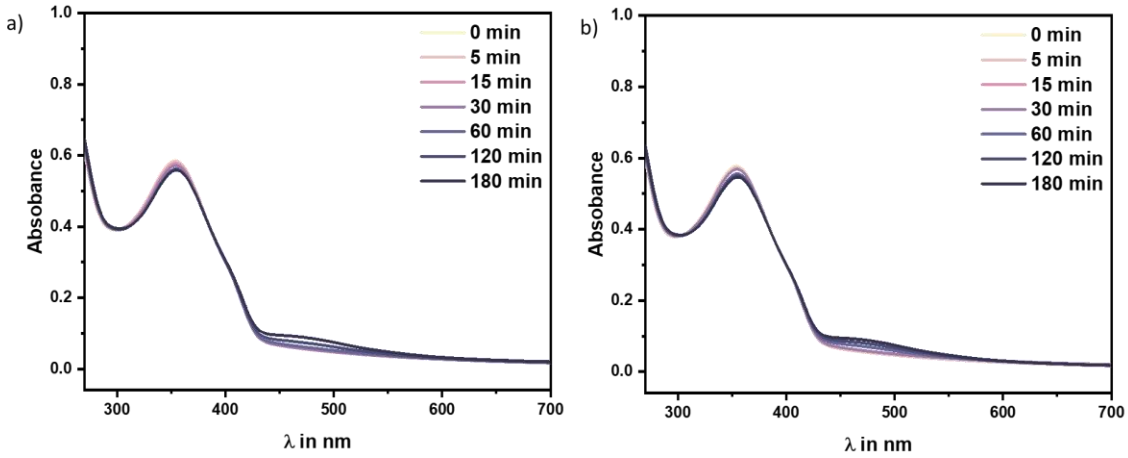


Figure S27. Temporal UV-vis spectra of NADH/**1**^{H}/XTT in phosphate buffer pH 7.0, irradiated with a) 470 nm LED; b) 370 nm LED.

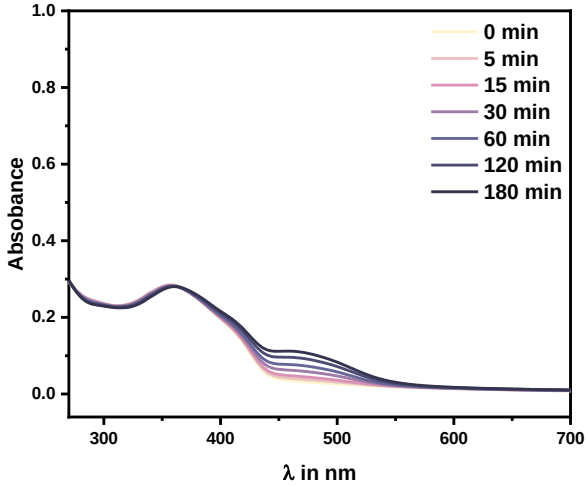


Figure S28. Temporal UV-vis spectra of XTT/**2**^{H}/NADH in phosphate buffer pH 7.0, irradiated with 470 nm LED.

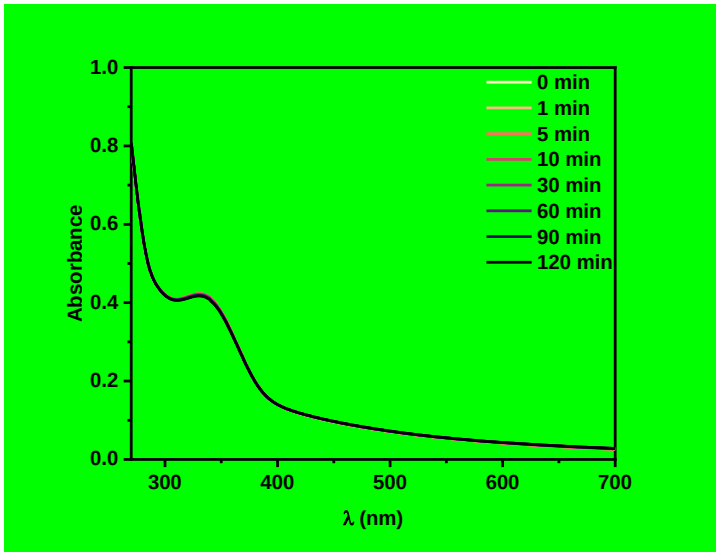


Figure S29. Temporal UV-vis spectra of NADH/-/XTT, NADH encapsulated inside DPPC liposome and XTT at the bulk solution in phosphate buffer pH 7.0, irradiated with 470 nm LED.

S10 Stern-Volmer Quenching Experiment

Liposomes were prepared as described in the methods section.

In cuvette:

V = 0.5 mL

2^{H} = 5 μM

[DPPC] = 500 μM

[14:0 PEG2000 PE] = 5 μM

Encapsulated NADH (NADH/2^{H})

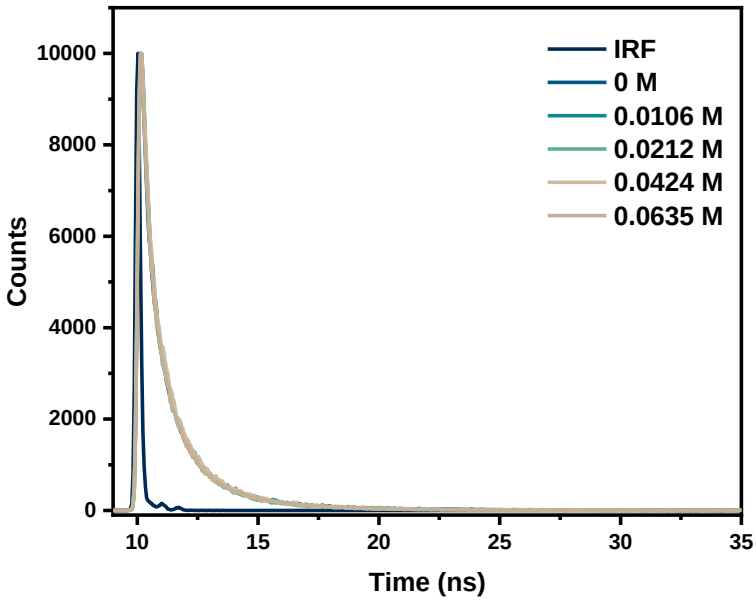


Figure S30. Kinetic traces of luminescence decay upon excitation at 371 nm with various concentrations of encapsulated NADH inside liposome as a quencher.

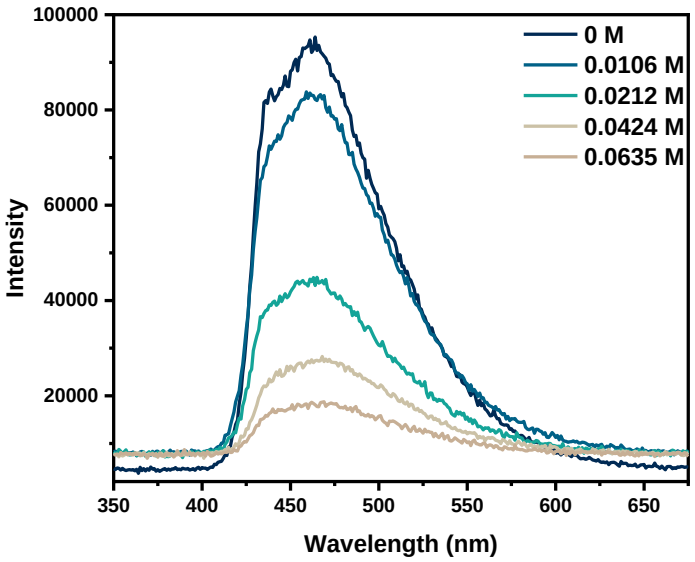


Figure S31. Luminescence quenching upon encapsulation of various concentrations of NADH inside liposome as a quencher.

XTT as quencher at the bulk solution (2^H/XTT)

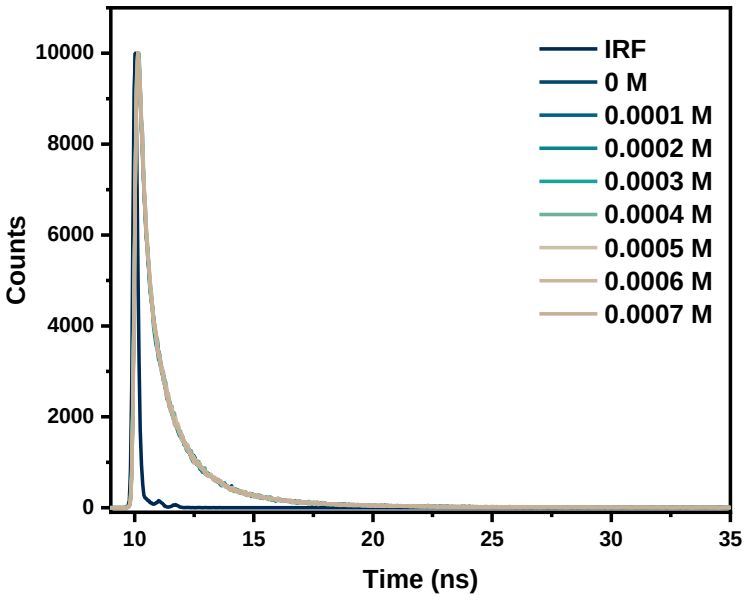


Figure S32. Kinetic traces of luminescence decay upon excitation at 371 nm with various concentrations of XTT as a quencher.

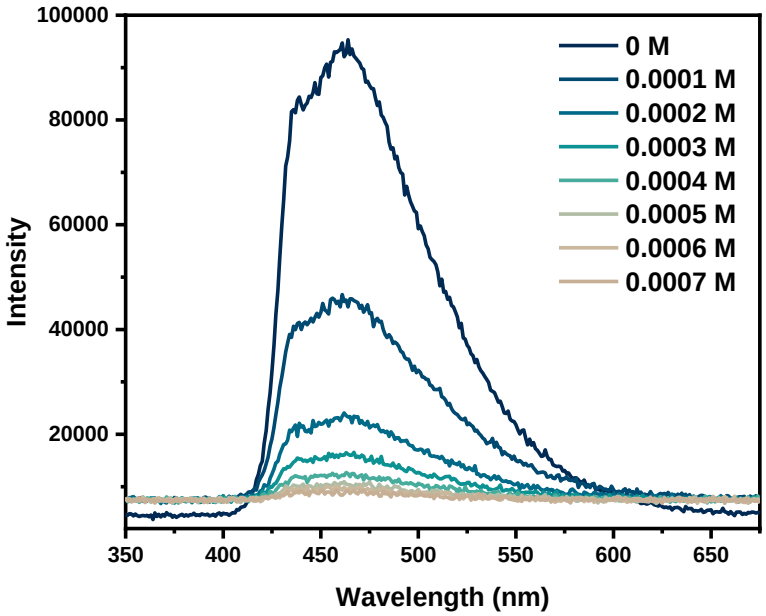


Figure S33. Luminescence quenching upon the addition of various concentrations of XTT as a quencher

S11 Atomic Coordinates of DFT Geometry-Optimized Structures

Table S6. Atomic coordinates of $\mathbf{1}^{Me}$ from its DFT geometry-optimized structure.

Atom	x	y	z
C	-3.52246	0.11964	2.41936
C	-3.12193	0.11601	1.06722
C	-4.10308	0.09554	0.05334
C	-5.44354	0.07973	0.39980
C	-5.83017	0.08295	1.75365
C	-4.86826	0.10304	2.76564
H	-2.76117	0.13558	3.19614
H	-3.79000	0.09292	-0.98897
H	-5.15886	0.10600	3.81463
C	-6.66259	0.05788	-0.51846
C	-7.79627	0.04883	0.50358
C	-9.16196	0.02982	0.27636
C	-10.05028	0.02419	1.37266
C	-9.53254	0.03787	2.68435
C	-8.16153	0.05746	2.91095
C	-7.29223	0.06319	1.81817
H	-9.56536	0.01904	-0.73440
H	-10.22272	0.03329	3.52508
H	-7.77990	0.06816	3.93035
C	-1.73480	0.13351	0.72725
C	-0.55539	0.14909	0.43800
C	-11.46193	0.00523	1.15604
C	-12.66223	-0.01031	0.97176
C	-14.07369	-0.02815	0.75655
C	-14.60629	-0.01112	-0.54583
C	-14.96886	-0.06299	1.84171
C	-15.97774	-0.03523	-0.75383
H	-13.93236	0.00755	-1.39943
C	-16.34027	-0.07279	1.63245
H	-14.57883	-0.06849	2.85709
C	-16.86290	-0.06267	0.33224
H	-16.37038	-0.03550	-1.76793

H	-17.01649	-0.08583	2.48399
C	0.83123	0.16849	0.09783
C	1.81955	0.22633	1.09782
C	1.24547	0.13115	-1.24647
C	3.16670	0.23932	0.76650
H	1.52202	0.24764	2.14387
C	2.59265	0.15834	-1.57677
H	0.49810	0.09447	-2.03595
C	3.57115	0.20949	-0.57489
H	3.91617	0.27065	1.55383
H	2.89286	0.14295	-2.62186
N	-18.26590	-0.08026	0.11900
N	4.94927	0.23112	-0.91325
C	-19.06681	-0.99966	0.82938
C	-20.32685	-0.62335	1.32205
C	-18.61060	-2.30699	1.06496
C	-21.11068	-1.53094	2.01994
H	-20.68833	0.38892	1.16079
C	-19.39385	-3.20583	1.77274
H	-17.64065	-2.61616	0.68422
C	-20.65365	-2.83349	2.25628
H	-22.08137	-1.22442	2.39977
H	-19.04143	-4.21936	1.94867
C	-18.84284	0.82158	-0.80009
C	-19.89396	0.41727	-1.63906
C	-18.36688	2.13942	-0.89844
C	-20.45820	1.30765	-2.54125
H	-20.26430	-0.60319	-1.58580
C	-18.92750	3.02107	-1.80991
H	-17.55873	2.47028	-0.25132
C	-19.98110	2.62064	-2.64011
H	-21.26746	0.97949	-3.18767
H	-18.56154	4.04266	-1.88003
C	5.44732	-0.68355	-1.86545
C	6.41083	-0.28620	-2.80731
C	4.97830	-2.00664	-1.89388

C	6.89316	-1.19093	-3.74036
H	6.77458	0.73802	-2.80844
C	5.45708	-2.90456	-2.83745
H	4.23847	-2.33105	-1.16670
C	6.42327	-2.50948	-3.77071
H	7.63491	-0.87996	-4.47218
H	5.08966	-3.92702	-2.84374
C	5.80438	1.16725	-0.29410
C	7.10817	0.80811	0.08451
C	5.36043	2.47462	-0.03604
C	7.94506	1.73198	0.69386
H	7.46243	-0.20361	-0.09518
C	6.19775	3.38978	0.58326
H	4.35674	2.77083	-0.32965
C	7.50012	3.03424	0.95347
H	8.94951	1.43856	0.98624
H	5.85424	4.40324	0.77646
C	-21.45410	-3.83841	3.00156
C	-20.54971	3.60772	-3.59310
C	8.35638	4.05606	1.60805
C	6.97034	-3.43500	-4.79543
O	8.00075	5.18313	1.85749
O	9.57722	3.60159	1.89827
O	6.43617	-4.65626	-4.72970
O	7.80968	-3.13009	-5.60877
O	-21.55411	3.11004	-4.31754
O	-20.15689	4.74379	-3.71145
O	-22.63789	-3.36737	3.39904
O	-21.08730	-4.96615	3.23097
C	-6.68424	-1.21022	-1.39173
H	-7.59811	-1.24587	-1.99840
H	-5.82621	-1.22260	-2.07594
C	-6.71854	1.31455	-1.40662
H	-7.63343	1.31847	-2.01283
H	-5.86156	1.34202	-2.09168
C	-22.16463	3.98188	-5.26208

H	-21.43410	4.32286	-6.00429
H	-22.95209	3.40197	-5.74849
H	-22.59489	4.85641	-4.76120
C	-23.47811	-4.25799	4.12426
H	-22.99084	-4.58372	5.05016
H	-24.38818	-3.69974	4.35470
H	-23.71932	-5.14087	3.52172
C	6.90007	-5.61670	-5.67179
H	7.97829	-5.77840	-5.56207
H	6.35748	-6.54036	-5.45867
H	6.69427	-5.28613	-6.69608
C	10.47181	4.51014	2.53026
H	10.06800	4.84663	3.49178
H	11.40437	3.96292	2.68470
H	10.64860	5.38534	1.89502
H	-6.64534	-2.11678	-0.77566
H	-6.70375	2.22900	-0.80126

Table S7. Atomic coordinates of $\mathbf{1}^{Me+}$ from its DFT geometry-optimized structure.

Atom	**x**	**y**	**z**
C	0.36125	-0.03376	0.04424
C	0.77363	0.00954	-1.31293
C	-0.19875	0.00798	-2.34688
C	-1.53488	-0.03550	-2.01529
C	-1.93260	-0.08093	-0.65747
C	-0.98082	-0.07957	0.37251
H	1.11795	-0.03116	0.82507
H	0.13027	0.04227	-3.38322
H	-1.28683	-0.11329	1.41581

C	-2.74872	-0.04294	-2.93908
C	-3.88354	-0.10021	-1.92163
C	-5.24706	-0.12890	-2.15274
C	-6.13576	-0.18220	-1.05723
C	-5.62183	-0.20630	0.25984
C	-4.25575	-0.17649	0.49119
C	-3.38390	-0.12256	-0.60282
H	-5.64993	-0.11110	-3.16318
H	-6.31585	-0.24793	1.09593
H	-3.87536	-0.19491	1.51058
C	2.14286	0.05408	-1.62943
C	3.33583	0.09284	-1.90407
C	4.69694	0.13761	-2.21696
C	5.68152	0.15292	-1.19019
C	5.13400	0.16945	-3.57044
C	7.01708	0.20453	-1.49411
H	5.36491	0.10640	-0.15134
C	6.46869	0.20728	-3.88043
H	4.39365	0.18047	-4.36628
C	7.45054	0.22988	-2.84987
H	7.75107	0.18934	-0.69467
H	6.77789	0.25724	-4.91967
N	8.78670	0.27498	-3.15669

C	9.27671	-0.20677	-4.40727
C	10.14703	0.58790	-5.16240
C	8.91182	-1.48052	-4.85842
C	10.63567	0.11048	-6.36952
H	10.42639	1.57685	-4.80834
C	9.40557	-1.95085	-6.06846
H	8.25820	-2.10519	-4.25465
C	10.26919	-1.15835	-6.83189
H	11.30382	0.71912	-6.97319
H	9.13078	-2.94176	-6.41772
C	9.74088	0.80365	-2.23678
C	10.90148	0.07671	-1.94969
C	9.52791	2.05643	-1.64874
C	11.83787	0.59535	-1.06555
H	11.06071	-0.89560	-2.40861
C	10.46875	2.56731	-0.76598
H	8.63878	2.63101	-1.89630
C	11.62675	1.84258	-0.46665
H	12.73448	0.02916	-0.83131
H	10.32183	3.54130	-0.30654
C	12.60496	2.44144	0.49010
C	10.82877	-1.62138	-8.13701
O	12.45147	3.51267	1.02132

O	13.66387	1.66465	0.69399
O	10.41134	-2.83824	-8.47106
O	11.57810	-0.96401	-8.81490
C	-2.75062	-1.28263	-3.85295
H	-3.66284	-1.30878	-4.46193
H	-1.89192	-1.26013	-4.53570
C	-2.81768	1.24295	-3.78402
H	-3.73264	1.25510	-4.38936
H	-1.96166	1.30194	-4.46792
C	10.89223	-3.37553	-9.70118
H	11.98495	-3.45111	-9.68652
H	10.44568	-4.36744	-9.79472
H	10.58927	-2.74217	-10.54203
C	14.65886	2.14513	1.59528
H	14.23242	2.29823	2.59262
H	15.43434	1.37734	1.62921
H	15.07749	3.09176	1.23669
H	-2.70131	-2.20845	-3.26732
H	-2.81372	2.13679	-3.14871
C	-7.54303	-0.21023	-1.27586
C	-8.74368	-0.23218	-1.46222
C	-10.15221	-0.25631	-1.68046
C	-10.68272	-0.18421	-2.98239

C	-11.04884	-0.35176	-0.59946
C	-12.05239	-0.21216	-3.19428
H	-10.00766	-0.11952	-3.83280
C	-12.41868	-0.36756	-0.81157
H	-10.66057	-0.39928	0.41546
C	-12.94088	-0.30091	-2.11207
H	-12.44187	-0.16951	-4.20841
H	-13.09481	-0.42719	0.03770
N	-14.33887	-0.32283	-2.32843
C	-15.14778	-1.22951	-1.60713
C	-16.39607	-0.82987	-1.10517
C	-14.71300	-2.54466	-1.37820
C	-17.19067	-1.72363	-0.40106
H	-16.73998	0.18886	-1.26469
C	-15.50621	-3.42968	-0.66385
H	-13.75277	-2.87112	-1.76928
C	-16.75446	-3.03389	-0.16934
H	-18.15286	-1.40053	-0.01351
H	-15.17166	-4.44988	-0.49184
C	-14.91971	0.56190	-3.26449
C	-15.94747	0.12723	-4.11585
C	-14.47470	1.89007	-3.36007
C	-16.51932	0.99932	-5.03146

H	-16.29376	-0.90165	-4.06110
C	-15.04183	2.75348	-4.28508
H	-13.68632	2.24352	-2.70047
C	-16.07177	2.32252	-5.12944
H	-17.31083	0.64924	-5.68822
H	-14.70071	3.78363	-4.35470
C	-17.56693	-4.02531	0.58254
C	-16.64897	3.29144	-6.09699
O	-17.63064	2.76697	-6.83254
O	-16.27957	4.43513	-6.21560
O	-18.73803	-3.53332	0.99019
O	-17.21760	-5.15927	0.80756
C	-18.24752	3.61927	-7.79113
H	-17.51458	3.97096	-8.52589
H	-19.01567	3.01910	-8.28369
H	-18.70298	4.48743	-7.30168
C	-19.58879	-4.40931	1.72148
H	-19.09937	-4.74593	2.64228
H	-20.48588	-3.83417	1.96091
H	-19.85196	-5.28607	1.11927

Table S8. Atomic coordinates of $\mathbf{1}^{Me2+}$ (closed-shell singlet) from its DFT geometry-optimized structure.

Atom	x	y	z
C	-3.58344	0.13832	2.31610
C	-3.16579	0.11762	0.94432
C	-4.13962	0.05867	-0.09852
C	-5.46739	0.02357	0.23037
C	-5.87104	0.04210	1.60162
C	-4.91249	0.10043	2.64339
H	-2.82285	0.18403	3.09109
H	-3.80269	0.04343	-1.13208
H	-5.22427	0.11548	3.68489
C	-6.68068	-0.03767	-0.68871
C	-7.80909	-0.04773	0.33467
C	-9.16070	-0.08785	0.12491
C	-10.03968	-0.08724	1.25028
C	-9.50378	-0.04950	2.57992
C	-8.15102	-0.00729	2.78796
C	-7.28722	-0.00352	1.66481
H	-9.58686	-0.11866	-0.87487
H	-10.19396	-0.05239	3.41944
H	-7.74932	0.02346	3.79789
C	-1.81269	0.15555	0.63832
C	-0.61246	0.18993	0.37133

C	-11.41479	-0.11799	1.06468
C	-12.63390	-0.13726	0.90289
C	-14.01064	-0.15207	0.72145
C	-14.57636	-0.17166	-0.58559
C	-14.89470	-0.14284	1.83825
C	-15.93410	-0.17037	-0.76572
H	-13.91604	-0.20293	-1.44862
C	-16.25297	-0.15508	1.66235
H	-14.47925	-0.10793	2.84226
C	-16.81542	-0.16286	0.35354
H	-16.34221	-0.20678	-1.77056
H	-16.90629	-0.12412	2.52826
C	0.74236	0.22989	0.07012
C	1.71998	0.28690	1.10467
C	1.19198	0.21612	-1.28149
C	3.05645	0.33450	0.80951
H	1.39519	0.27566	2.14211
C	2.52806	0.25125	-1.58047
H	0.45849	0.19447	-2.08365
C	3.50299	0.31539	-0.54340
H	3.78310	0.35448	1.61519
H	2.84530	0.26339	-2.61817
N	-18.17306	-0.16189	0.17493

N	4.83866	0.35741	-0.84002
C	-19.05771	-0.63183	1.19240
C	-20.14056	0.15986	1.58919
C	-18.86059	-1.89376	1.76577
C	-21.01474	-0.30393	2.56346
H	-20.28952	1.13905	1.14131
C	-19.73615	-2.34904	2.74133
H	-18.03360	-2.51819	1.43641
C	-20.81714	-1.56011	3.14781
H	-21.85116	0.31250	2.87954
H	-19.59949	-3.32914	3.19097
C	-18.76358	0.31067	-1.03595
C	-19.71440	-0.47476	-1.69622
C	-18.41677	1.56942	-1.54156
C	-20.30495	-0.00844	-2.86341
H	-19.98124	-1.45108	-1.29964
C	-19.00839	2.02725	-2.71021
H	-17.69790	2.18954	-1.01156
C	-19.95411	1.24403	-3.37986
H	-21.03666	-0.62012	-3.38293
H	-18.75333	3.00488	-3.11108
C	5.34092	-0.12913	-2.08506
C	6.19396	0.67471	-2.84940

C	5.00903	-1.41691	-2.52104
C	6.69859	0.19309	-4.04863
H	6.45001	1.67412	-2.50700
C	5.51597	-1.89137	-3.72407
H	4.36770	-2.04871	-1.91127
C	6.36329	-1.08944	-4.49613
H	7.35491	0.80923	-4.65774
H	5.26511	-2.89291	-4.06102
C	5.79038	0.88764	0.08323
C	6.93264	0.14597	0.40251
C	5.59673	2.15730	0.64049
C	7.86918	0.66613	1.28613
H	7.07917	-0.83879	-0.03377
C	6.53545	2.66937	1.52491
H	4.72176	2.74320	0.36960
C	7.67557	1.92978	1.85545
H	8.75200	0.08819	1.54324
H	6.40165	3.65596	1.96102
C	-21.72919	-2.10174	4.19838
C	-20.56041	1.78740	-4.63123
C	8.65261	2.53034	2.81132
C	6.93645	-1.55573	-5.79342
O	8.51299	3.61497	3.31918

O	9.69512	1.73909	3.04447
O	6.54775	-2.78629	-6.11367
O	7.67228	-0.89053	-6.47873
O	-21.45145	0.96137	-5.17064
O	-20.27425	2.85917	-5.10386
O	-22.72474	-1.27110	4.49184
O	-21.58100	-3.17608	4.72541
C	-6.67761	-1.32625	-1.53358
H	-7.58967	-1.38767	-2.13935
H	-5.81948	-1.33179	-2.21647
C	-6.76045	1.20340	-1.59816
H	-7.67547	1.17510	-2.20207
H	-5.90575	1.22975	-2.28474
C	-22.08943	1.38779	-6.37222
H	-21.34972	1.55107	-7.16355
H	-22.77399	0.58534	-6.65421
H	-22.64366	2.31764	-6.20426
C	-23.65375	-1.69577	5.48642
H	-23.14432	-1.86539	6.44127
H	-24.38332	-0.88950	5.58501
H	-24.15111	-2.62172	5.17779
C	7.04420	-3.32678	-7.33597
H	8.13838	-3.37604	-7.31845

H	6.62180	-4.33022	-7.41845
H	6.72826	-2.71124	-8.18529
C	10.68762	2.22063	3.94766
H	10.25200	2.40398	4.93591
H	11.44792	1.43939	4.00852
H	11.12889	3.15099	3.57391
H	-6.62163	-2.21942	-0.90022
H	-6.76171	2.12936	-1.01127
C	-3.58344	0.13832	2.31610
C	-3.16579	0.11762	0.94432
C	-4.13962	0.05867	-0.09852
C	-5.46739	0.02357	0.23037
C	-5.87104	0.04210	1.60162
C	-4.91249	0.10043	2.64339
H	-2.82285	0.18403	3.09109
H	-3.80269	0.04343	-1.13208
H	-5.22427	0.11548	3.68489
C	-6.68068	-0.03767	-0.68871
C	-7.80909	-0.04773	0.33467
C	-9.16070	-0.08785	0.12491
C	-10.03968	-0.08724	1.25028
C	-9.50378	-0.04950	2.57992
C	-8.15102	-0.00729	2.78796

C	-7.28722	-0.00352	1.66481
H	-9.58686	-0.11866	-0.87487
H	-10.19396	-0.05239	3.41944
H	-7.74932	0.02346	3.79789
C	-1.81269	0.15555	0.63832
C	-0.61246	0.18993	0.37133
C	-11.41479	-0.11799	1.06468
C	-12.63390	-0.13726	0.90289
C	-14.01064	-0.15207	0.72145
C	-14.57636	-0.17166	-0.58559
C	-14.89470	-0.14284	1.83825
C	-15.93410	-0.17037	-0.76572
H	-13.91604	-0.20293	-1.44862
C	-16.25297	-0.15508	1.66235
H	-14.47925	-0.10793	2.84226
C	-16.81542	-0.16286	0.35354
H	-16.34221	-0.20678	-1.77056
H	-16.90629	-0.12412	2.52826
C	0.74236	0.22989	0.07012
C	1.71998	0.28690	1.10467
C	1.19198	0.21612	-1.28149
C	3.05645	0.33450	0.80951
H	1.39519	0.27566	2.14211

C	2.52806	0.25125	-1.58047
H	0.45849	0.19447	-2.08365
C	3.50299	0.31539	-0.54340
H	3.78310	0.35448	1.61519
H	2.84530	0.26339	-2.61817
N	-18.17306	-0.16189	0.17493
N	4.83866	0.35741	-0.84002
C	-19.05771	-0.63183	1.19240
C	-20.14056	0.15986	1.58919
C	-18.86059	-1.89376	1.76577
C	-21.01474	-0.30393	2.56346
H	-20.28952	1.13905	1.14131
C	-19.73615	-2.34904	2.74133
H	-18.03360	-2.51819	1.43641
C	-20.81714	-1.56011	3.14781
H	-21.85116	0.31250	2.87954
H	-19.59949	-3.32914	3.19097
C	-18.76358	0.31067	-1.03595
C	-19.71440	-0.47476	-1.69622
C	-18.41677	1.56942	-1.54156
C	-20.30495	-0.00844	-2.86341
H	-19.98124	-1.45108	-1.29964
C	-19.00839	2.02725	-2.71021

H	-17.69790	2.18954	-1.01156
C	-19.95411	1.24403	-3.37986
H	-21.03666	-0.62012	-3.38293
H	-18.75333	3.00488	-3.11108
C	5.34092	-0.12913	-2.08506
C	6.19396	0.67471	-2.84940
C	5.00903	-1.41691	-2.52104
C	6.69859	0.19309	-4.04863
H	6.45001	1.67412	-2.50700
C	5.51597	-1.89137	-3.72407
H	4.36770	-2.04871	-1.91127
C	6.36329	-1.08944	-4.49613
H	7.35491	0.80923	-4.65774
H	5.26511	-2.89291	-4.06102
C	5.79038	0.88764	0.08323
C	6.93264	0.14597	0.40251
C	5.59673	2.15730	0.64049
C	7.86918	0.66613	1.28613
H	7.07917	-0.83879	-0.03377
C	6.53545	2.66937	1.52491
H	4.72176	2.74320	0.36960
C	7.67557	1.92978	1.85545
H	8.75200	0.08819	1.54324

H	6.40165	3.65596	1.96102
C	-21.72919	-2.10174	4.19838
C	-20.56041	1.78740	-4.63123
C	8.65261	2.53034	2.81132
C	6.93645	-1.55573	-5.79342
O	8.51299	3.61497	3.31918
O	9.69512	1.73909	3.04447
O	6.54775	-2.78629	-6.11367
O	7.67228	-0.89053	-6.47873
O	-21.45145	0.96137	-5.17064
O	-20.27425	2.85917	-5.10386
O	-22.72474	-1.27110	4.49184
O	-21.58100	-3.17608	4.72541
C	-6.67761	-1.32625	-1.53358
H	-7.58967	-1.38767	-2.13935
H	-5.81948	-1.33179	-2.21647
C	-6.76045	1.20340	-1.59816
H	-7.67547	1.17510	-2.20207
H	-5.90575	1.22975	-2.28474
C	-22.08943	1.38779	-6.37222
H	-21.34972	1.55107	-7.16355
H	-22.77399	0.58534	-6.65421
H	-22.64366	2.31764	-6.20426

C	-23.65375	-1.69577	5.48642
H	-23.14432	-1.86539	6.44127
H	-24.38332	-0.88950	5.58501
H	-24.15111	-2.62172	5.17779
C	7.04420	-3.32678	-7.33597
H	8.13838	-3.37604	-7.31845
H	6.62180	-4.33022	-7.41845
H	6.72826	-2.71124	-8.18529
C	10.68762	2.22063	3.94766
H	10.25200	2.40398	4.93591
H	11.44792	1.43939	4.00852
H	11.12889	3.15099	3.57391
H	-6.62163	-2.21942	-0.90022
H	-6.76171	2.12936	-1.01127

Table S9. Atomic coordinates of $\mathbf{1}^{Me2+}$ (open-shell singlet) from its DFT geometry-optimized structure.

Atom	x	y	z
C	-3.58344	0.13832	2.31610
C	-3.16579	0.11762	0.94432
C	-4.13962	0.05867	-0.09852
C	-5.46739	0.02357	0.23037
C	-5.87104	0.04210	1.60162
C	-4.91249	0.10043	2.64339
H	-2.82285	0.18403	3.09109
H	-3.80269	0.04343	-1.13208
H	-5.22427	0.11548	3.68489
C	-6.68068	-0.03767	-0.68871
C	-7.80909	-0.04773	0.33467
C	-9.16070	-0.08785	0.12491
C	-10.03968	-0.08724	1.25028
C	-9.50378	-0.04950	2.57992
C	-8.15102	-0.00729	2.78796
C	-7.28722	-0.00352	1.66481
H	-9.58686	-0.11866	-0.87487
H	-10.19396	-0.05239	3.41944
H	-7.74932	0.02346	3.79789
C	-1.81269	0.15555	0.63832
C	-0.61246	0.18993	0.37133

C	-11.41479	-0.11799	1.06468
C	-12.63390	-0.13726	0.90289
C	-14.01064	-0.15207	0.72145
C	-14.57636	-0.17166	-0.58559
C	-14.89470	-0.14284	1.83825
C	-15.93410	-0.17037	-0.76572
H	-13.91604	-0.20293	-1.44862
C	-16.25297	-0.15508	1.66235
H	-14.47925	-0.10793	2.84226
C	-16.81542	-0.16286	0.35354
H	-16.34221	-0.20678	-1.77056
H	-16.90629	-0.12412	2.52826
C	0.74236	0.22989	0.07012
C	1.71998	0.28690	1.10467
C	1.19198	0.21612	-1.28149
C	3.05645	0.33450	0.80951
H	1.39519	0.27566	2.14211
C	2.52806	0.25125	-1.58047
H	0.45849	0.19447	-2.08365
C	3.50299	0.31539	-0.54340
H	3.78310	0.35448	1.61519
H	2.84530	0.26339	-2.61817
N	-18.17306	-0.16189	0.17493

N	4.83866	0.35741	-0.84002
C	-19.05771	-0.63183	1.19240
C	-20.14056	0.15986	1.58919
C	-18.86059	-1.89376	1.76577
C	-21.01474	-0.30393	2.56346
H	-20.28952	1.13905	1.14131
C	-19.73615	-2.34904	2.74133
H	-18.03360	-2.51819	1.43641
C	-20.81714	-1.56011	3.14781
H	-21.85116	0.31250	2.87954
H	-19.59949	-3.32914	3.19097
C	-18.76358	0.31067	-1.03595
C	-19.71440	-0.47476	-1.69622
C	-18.41677	1.56942	-1.54156
C	-20.30495	-0.00844	-2.86341
H	-19.98124	-1.45108	-1.29964
C	-19.00839	2.02725	-2.71021
H	-17.69790	2.18954	-1.01156
C	-19.95411	1.24403	-3.37986
H	-21.03666	-0.62012	-3.38293
H	-18.75333	3.00488	-3.11108
C	5.34092	-0.12913	-2.08506
C	6.19396	0.67471	-2.84940

C	5.00903	-1.41691	-2.52104
C	6.69859	0.19309	-4.04863
H	6.45001	1.67412	-2.50700
C	5.51597	-1.89137	-3.72407
H	4.36770	-2.04871	-1.91127
C	6.36329	-1.08944	-4.49613
H	7.35491	0.80923	-4.65774
H	5.26511	-2.89291	-4.06102
C	5.79038	0.88764	0.08323
C	6.93264	0.14597	0.40251
C	5.59673	2.15730	0.64049
C	7.86918	0.66613	1.28613
H	7.07917	-0.83879	-0.03377
C	6.53545	2.66937	1.52491
H	4.72176	2.74320	0.36960
C	7.67557	1.92978	1.85545
H	8.75200	0.08819	1.54324
H	6.40165	3.65596	1.96102
C	-21.72919	-2.10174	4.19838
C	-20.56041	1.78740	-4.63123
C	8.65261	2.53034	2.81132
C	6.93645	-1.55573	-5.79342
O	8.51299	3.61497	3.31918

O	9.69512	1.73909	3.04447
O	6.54775	-2.78629	-6.11367
O	7.67228	-0.89053	-6.47873
O	-21.45145	0.96137	-5.17064
O	-20.27425	2.85917	-5.10386
O	-22.72474	-1.27110	4.49184
O	-21.58100	-3.17608	4.72541
C	-6.67761	-1.32625	-1.53358
H	-7.58967	-1.38767	-2.13935
H	-5.81948	-1.33179	-2.21647
C	-6.76045	1.20340	-1.59816
H	-7.67547	1.17510	-2.20207
H	-5.90575	1.22975	-2.28474
C	-22.08943	1.38779	-6.37222
H	-21.34972	1.55107	-7.16355
H	-22.77399	0.58534	-6.65421
H	-22.64366	2.31764	-6.20426
C	-23.65375	-1.69577	5.48642
H	-23.14432	-1.86539	6.44127
H	-24.38332	-0.88950	5.58501
H	-24.15111	-2.62172	5.17779
C	7.04420	-3.32678	-7.33597
H	8.13838	-3.37604	-7.31845

H	6.62180	-4.33022	-7.41845
H	6.72826	-2.71124	-8.18529
C	10.68762	2.22063	3.94766
H	10.25200	2.40398	4.93591
H	11.44792	1.43939	4.00852
H	11.12889	3.15099	3.57391
H	-6.62163	-2.21942	-0.90022
H	-6.76171	2.12936	-1.01127
C	-3.58344	0.13832	2.31610
C	-3.16579	0.11762	0.94432
C	-4.13962	0.05867	-0.09852
C	-5.46739	0.02357	0.23037
C	-5.87104	0.04210	1.60162
C	-4.91249	0.10043	2.64339
H	-2.82285	0.18403	3.09109
H	-3.80269	0.04343	-1.13208
H	-5.22427	0.11548	3.68489
C	-6.68068	-0.03767	-0.68871
C	-7.80909	-0.04773	0.33467
C	-9.16070	-0.08785	0.12491
C	-10.03968	-0.08724	1.25028
C	-9.50378	-0.04950	2.57992
C	-8.15102	-0.00729	2.78796

C	-7.28722	-0.00352	1.66481
H	-9.58686	-0.11866	-0.87487
H	-10.19396	-0.05239	3.41944
H	-7.74932	0.02346	3.79789
C	-1.81269	0.15555	0.63832
C	-0.61246	0.18993	0.37133
C	-11.41479	-0.11799	1.06468
C	-12.63390	-0.13726	0.90289
C	-14.01064	-0.15207	0.72145
C	-14.57636	-0.17166	-0.58559
C	-14.89470	-0.14284	1.83825
C	-15.93410	-0.17037	-0.76572
H	-13.91604	-0.20293	-1.44862
C	-16.25297	-0.15508	1.66235
H	-14.47925	-0.10793	2.84226
C	-16.81542	-0.16286	0.35354
H	-16.34221	-0.20678	-1.77056
H	-16.90629	-0.12412	2.52826
C	0.74236	0.22989	0.07012
C	1.71998	0.28690	1.10467
C	1.19198	0.21612	-1.28149
C	3.05645	0.33450	0.80951
H	1.39519	0.27566	2.14211

C	2.52806	0.25125	-1.58047
H	0.45849	0.19447	-2.08365
C	3.50299	0.31539	-0.54340
H	3.78310	0.35448	1.61519
H	2.84530	0.26339	-2.61817
N	-18.17306	-0.16189	0.17493
N	4.83866	0.35741	-0.84002
C	-19.05771	-0.63183	1.19240
C	-20.14056	0.15986	1.58919
C	-18.86059	-1.89376	1.76577
C	-21.01474	-0.30393	2.56346
H	-20.28952	1.13905	1.14131
C	-19.73615	-2.34904	2.74133
H	-18.03360	-2.51819	1.43641
C	-20.81714	-1.56011	3.14781
H	-21.85116	0.31250	2.87954
H	-19.59949	-3.32914	3.19097
C	-18.76358	0.31067	-1.03595
C	-19.71440	-0.47476	-1.69622
C	-18.41677	1.56942	-1.54156
C	-20.30495	-0.00844	-2.86341
H	-19.98124	-1.45108	-1.29964
C	-19.00839	2.02725	-2.71021

H	-17.69790	2.18954	-1.01156
C	-19.95411	1.24403	-3.37986
H	-21.03666	-0.62012	-3.38293
H	-18.75333	3.00488	-3.11108
C	5.34092	-0.12913	-2.08506
C	6.19396	0.67471	-2.84940
C	5.00903	-1.41691	-2.52104
C	6.69859	0.19309	-4.04863
H	6.45001	1.67412	-2.50700
C	5.51597	-1.89137	-3.72407
H	4.36770	-2.04871	-1.91127
C	6.36329	-1.08944	-4.49613
H	7.35491	0.80923	-4.65774
H	5.26511	-2.89291	-4.06102
C	5.79038	0.88764	0.08323
C	6.93264	0.14597	0.40251
C	5.59673	2.15730	0.64049
C	7.86918	0.66613	1.28613
H	7.07917	-0.83879	-0.03377
C	6.53545	2.66937	1.52491
H	4.72176	2.74320	0.36960
C	7.67557	1.92978	1.85545
H	8.75200	0.08819	1.54324

H	6.40165	3.65596	1.96102
C	-21.72919	-2.10174	4.19838
C	-20.56041	1.78740	-4.63123
C	8.65261	2.53034	2.81132
C	6.93645	-1.55573	-5.79342
O	8.51299	3.61497	3.31918
O	9.69512	1.73909	3.04447
O	6.54775	-2.78629	-6.11367
O	7.67228	-0.89053	-6.47873
O	-21.45145	0.96137	-5.17064
O	-20.27425	2.85917	-5.10386
O	-22.72474	-1.27110	4.49184
O	-21.58100	-3.17608	4.72541
C	-6.67761	-1.32625	-1.53358
H	-7.58967	-1.38767	-2.13935
H	-5.81948	-1.33179	-2.21647
C	-6.76045	1.20340	-1.59816
H	-7.67547	1.17510	-2.20207
H	-5.90575	1.22975	-2.28474
C	-22.08943	1.38779	-6.37222
H	-21.34972	1.55107	-7.16355
H	-22.77399	0.58534	-6.65421
H	-22.64366	2.31764	-6.20426

C	-23.65375	-1.69577	5.48642
H	-23.14432	-1.86539	6.44127
H	-24.38332	-0.88950	5.58501
H	-24.15111	-2.62172	5.17779
C	7.04420	-3.32678	-7.33597
H	8.13838	-3.37604	-7.31845
H	6.62180	-4.33022	-7.41845
H	6.72826	-2.71124	-8.18529
C	10.68762	2.22063	3.94766
H	10.25200	2.40398	4.93591
H	11.44792	1.43939	4.00852
H	11.12889	3.15099	3.57391
H	-6.62163	-2.21942	-0.90022
H	-6.76171	2.12936	-1.01127

Table S10. Atomic coordinates of $\mathbf{1}^{Me2+}$ (triplet) from its DFT geometry-optimized structure.

Atom	x	y	z
C	-3.54489	0.12345	2.40937
C	-3.14339	0.11350	1.05304
C	-4.11650	0.07684	0.02759
C	-5.45540	0.05240	0.36851
C	-5.84248	0.06208	1.72503
C	-4.88844	0.09745	2.74762
H	-2.78470	0.15196	3.18620
H	-3.79426	0.06917	-1.01137
H	-5.18748	0.10535	3.79351
C	-6.67164	0.01397	-0.55102
C	-7.80343	0.00397	0.47140
C	-9.16688	-0.02530	0.24871
C	-10.04733	-0.02820	1.35533
C	-9.52961	-0.00240	2.67149
C	-8.16173	0.02752	2.89113
C	-7.30007	0.03138	1.78895
H	-9.57814	-0.04546	-0.75819
H	-10.21960	-0.00553	3.51176
H	-7.77298	0.04783	3.90699
C	-1.76641	0.14235	0.72376
C	-0.57922	0.16948	0.44089

C	-11.44780	-0.05483	1.14725
C	-12.65518	-0.07554	0.96839
C	-14.04441	-0.09662	0.76332
C	-14.58410	-0.12299	-0.55053
C	-14.94071	-0.09057	1.86555
C	-15.94081	-0.13400	-0.75439
H	-13.90911	-0.15208	-1.40182
C	-16.29845	-0.11547	1.66965
H	-14.54055	-0.04734	2.87507
C	-16.83472	-0.13354	0.35220
H	-16.33421	-0.18525	-1.76483
H	-16.96747	-0.07848	2.52374
C	0.78645	0.20470	0.11514
C	1.77528	0.24690	1.13432
C	1.20930	0.20107	-1.24112
C	3.10985	0.29276	0.81925
H	1.46624	0.22521	2.17608
C	2.54250	0.23289	-1.56364
H	0.46227	0.19167	-2.03049
C	3.52914	0.28465	-0.54011
H	3.85120	0.29308	1.61224
H	2.84460	0.26213	-2.60593
N	-18.19420	-0.14962	0.15114

N	4.86508	0.32629	-0.85944
C	-19.07508	-0.70259	1.12321
C	-20.22875	0.00150	1.49123
C	-18.79761	-1.95584	1.68606
C	-21.09246	-0.54118	2.43174
H	-20.43466	0.97534	1.05504
C	-19.66934	-2.49075	2.62274
H	-17.91882	-2.51342	1.37242
C	-20.81792	-1.78926	3.00344
H	-21.98110	0.00615	2.73154
H	-19.47610	-3.46584	3.06199
C	-18.76730	0.38729	-1.03653
C	-19.74448	-0.34297	-1.72477
C	-18.37006	1.65079	-1.49478
C	-20.30946	0.18455	-2.87704
H	-20.04379	-1.32456	-1.36702
C	-18.94370	2.17043	-2.64559
H	-17.63576	2.22767	-0.93848
C	-19.91244	1.44301	-3.34458
H	-21.05736	-0.38258	-3.42304
H	-18.65572	3.15308	-3.00975
C	5.34661	-0.22865	-2.07927
C	6.23758	0.50827	-2.87060

C	4.94858	-1.51471	-2.46688
C	6.71184	-0.03929	-4.05245
H	6.53827	1.50757	-2.56725
C	5.43281	-2.05548	-3.65028
H	4.28338	-2.09448	-1.83213
C	6.31428	-1.32089	-4.45056
H	7.39253	0.52279	-4.68635
H	5.13668	-3.05620	-3.95026
C	5.81276	0.92662	0.01703
C	7.01250	0.26088	0.29908
C	5.55286	2.18779	0.57059
C	7.94104	0.85001	1.14515
H	7.20491	-0.71932	-0.12884
C	6.48905	2.76907	1.41261
H	4.63555	2.71528	0.32199
C	7.68502	2.10638	1.70719
H	8.86690	0.33288	1.37857
H	6.30938	3.75082	1.84267
C	-21.72054	-2.41504	4.01798
C	-20.49576	2.05282	-4.57886
C	8.65711	2.78205	2.62048
C	6.86191	-1.86128	-5.73260
O	8.46096	3.85974	3.12278

O	9.75755	2.06554	2.81623
O	6.41575	-3.08201	-6.00462
O	7.62462	-1.25353	-6.44036
O	-21.40826	1.27600	-5.15033
O	-20.17119	3.13170	-5.00654
O	-22.78012	-1.66352	4.29217
O	-21.50719	-3.48490	4.52993
C	-6.68237	-1.26240	-1.41318
H	-7.59504	-1.30888	-2.02027
H	-5.82427	-1.27161	-2.09681
C	-6.73752	1.26467	-1.44766
H	-7.65197	1.25522	-2.05385
H	-5.88136	1.29243	-2.13317
C	-22.02856	1.76529	-6.33817
H	-21.28003	1.93642	-7.11929
H	-22.73411	0.99363	-6.65205
H	-22.55661	2.70351	-6.13641
C	-23.70674	-2.16986	5.25146
H	-23.21541	-2.31539	6.21955
H	-24.49592	-1.42031	5.33609
H	-24.12403	-3.12491	4.91457
C	6.88076	-3.69212	-7.20737
H	7.97115	-3.79448	-7.18880

H	6.40881	-4.67558	-7.25093
H	6.59214	-3.09317	-8.07784
C	10.75284	2.62202	3.67358
H	10.34744	2.78235	4.67844
H	11.56696	1.89538	3.70505
H	11.11122	3.57743	3.27541
H	-6.63640	-2.16378	-0.79034
H	-6.73006	2.18379	-0.84964
C	-3.54489	0.12345	2.40937
C	-3.14339	0.11350	1.05304
C	-4.11650	0.07684	0.02759
C	-5.45540	0.05240	0.36851
C	-5.84248	0.06208	1.72503
C	-4.88844	0.09745	2.74762
H	-2.78470	0.15196	3.18620
H	-3.79426	0.06917	-1.01137
H	-5.18748	0.10535	3.79351
C	-6.67164	0.01397	-0.55102
C	-7.80343	0.00397	0.47140
C	-9.16688	-0.02530	0.24871
C	-10.04733	-0.02820	1.35533
C	-9.52961	-0.00240	2.67149
C	-8.16173	0.02752	2.89113

C	-7.30007	0.03138	1.78895
H	-9.57814	-0.04546	-0.75819
H	-10.21960	-0.00553	3.51176
H	-7.77298	0.04783	3.90699
C	-1.76641	0.14235	0.72376
C	-0.57922	0.16948	0.44089
C	-11.44780	-0.05483	1.14725
C	-12.65518	-0.07554	0.96839
C	-14.04441	-0.09662	0.76332
C	-14.58410	-0.12299	-0.55053
C	-14.94071	-0.09057	1.86555
C	-15.94081	-0.13400	-0.75439
H	-13.90911	-0.15208	-1.40182
C	-16.29845	-0.11547	1.66965
H	-14.54055	-0.04734	2.87507
C	-16.83472	-0.13354	0.35220
H	-16.33421	-0.18525	-1.76483
H	-16.96747	-0.07848	2.52374
C	0.78645	0.20470	0.11514
C	1.77528	0.24690	1.13432
C	1.20930	0.20107	-1.24112
C	3.10985	0.29276	0.81925
H	1.46624	0.22521	2.17608

C	2.54250	0.23289	-1.56364
H	0.46227	0.19167	-2.03049
C	3.52914	0.28465	-0.54011
H	3.85120	0.29308	1.61224
H	2.84460	0.26213	-2.60593
N	-18.19420	-0.14962	0.15114
N	4.86508	0.32629	-0.85944
C	-19.07508	-0.70259	1.12321
C	-20.22875	0.00150	1.49123
C	-18.79761	-1.95584	1.68606
C	-21.09246	-0.54118	2.43174
H	-20.43466	0.97534	1.05504
C	-19.66934	-2.49075	2.62274
H	-17.91882	-2.51342	1.37242
C	-20.81792	-1.78926	3.00344
H	-21.98110	0.00615	2.73154
H	-19.47610	-3.46584	3.06199
C	-18.76730	0.38729	-1.03653
C	-19.74448	-0.34297	-1.72477
C	-18.37006	1.65079	-1.49478
C	-20.30946	0.18455	-2.87704
H	-20.04379	-1.32456	-1.36702
C	-18.94370	2.17043	-2.64559

H	-17.63576	2.22767	-0.93848
C	-19.91244	1.44301	-3.34458
H	-21.05736	-0.38258	-3.42304
H	-18.65572	3.15308	-3.00975
C	5.34661	-0.22865	-2.07927
C	6.23758	0.50827	-2.87060
C	4.94858	-1.51471	-2.46688
C	6.71184	-0.03929	-4.05245
H	6.53827	1.50757	-2.56725
C	5.43281	-2.05548	-3.65028
H	4.28338	-2.09448	-1.83213
C	6.31428	-1.32089	-4.45056
H	7.39253	0.52279	-4.68635
H	5.13668	-3.05620	-3.95026
C	5.81276	0.92662	0.01703
C	7.01250	0.26088	0.29908
C	5.55286	2.18779	0.57059
C	7.94104	0.85001	1.14515
H	7.20491	-0.71932	-0.12884
C	6.48905	2.76907	1.41261
H	4.63555	2.71528	0.32199
C	7.68502	2.10638	1.70719
H	8.86690	0.33288	1.37857

H	6.30938	3.75082	1.84267
C	-21.72054	-2.41504	4.01798
C	-20.49576	2.05282	-4.57886
C	8.65711	2.78205	2.62048
C	6.86191	-1.86128	-5.73260
O	8.46096	3.85974	3.12278
O	9.75755	2.06554	2.81623
O	6.41575	-3.08201	-6.00462
O	7.62462	-1.25353	-6.44036
O	-21.40826	1.27600	-5.15033
O	-20.17119	3.13170	-5.00654
O	-22.78012	-1.66352	4.29217
O	-21.50719	-3.48490	4.52993
C	-6.68237	-1.26240	-1.41318
H	-7.59504	-1.30888	-2.02027
H	-5.82427	-1.27161	-2.09681
C	-6.73752	1.26467	-1.44766
H	-7.65197	1.25522	-2.05385
H	-5.88136	1.29243	-2.13317
C	-22.02856	1.76529	-6.33817
H	-21.28003	1.93642	-7.11929
H	-22.73411	0.99363	-6.65205
H	-22.55661	2.70351	-6.13641

C	-23.70674	-2.16986	5.25146
H	-23.21541	-2.31539	6.21955
H	-24.49592	-1.42031	5.33609
H	-24.12403	-3.12491	4.91457
C	6.88076	-3.69212	-7.20737
H	7.97115	-3.79448	-7.18880
H	6.40881	-4.67558	-7.25093
H	6.59214	-3.09317	-8.07784
C	10.75284	2.62202	3.67358
H	10.34744	2.78235	4.67844
H	11.56696	1.89538	3.70505
H	11.11122	3.57743	3.27541
H	-6.63640	-2.16378	-0.79034
H	-6.73006	2.18379	-0.84964

Table S11. Atomic coordinates of **2**^{Me} from its DFT geometry-optimized structure.

Atom	x	y	z
C	-2.28356	-0.56735	1.29178
C	-2.65838	0.78184	1.46330
C	-1.66265	1.76214	1.66461
C	-0.33134	1.38465	1.69084
C	0.03036	0.03454	1.51814
C	-0.94645	-0.94334	1.31832
H	-3.05710	-1.31617	1.13735
H	-1.95773	2.80126	1.79628
H	-0.67374	-1.98846	1.18424
C	0.90173	2.26119	1.89251
C	2.01465	1.22023	1.80828
C	3.38214	1.40934	1.91574
C	4.24864	0.30132	1.80581
C	3.70817	-0.98328	1.58871
C	2.33570	-1.17159	1.48115
C	1.48821	-0.06721	1.59085
H	3.80292	2.39895	2.08298
H	4.38211	-1.83294	1.50514
H	1.93584	-2.16996	1.31327
C	-4.03418	1.15155	1.43342
C	-5.21170	1.46540	1.40749

C	-6.53369	1.81559	1.37772
C	-9.09036	2.48613	1.31732
C	-10.07674	1.49924	1.10255
C	-9.47750	3.83058	1.49803
C	-11.41094	1.86568	1.07190
H	-9.77219	0.46377	0.96387
C	-10.81768	4.19549	1.46714
H	-8.71124	4.58464	1.66291
C	-12.63504	0.98022	0.85579
C	-11.78516	3.21122	1.25358
H	-11.09991	5.23714	1.60833
C	-13.75724	2.01094	0.94106
C	-13.24346	3.30107	1.17258
C	-15.12216	1.81088	0.82255
C	-14.10148	4.39698	1.28572
C	-15.99918	2.91030	0.93553
H	-15.53306	0.81909	0.64407
C	-15.47157	4.19763	1.16720
H	-13.71161	5.39742	1.46450
H	-16.15344	5.04072	1.25309
C	-7.71210	2.12596	1.35052
C	5.66192	0.47791	1.91203
C	-17.40974	2.72041	0.81683

C	6.86396	0.62654	2.00077
C	-18.60877	2.55608	0.71605
C	8.27771	0.79777	2.10362
C	8.83748	2.06789	2.33491
C	9.14837	-0.30027	1.97564
C	10.21105	2.23129	2.44111
H	8.18259	2.92934	2.44535
C	10.52243	-0.13316	2.06740
H	8.73756	-1.28987	1.78835
C	11.07223	1.13395	2.30496
H	10.62390	3.21860	2.63424
H	11.17951	-0.99180	1.95143
C	-20.01829	2.36131	0.59763
C	-20.55131	1.08395	0.34398
C	-20.91080	3.44095	0.73152
C	-21.92123	0.89354	0.23611
H	-19.87990	0.23391	0.24501
C	-22.27969	3.25143	0.60941
H	-20.51976	4.43840	0.91950
C	-22.80335	1.97495	0.36379
H	-22.31524	-0.10340	0.05342
H	-22.95291	4.10038	0.70210
N	12.47731	1.30254	2.40616

N	-24.20411	1.78034	0.24578
C	13.23116	0.41050	3.19866
C	14.49009	-0.04088	2.77081
C	12.72795	-0.04961	4.42649
C	15.22672	-0.91965	3.55215
H	14.88759	0.29535	1.81667
C	13.46407	-0.93613	5.19756
H	11.75851	0.29663	4.77535
C	14.72214	-1.38087	4.77440
H	16.19682	-1.26539	3.20593
H	13.07553	-1.28680	6.15071
C	13.10576	2.35867	1.71261
C	14.15551	3.08034	2.30353
C	12.68393	2.71266	0.42054
C	14.77025	4.11879	1.61872
H	14.48461	2.82771	3.30814
C	13.29478	3.75865	-0.25406
H	11.87810	2.15890	-0.05415
C	14.34616	4.47333	0.33197
H	15.57752	4.67216	2.09054
H	12.97085	4.02734	-1.25670
C	-25.07067	2.35291	1.20088
C	-26.30096	2.90866	0.81231

C	-24.71145	2.38629	2.55784
C	-27.14531	3.47093	1.75715
H	-26.58865	2.90386	-0.23581
C	-25.55622	2.96039	3.49722
H	-23.76624	1.95352	2.87509
C	-26.78571	3.50712	3.10982
H	-28.09470	3.90558	1.45354
H	-25.26773	2.97376	4.54462
C	-24.71280	1.01404	-0.82454
C	-25.78777	0.13193	-0.62905
C	-24.14268	1.11363	-2.10428
C	-26.28266	-0.62092	-1.68435
H	-26.23132	0.03294	0.35828
C	-24.63465	0.35056	-3.15209
H	-23.31508	1.79751	-2.27382
C	-25.71093	-0.52348	-2.95905
H	-27.11122	-1.30363	-1.51739
H	-24.19576	0.43361	-4.14348
C	15.46962	-2.32691	5.64180
C	14.96795	5.58091	-0.43784
C	-26.20118	-1.31332	-4.11746
C	-27.72535	4.12721	4.07859
O	-25.72609	-1.26081	-5.22672

O	-27.23454	-2.09966	-3.80919
O	-27.26549	4.10893	5.33138
O	-28.79520	4.60202	3.78031
O	15.96730	6.17263	0.21971
O	14.61823	5.92172	-1.54259
O	16.65661	-2.66776	5.13587
O	15.06047	-2.75185	6.69580
C	0.88007	2.94964	3.26979
H	1.80180	3.52370	3.42875
H	0.03433	3.64552	3.34016
C	1.03216	3.31290	0.77544
H	1.95821	3.88955	0.89530
H	0.19118	4.01726	0.80779
C	-12.59895	0.30234	-0.52640
H	-11.74689	-0.38579	-0.59667
H	-13.51471	-0.27837	-0.69540
C	-12.76330	-0.08094	1.96418
H	-13.68342	-0.66481	1.83408
H	-11.91588	-0.77754	1.93202
C	16.62532	7.25006	-0.43703
H	15.92116	8.06178	-0.65167
H	17.40159	7.59718	0.24846
H	17.07548	6.91405	-1.37787

C	17.44646	-3.57548	5.89570
H	16.92102	-4.52756	6.03083
H	18.36583	-3.73063	5.32680
H	17.67866	-3.15653	6.88125
C	-28.09751	4.68024	6.33456
H	-29.05998	4.15872	6.38382
H	-27.55959	4.56706	7.27838
H	-28.27991	5.74110	6.12936
C	-27.77358	-2.89907	-4.85589
H	-27.01462	-3.58339	-5.25150
H	-28.59716	-3.46492	-4.41490
H	-28.14317	-2.26989	-5.67336
H	0.78886	2.21498	4.07899
H	-12.50903	1.04376	-1.32954
H	-12.78883	0.38383	2.95724
H	1.04721	2.84057	-0.21426
C	-2.28356	-0.56735	1.29178
C	-2.65838	0.78184	1.46330
C	-1.66265	1.76214	1.66461
C	-0.33134	1.38465	1.69084
C	0.03036	0.03454	1.51814
C	-0.94645	-0.94334	1.31832
H	-3.05710	-1.31617	1.13735

H	-1.95773	2.80126	1.79628
H	-0.67374	-1.98846	1.18424
C	0.90173	2.26119	1.89251
C	2.01465	1.22023	1.80828
C	3.38214	1.40934	1.91574
C	4.24864	0.30132	1.80581
C	3.70817	-0.98328	1.58871
C	2.33570	-1.17159	1.48115
C	1.48821	-0.06721	1.59085
H	3.80292	2.39895	2.08298
H	4.38211	-1.83294	1.50514
H	1.93584	-2.16996	1.31327
C	-4.03418	1.15155	1.43342
C	-5.21170	1.46540	1.40749
C	-6.53369	1.81559	1.37772
C	-9.09036	2.48613	1.31732
C	-10.07674	1.49924	1.10255
C	-9.47750	3.83058	1.49803
C	-11.41094	1.86568	1.07190
H	-9.77219	0.46377	0.96387
C	-10.81768	4.19549	1.46714
H	-8.71124	4.58464	1.66291
C	-12.63504	0.98022	0.85579

C	-11.78516	3.21122	1.25358
H	-11.09991	5.23714	1.60833
C	-13.75724	2.01094	0.94106
C	-13.24346	3.30107	1.17258
C	-15.12216	1.81088	0.82255
C	-14.10148	4.39698	1.28572
C	-15.99918	2.91030	0.93553
H	-15.53306	0.81909	0.64407
C	-15.47157	4.19763	1.16720
H	-13.71161	5.39742	1.46450
H	-16.15344	5.04072	1.25309
C	-7.71210	2.12596	1.35052
C	5.66192	0.47791	1.91203
C	-17.40974	2.72041	0.81683
C	6.86396	0.62654	2.00077
C	-18.60877	2.55608	0.71605
C	8.27771	0.79777	2.10362
C	8.83748	2.06789	2.33491
C	9.14837	-0.30027	1.97564
C	10.21105	2.23129	2.44111
H	8.18259	2.92934	2.44535
C	10.52243	-0.13316	2.06740
H	8.73756	-1.28987	1.78835

C	11.07223	1.13395	2.30496
H	10.62390	3.21860	2.63424
H	11.17951	-0.99180	1.95143
C	-20.01829	2.36131	0.59763
C	-20.55131	1.08395	0.34398
C	-20.91080	3.44095	0.73152
C	-21.92123	0.89354	0.23611
H	-19.87990	0.23391	0.24501
C	-22.27969	3.25143	0.60941
H	-20.51976	4.43840	0.91950
C	-22.80335	1.97495	0.36379
H	-22.31524	-0.10340	0.05342
H	-22.95291	4.10038	0.70210
N	12.47731	1.30254	2.40616
N	-24.20411	1.78034	0.24578
C	13.23116	0.41050	3.19866
C	14.49009	-0.04088	2.77081
C	12.72795	-0.04961	4.42649
C	15.22672	-0.91965	3.55215
H	14.88759	0.29535	1.81667
C	13.46407	-0.93613	5.19756
H	11.75851	0.29663	4.77535
C	14.72214	-1.38087	4.77440

H	16.19682	-1.26539	3.20593
H	13.07553	-1.28680	6.15071
C	13.10576	2.35867	1.71261
C	14.15551	3.08034	2.30353
C	12.68393	2.71266	0.42054
C	14.77025	4.11879	1.61872
H	14.48461	2.82771	3.30814
C	13.29478	3.75865	-0.25406
H	11.87810	2.15890	-0.05415
C	14.34616	4.47333	0.33197
H	15.57752	4.67216	2.09054
H	12.97085	4.02734	-1.25670
C	-25.07067	2.35291	1.20088
C	-26.30096	2.90866	0.81231
C	-24.71145	2.38629	2.55784
C	-27.14531	3.47093	1.75715
H	-26.58865	2.90386	-0.23581
C	-25.55622	2.96039	3.49722
H	-23.76624	1.95352	2.87509
C	-26.78571	3.50712	3.10982
H	-28.09470	3.90558	1.45354
H	-25.26773	2.97376	4.54462
C	-24.71280	1.01404	-0.82454

C	-25.78777	0.13193	-0.62905
C	-24.14268	1.11363	-2.10428
C	-26.28266	-0.62092	-1.68435
H	-26.23132	0.03294	0.35828
C	-24.63465	0.35056	-3.15209
H	-23.31508	1.79751	-2.27382
C	-25.71093	-0.52348	-2.95905
H	-27.11122	-1.30363	-1.51739
H	-24.19576	0.43361	-4.14348
C	15.46962	-2.32691	5.64180
C	14.96795	5.58091	-0.43784
C	-26.20118	-1.31332	-4.11746
C	-27.72535	4.12721	4.07859
O	-25.72609	-1.26081	-5.22672
O	-27.23454	-2.09966	-3.80919
O	-27.26549	4.10893	5.33138
O	-28.79520	4.60202	3.78031
O	15.96730	6.17263	0.21971
O	14.61823	5.92172	-1.54259
O	16.65661	-2.66776	5.13587
O	15.06047	-2.75185	6.69580
C	0.88007	2.94964	3.26979
H	1.80180	3.52370	3.42875

H	0.03433	3.64552	3.34016
C	1.03216	3.31290	0.77544
H	1.95821	3.88955	0.89530
H	0.19118	4.01726	0.80779
C	-12.59895	0.30234	-0.52640
H	-11.74689	-0.38579	-0.59667
H	-13.51471	-0.27837	-0.69540
C	-12.76330	-0.08094	1.96418
H	-13.68342	-0.66481	1.83408
H	-11.91588	-0.77754	1.93202
C	16.62532	7.25006	-0.43703
H	15.92116	8.06178	-0.65167
H	17.40159	7.59718	0.24846
H	17.07548	6.91405	-1.37787
C	17.44646	-3.57548	5.89570
H	16.92102	-4.52756	6.03083
H	18.36583	-3.73063	5.32680
H	17.67866	-3.15653	6.88125
C	-28.09751	4.68024	6.33456
H	-29.05998	4.15872	6.38382
H	-27.55959	4.56706	7.27838
H	-28.27991	5.74110	6.12936
C	-27.77358	-2.89907	-4.85589

H	-27.01462	-3.58339	-5.25150
H	-28.59716	-3.46492	-4.41490
H	-28.14317	-2.26989	-5.67336
H	0.78886	2.21498	4.07899
H	-12.50903	1.04376	-1.32954
H	-12.78883	0.38383	2.95724
H	1.04721	2.84057	-0.21426

Table S12. Atomic coordinates of **2**$^{Me+}$ from its DFT geometry-optimized structure.

Atom	**x**	**y**	**z**
C	8.51725	15.94718	0.17346
C	5.95748	16.60217	0.10907
C	4.97787	15.60921	-0.11066
C	5.56259	17.94393	0.29435
C	3.64183	15.96747	-0.14120
H	5.28928	14.57625	-0.25265
C	4.22047	18.30043	0.26343
H	6.32418	18.70185	0.46291
C	2.42313	15.07570	-0.36117
C	3.25951	17.31046	0.04533
H	3.93130	19.33960	0.40831
C	1.29510	16.09959	-0.27218
C	1.80107	17.39189	-0.03583

C	-0.06866	15.89188	-0.39124
C	0.93678	18.48255	0.08148
C	-0.95193	16.98571	-0.27374
H	-0.47386	14.89844	-0.57330
C	-0.43194	18.27550	-0.03743
H	1.32076	19.48459	0.26387
H	-1.11887	19.11409	0.05179
C	7.33678	16.25062	0.14373
C	-2.36130	16.78788	-0.39215
C	-3.55941	16.61661	-0.49229
C	-4.96775	16.41340	-0.60979
C	-5.49239	15.13504	-0.87557
C	-5.86740	17.48537	-0.46272
C	-6.86111	14.93621	-0.98259
H	-4.81533	14.29074	-0.98473
C	-7.23516	17.28758	-0.58375
H	-5.48293	18.48355	-0.26524
C	-7.75060	16.01006	-0.84171
H	-7.24847	13.93847	-1.17481
H	-7.91397	18.13085	-0.48074
N	-9.14987	15.80702	-0.95878
C	-10.01910	16.36841	0.00082
C	-11.25197	16.92109	-0.38364

C	-9.66006	16.39284	1.35795
C	-12.09909	17.47196	0.56547
H	-11.53957	16.92281	-1.43181
C	-10.50758	16.95566	2.30171
H	-8.71285	15.96197	1.67187
C	-11.73961	17.49947	1.91835
H	-13.05060	17.90428	0.26521
H	-10.21930	16.96229	3.34923
C	-9.65572	15.04375	-2.03279
C	-10.72400	14.15304	-1.84013
C	-9.08970	15.15568	-3.31329
C	-11.21641	13.40352	-2.89899
H	-11.16434	14.04482	-0.85233
C	-9.57898	14.39582	-4.36469
H	-8.26751	15.84662	-3.48059
C	-10.64858	13.51304	-4.17443
H	-12.03987	12.71410	-2.73436
H	-9.14337	14.48827	-5.35669
C	-11.13621	12.72713	-5.33671
C	-12.68223	18.10775	2.89186
O	-10.66363	12.78959	-6.44652
O	-12.16380	11.93236	-5.03119
O	-12.22218	18.08226	4.14440

O	-13.75427	18.57967	2.59708
C	2.46363	14.40353	-1.74606
H	3.31944	13.72030	-1.81867
H	1.55115	13.81848	-1.91752
C	2.30084	14.00956	0.74313
H	1.38409	13.42107	0.61043
H	3.15214	13.31784	0.70835
C	-13.05679	18.64224	5.15187
H	-14.01667	18.11568	5.19752
H	-12.51812	18.52486	6.09476
H	-13.24442	19.70364	4.95432
C	-12.70012	11.13609	-6.08172
H	-11.93775	10.45903	-6.48319
H	-13.51918	10.56237	-5.64249
H	-13.07543	11.76806	-6.89442
H	2.54962	15.14855	-2.54628
H	2.27237	14.47027	1.73799
C	12.77646	13.58858	0.08597
C	12.39472	14.93601	0.27768
C	13.38135	15.91882	0.50886
C	14.71334	15.54676	0.54586
C	15.08141	14.19936	0.35394
C	14.11167	13.21758	0.12286

H	12.00683	12.84127	-0.09141
H	13.07832	16.95337	0.65501
H	14.39174	12.17674	-0.02611
C	15.93854	16.42449	0.77964
C	17.05448	15.38820	0.69414
C	18.41411	15.57214	0.82461
C	19.27955	14.45457	0.70617
C	18.74037	13.16681	0.45642
C	17.37513	12.98687	0.32645
C	16.52996	14.09852	0.44500
H	18.83965	16.55489	1.01585
H	19.41671	12.32002	0.36848
H	16.97080	11.99525	0.13523
C	11.01928	15.29807	0.23911
C	9.83983	15.60505	0.20770
C	20.67140	14.61983	0.83604
C	21.88224	14.76126	0.94924
C	23.26487	14.91980	1.07960
C	23.83089	16.19598	1.35415
C	24.14197	13.80798	0.94180
C	25.18640	16.35430	1.47927
H	23.17239	17.05105	1.48341
C	25.49738	13.95787	1.07703

H	23.72644	12.83099	0.70873
C	26.06048	15.23754	1.34828
H	25.59376	17.33179	1.71706
H	26.14935	13.10108	0.94000
N	27.41611	15.39092	1.48093
C	28.25260	14.29883	1.86090
C	29.41195	14.02766	1.12575
C	27.92797	13.52474	2.98168
C	30.23535	12.97556	1.50311
H	29.65792	14.63096	0.25578
C	28.75666	12.47511	3.35163
H	27.04203	13.75692	3.56740
C	29.91239	12.19197	2.61693
H	31.13011	12.75436	0.92887
H	28.52303	11.86947	4.22335
C	28.04661	16.64951	1.24535
C	28.94889	17.15777	2.18635
C	27.78416	17.35352	0.06387
C	29.57516	18.37426	1.95124
H	29.14715	16.60746	3.10243
C	28.41491	18.56845	-0.16312
H	27.10445	16.94089	-0.67744
C	29.31133	19.08764	0.77632

H	30.26763	18.77828	2.68373
H	28.22820	19.12372	-1.07860
C	30.76841	11.05149	3.06234
C	29.96295	20.39864	0.47862
O	30.79611	20.78632	1.43838
O	29.75583	21.03622	-0.52321
O	31.84199	10.88713	2.29684
O	30.51362	10.35560	4.01309
C	15.89510	17.08949	2.16813
H	16.81070	17.66678	2.34806
H	15.04448	17.77909	2.23641
C	16.08226	17.49353	-0.31961
H	17.00280	18.07298	-0.17506
H	15.23704	18.19228	-0.28824
C	31.47112	22.02843	1.25115
H	30.75003	22.84826	1.16256
H	32.09800	22.16958	2.13381
H	32.08950	21.99719	0.34751
C	32.72729	9.82261	2.63819
H	32.20668	8.85993	2.59180
H	33.53481	9.85177	1.90400
H	33.12710	9.96442	3.64814
H	15.79658	16.34177	2.96417

H	16.11492	17.03717	-1.31619
C	8.51725	15.94718	0.17346
C	5.95748	16.60217	0.10907
C	4.97787	15.60921	-0.11066
C	5.56259	17.94393	0.29435
C	3.64183	15.96747	-0.14120
H	5.28928	14.57625	-0.25265
C	4.22047	18.30043	0.26343
H	6.32418	18.70185	0.46291
C	2.42313	15.07570	-0.36117
C	3.25951	17.31046	0.04533
H	3.93130	19.33960	0.40831
C	1.29510	16.09959	-0.27218
C	1.80107	17.39189	-0.03583
C	-0.06866	15.89188	-0.39124
C	0.93678	18.48255	0.08148
C	-0.95193	16.98571	-0.27374
H	-0.47386	14.89844	-0.57330
C	-0.43194	18.27550	-0.03743
H	1.32076	19.48459	0.26387
H	-1.11887	19.11409	0.05179
C	7.33678	16.25062	0.14373
C	-2.36130	16.78788	-0.39215

C	-3.55941	16.61661	-0.49229
C	-4.96775	16.41340	-0.60979
C	-5.49239	15.13504	-0.87557
C	-5.86740	17.48537	-0.46272
C	-6.86111	14.93621	-0.98259
H	-4.81533	14.29074	-0.98473
C	-7.23516	17.28758	-0.58375
H	-5.48293	18.48355	-0.26524
C	-7.75060	16.01006	-0.84171
H	-7.24847	13.93847	-1.17481
H	-7.91397	18.13085	-0.48074
N	-9.14987	15.80702	-0.95878
C	-10.01910	16.36841	0.00082
C	-11.25197	16.92109	-0.38364
C	-9.66006	16.39284	1.35795
C	-12.09909	17.47196	0.56547
H	-11.53957	16.92281	-1.43181
C	-10.50758	16.95566	2.30171
H	-8.71285	15.96197	1.67187
C	-11.73961	17.49947	1.91835
H	-13.05060	17.90428	0.26521
H	-10.21930	16.96229	3.34923
C	-9.65572	15.04375	-2.03279

C	-10.72400	14.15304	-1.84013
C	-9.08970	15.15568	-3.31329
C	-11.21641	13.40352	-2.89899
H	-11.16434	14.04482	-0.85233
C	-9.57898	14.39582	-4.36469
H	-8.26751	15.84662	-3.48059
C	-10.64858	13.51304	-4.17443
H	-12.03987	12.71410	-2.73436
H	-9.14337	14.48827	-5.35669
C	-11.13621	12.72713	-5.33671
C	-12.68223	18.10775	2.89186
O	-10.66363	12.78959	-6.44652
O	-12.16380	11.93236	-5.03119
O	-12.22218	18.08226	4.14440
O	-13.75427	18.57967	2.59708
C	2.46363	14.40353	-1.74606
H	3.31944	13.72030	-1.81867
H	1.55115	13.81848	-1.91752
C	2.30084	14.00956	0.74313
H	1.38409	13.42107	0.61043
H	3.15214	13.31784	0.70835
C	-13.05679	18.64224	5.15187
H	-14.01667	18.11568	5.19752

H	-12.51812	18.52486	6.09476
H	-13.24442	19.70364	4.95432
C	-12.70012	11.13609	-6.08172
H	-11.93775	10.45903	-6.48319
H	-13.51918	10.56237	-5.64249
H	-13.07543	11.76806	-6.89442
H	2.54962	15.14855	-2.54628
H	2.27237	14.47027	1.73799
C	12.77646	13.58858	0.08597
C	12.39472	14.93601	0.27768
C	13.38135	15.91882	0.50886
C	14.71334	15.54676	0.54586
C	15.08141	14.19936	0.35394
C	14.11167	13.21758	0.12286
H	12.00683	12.84127	-0.09141
H	13.07832	16.95337	0.65501
H	14.39174	12.17674	-0.02611
C	15.93854	16.42449	0.77964
C	17.05448	15.38820	0.69414
C	18.41411	15.57214	0.82461
C	19.27955	14.45457	0.70617
C	18.74037	13.16681	0.45642
C	17.37513	12.98687	0.32645

C	16.52996	14.09852	0.44500
H	18.83965	16.55489	1.01585
H	19.41671	12.32002	0.36848
H	16.97080	11.99525	0.13523
C	11.01928	15.29807	0.23911
C	9.83983	15.60505	0.20770
C	20.67140	14.61983	0.83604
C	21.88224	14.76126	0.94924
C	23.26487	14.91980	1.07960
C	23.83089	16.19598	1.35415
C	24.14197	13.80798	0.94180
C	25.18640	16.35430	1.47927
H	23.17239	17.05105	1.48341
C	25.49738	13.95787	1.07703
H	23.72644	12.83099	0.70873
C	26.06048	15.23754	1.34828
H	25.59376	17.33179	1.71706
H	26.14935	13.10108	0.94000
N	27.41611	15.39092	1.48093
C	28.25260	14.29883	1.86090
C	29.41195	14.02766	1.12575
C	27.92797	13.52474	2.98168
C	30.23535	12.97556	1.50311

H	29.65792	14.63096	0.25578
C	28.75666	12.47511	3.35163
H	27.04203	13.75692	3.56740
C	29.91239	12.19197	2.61693
H	31.13011	12.75436	0.92887
H	28.52303	11.86947	4.22335
C	28.04661	16.64951	1.24535
C	28.94889	17.15777	2.18635
C	27.78416	17.35352	0.06387
C	29.57516	18.37426	1.95124
H	29.14715	16.60746	3.10243
C	28.41491	18.56845	-0.16312
H	27.10445	16.94089	-0.67744
C	29.31133	19.08764	0.77632
H	30.26763	18.77828	2.68373
H	28.22820	19.12372	-1.07860
C	30.76841	11.05149	3.06234
C	29.96295	20.39864	0.47862
O	30.79611	20.78632	1.43838
O	29.75583	21.03622	-0.52321
O	31.84199	10.88713	2.29684
O	30.51362	10.35560	4.01309
C	15.89510	17.08949	2.16813

H	16.81070	17.66678	2.34806
H	15.04448	17.77909	2.23641
C	16.08226	17.49353	-0.31961
H	17.00280	18.07298	-0.17506
H	15.23704	18.19228	-0.28824
C	31.47112	22.02843	1.25115
H	30.75003	22.84826	1.16256
H	32.09800	22.16958	2.13381
H	32.08950	21.99719	0.34751
C	32.72729	9.82261	2.63819
H	32.20668	8.85993	2.59180
H	33.53481	9.85177	1.90400
H	33.12710	9.96442	3.64814
H	15.79658	16.34177	2.96417
H	16.11492	17.03717	-1.31619

Table S13. Atomic coordinates of **2**$^{Me2+}$ (closed-shell singlet) from its DFT geometry-optimized structure.

Atom	**x**	**y**	**z**
C	-2.25032	-0.58261	1.16649
C	-2.64751	0.77278	1.35089
C	-1.66785	1.77780	1.57327
C	-0.34041	1.42281	1.60921
C	0.04383	0.06765	1.42410

C	-0.91963	-0.93513	1.20133
H	-3.01563	-1.33580	0.99756
H	-1.98769	2.80796	1.71159
H	-0.62354	-1.97184	1.05916
C	0.87916	2.30881	1.83310
C	1.99811	1.27766	1.74885
C	3.35415	1.46696	1.87086
C	4.22454	0.34995	1.75262
C	3.68655	-0.94761	1.51207
C	2.32799	-1.13532	1.39185
C	1.47459	-0.02092	1.50887
H	3.77876	2.45122	2.05414
H	4.36870	-1.78948	1.42536
H	1.92576	-2.12917	1.20926
C	-4.00656	1.11030	1.31367
C	-5.19840	1.40412	1.28249
C	-6.50618	1.72683	1.24930
C	-9.05742	2.35815	1.18576
C	-10.03825	1.35163	0.97631
C	-9.45369	3.71452	1.36195
C	-11.36613	1.70616	0.94626
H	-9.71922	0.32040	0.84414
C	-10.78493	4.06671	1.33146

H	-8.68769	4.46919	1.52100
C	-12.58711	0.81797	0.73871
C	-11.74935	3.06239	1.12273
H	-11.08022	5.10454	1.46705
C	-13.70599	1.84918	0.82408
C	-13.18179	3.14967	1.04752
C	-15.06352	1.65738	0.71657
C	-14.03501	4.26388	1.16056
C	-15.93370	2.77393	0.83210
H	-15.48840	0.67079	0.54682
C	-15.39496	4.07367	1.05388
H	-13.63252	5.25999	1.33001
H	-16.07687	4.91597	1.13844
C	-7.69802	2.02065	1.21955
C	5.61134	0.51873	1.87106
C	-17.32305	2.60190	0.73088
C	6.82269	0.66366	1.97349
C	-18.53472	2.45420	0.64604
C	8.20941	0.82785	2.09062
C	8.77247	2.10062	2.36473
C	9.08845	-0.27500	1.93838
C	10.13291	2.26288	2.47929
H	8.11404	2.95470	2.50308

C	10.44909	-0.11687	2.05536
H	8.67719	-1.25492	1.70873
C	11.00847	1.15736	2.32893
H	10.53752	3.24274	2.71313
H	11.10194	-0.97213	1.91118
C	-19.92451	2.28650	0.55103
C	-20.49081	1.00507	0.33448
C	-20.80056	3.39464	0.67046
C	-21.85335	0.84007	0.24020
H	-19.83640	0.14009	0.25870
C	-22.16372	3.23212	0.58213
H	-20.38437	4.38821	0.81807
C	-22.72575	1.94988	0.36324
H	-22.26413	-0.15450	0.09576
H	-22.81277	4.09936	0.65551
N	12.37593	1.31774	2.44664
N	-24.09720	1.78529	0.27203
C	13.21059	0.23843	2.85193
C	14.37643	-0.04880	2.13147
C	12.88447	-0.52120	3.98345
C	15.20247	-1.08961	2.53386
H	14.62730	0.53841	1.25178
C	13.71129	-1.56335	4.37652

H	11.99253	-0.28415	4.55814
C	14.87509	-1.85701	3.65766
H	16.10204	-1.31689	1.96928
H	13.47150	-2.15490	5.25640
C	12.99687	2.56748	2.16716
C	13.92758	3.09944	3.06807
C	12.70072	3.25489	0.98245
C	14.54881	4.30966	2.79076
H	14.15459	2.56742	3.98840
C	13.32105	4.46631	0.71431
H	11.99668	2.83137	0.27047
C	14.24846	5.00417	1.61328
H	15.26426	4.72535	3.49429
H	13.10393	5.00478	-0.20469
C	-24.98734	2.67253	0.93807
C	-26.08144	3.21141	0.24871
C	-24.78865	2.99143	2.28776
C	-26.95786	4.06414	0.90337
H	-26.23429	2.96746	-0.79948
C	-25.66670	3.84996	2.93549
H	-23.95360	2.55518	2.83029
C	-26.75835	4.39341	2.24876
H	-27.80495	4.49468	0.37547

H	-25.51503	4.09044	3.98374
C	-24.65925	0.72499	-0.49109
C	-25.68120	-0.06199	0.05461
C	-24.21240	0.47938	-1.79664
C	-26.24443	-1.08634	-0.69428
H	-26.02513	0.12568	1.06856
C	-24.77512	-0.54977	-2.53696
H	-23.43600	1.10434	-2.23089
C	-25.79414	-1.34068	-1.99494
H	-27.03140	-1.70072	-0.26669
H	-24.44073	-0.74411	-3.55286
C	15.72912	-2.98591	4.12755
C	14.88805	6.30772	1.27234
C	-26.36617	-2.43013	-2.83730
C	-27.72984	5.31735	2.90164
O	-25.99265	-2.68133	-3.95643
O	-27.33746	-3.09996	-2.22222
O	-27.43261	5.55981	4.17593
O	-28.68348	5.79704	2.34013
O	15.75804	6.71056	2.19466
O	14.64608	6.93320	0.26980
O	16.81332	-3.15797	3.37613
O	15.46928	-3.67174	5.08513

C	0.83659	2.97990	3.21904
H	1.75099	3.56069	3.39136
H	-0.01571	3.66729	3.28523
C	1.01264	3.37154	0.72611
H	1.93197	3.95376	0.86432
H	0.16563	4.06767	0.75925
C	-12.55541	0.13694	-0.64270
H	-11.70332	-0.55053	-0.71103
H	-13.47096	-0.44537	-0.80348
C	-12.71109	-0.23693	1.85418
H	-13.63142	-0.82030	1.72783
H	-11.86430	-0.93328	1.81908
C	16.42459	7.94861	1.96200
H	15.70117	8.76809	1.88924
H	17.08601	8.10342	2.81687
H	17.00720	7.90420	1.03531
C	17.69669	-4.21448	3.74299
H	17.18010	-5.17977	3.70398
H	18.51339	-4.19365	3.01855
H	18.08428	-4.05832	4.75568
C	-28.30306	6.43282	4.89079
H	-29.32050	6.02743	4.91569
H	-27.89962	6.50303	5.90302

H	-28.32560	7.42292	4.42240
C	-27.95106	-4.16403	-2.94482
H	-27.21194	-4.92945	-3.20566
H	-28.71115	-4.58315	-2.28236
H	-28.41465	-3.78868	-3.86372
H	0.74354	2.23623	4.01928
H	-12.46927	0.87499	-1.44892
H	-12.73256	0.23166	2.84519
H	1.04223	2.91003	-0.26799
C	-2.25032	-0.58261	1.16649
C	-2.64751	0.77278	1.35089
C	-1.66785	1.77780	1.57327
C	-0.34041	1.42281	1.60921
C	0.04383	0.06765	1.42410
C	-0.91963	-0.93513	1.20133
H	-3.01563	-1.33580	0.99756
H	-1.98769	2.80796	1.71159
H	-0.62354	-1.97184	1.05916
C	0.87916	2.30881	1.83310
C	1.99811	1.27766	1.74885
C	3.35415	1.46696	1.87086
C	4.22454	0.34995	1.75262
C	3.68655	-0.94761	1.51207

C	2.32799	-1.13532	1.39185
C	1.47459	-0.02092	1.50887
H	3.77876	2.45122	2.05414
H	4.36870	-1.78948	1.42536
H	1.92576	-2.12917	1.20926
C	-4.00656	1.11030	1.31367
C	-5.19840	1.40412	1.28249
C	-6.50618	1.72683	1.24930
C	-9.05742	2.35815	1.18576
C	-10.03825	1.35163	0.97631
C	-9.45369	3.71452	1.36195
C	-11.36613	1.70616	0.94626
H	-9.71922	0.32040	0.84414
C	-10.78493	4.06671	1.33146
H	-8.68769	4.46919	1.52100
C	-12.58711	0.81797	0.73871
C	-11.74935	3.06239	1.12273
H	-11.08022	5.10454	1.46705
C	-13.70599	1.84918	0.82408
C	-13.18179	3.14967	1.04752
C	-15.06352	1.65738	0.71657
C	-14.03501	4.26388	1.16056
C	-15.93370	2.77393	0.83210

H	-15.48840	0.67079	0.54682
C	-15.39496	4.07367	1.05388
H	-13.63252	5.25999	1.33001
H	-16.07687	4.91597	1.13844
C	-7.69802	2.02065	1.21955
C	5.61134	0.51873	1.87106
C	-17.32305	2.60190	0.73088
C	6.82269	0.66366	1.97349
C	-18.53472	2.45420	0.64604
C	8.20941	0.82785	2.09062
C	8.77247	2.10062	2.36473
C	9.08845	-0.27500	1.93838
C	10.13291	2.26288	2.47929
H	8.11404	2.95470	2.50308
C	10.44909	-0.11687	2.05536
H	8.67719	-1.25492	1.70873
C	11.00847	1.15736	2.32893
H	10.53752	3.24274	2.71313
H	11.10194	-0.97213	1.91118
C	-19.92451	2.28650	0.55103
C	-20.49081	1.00507	0.33448
C	-20.80056	3.39464	0.67046
C	-21.85335	0.84007	0.24020

H	-19.83640	0.14009	0.25870
C	-22.16372	3.23212	0.58213
H	-20.38437	4.38821	0.81807
C	-22.72575	1.94988	0.36324
H	-22.26413	-0.15450	0.09576
H	-22.81277	4.09936	0.65551
N	12.37593	1.31774	2.44664
N	-24.09720	1.78529	0.27203
C	13.21059	0.23843	2.85193
C	14.37643	-0.04880	2.13147
C	12.88447	-0.52120	3.98345
C	15.20247	-1.08961	2.53386
H	14.62730	0.53841	1.25178
C	13.71129	-1.56335	4.37652
H	11.99253	-0.28415	4.55814
C	14.87509	-1.85701	3.65766
H	16.10204	-1.31689	1.96928
H	13.47150	-2.15490	5.25640
C	12.99687	2.56748	2.16716
C	13.92758	3.09944	3.06807
C	12.70072	3.25489	0.98245
C	14.54881	4.30966	2.79076
H	14.15459	2.56742	3.98840

C	13.32105	4.46631	0.71431
H	11.99668	2.83137	0.27047
C	14.24846	5.00417	1.61328
H	15.26426	4.72535	3.49429
H	13.10393	5.00478	-0.20469
C	-24.98734	2.67253	0.93807
C	-26.08144	3.21141	0.24871
C	-24.78865	2.99143	2.28776
C	-26.95786	4.06414	0.90337
H	-26.23429	2.96746	-0.79948
C	-25.66670	3.84996	2.93549
H	-23.95360	2.55518	2.83029
C	-26.75835	4.39341	2.24876
H	-27.80495	4.49468	0.37547
H	-25.51503	4.09044	3.98374
C	-24.65925	0.72499	-0.49109
C	-25.68120	-0.06199	0.05461
C	-24.21240	0.47938	-1.79664
C	-26.24443	-1.08634	-0.69428
H	-26.02513	0.12568	1.06856
C	-24.77512	-0.54977	-2.53696
H	-23.43600	1.10434	-2.23089
C	-25.79414	-1.34068	-1.99494

H	-27.03140	-1.70072	-0.26669
H	-24.44073	-0.74411	-3.55286
C	15.72912	-2.98591	4.12755
C	14.88805	6.30772	1.27234
C	-26.36617	-2.43013	-2.83730
C	-27.72984	5.31735	2.90164
O	-25.99265	-2.68133	-3.95643
O	-27.33746	-3.09996	-2.22222
O	-27.43261	5.55981	4.17593
O	-28.68348	5.79704	2.34013
O	15.75804	6.71056	2.19466
O	14.64608	6.93320	0.26980
O	16.81332	-3.15797	3.37613
O	15.46928	-3.67174	5.08513
C	0.83659	2.97990	3.21904
H	1.75099	3.56069	3.39136
H	-0.01571	3.66729	3.28523
C	1.01264	3.37154	0.72611
H	1.93197	3.95376	0.86432
H	0.16563	4.06767	0.75925
C	-12.55541	0.13694	-0.64270
H	-11.70332	-0.55053	-0.71103
H	-13.47096	-0.44537	-0.80348

C	-12.71109	-0.23693	1.85418
H	-13.63142	-0.82030	1.72783
H	-11.86430	-0.93328	1.81908
C	16.42459	7.94861	1.96200
H	15.70117	8.76809	1.88924
H	17.08601	8.10342	2.81687
H	17.00720	7.90420	1.03531
C	17.69669	-4.21448	3.74299
H	17.18010	-5.17977	3.70398
H	18.51339	-4.19365	3.01855
H	18.08428	-4.05832	4.75568
C	-28.30306	6.43282	4.89079
H	-29.32050	6.02743	4.91569
H	-27.89962	6.50303	5.90302
H	-28.32560	7.42292	4.42240
C	-27.95106	-4.16403	-2.94482
H	-27.21194	-4.92945	-3.20566
H	-28.71115	-4.58315	-2.28236
H	-28.41465	-3.78868	-3.86372
H	0.74354	2.23623	4.01928
H	-12.46927	0.87499	-1.44892
H	-12.73256	0.23166	2.84519
H	1.04223	2.91003	-0.26799

Table S14. Atomic coordinates of $\mathbf{2}^{Me2+}$ (open-shell singlet) from its DFT geometry-optimized structure.

Atom	x	y	z
C	-2.25031	-0.58258	1.16699
C	-2.64748	0.77286	1.35113
C	-1.66782	1.77793	1.57330
C	-0.34038	1.42293	1.60930
C	0.04385	0.06771	1.42447
C	-0.91964	-0.93511	1.20190
H	-3.01564	-1.33580	0.99822
H	-1.98765	2.80811	1.71142
H	-0.62356	-1.97185	1.05994
C	0.87920	2.30896	1.83300
C	1.99813	1.27777	1.74896
C	3.35416	1.46706	1.87091
C	4.22452	0.34996	1.75293
C	3.68647	-0.94767	1.51267
C	2.32793	-1.13535	1.39249
C	1.47456	-0.02086	1.50926
H	3.77881	2.45134	2.05396
H	4.36860	-1.78956	1.42615
H	1.92566	-2.12922	1.21012
C	-4.00653	1.11038	1.31387

C	-5.19836	1.40421	1.28267
C	-6.50614	1.72693	1.24947
C	-9.05738	2.35826	1.18592
C	-10.03823	1.35173	0.97659
C	-9.45364	3.71463	1.36200
C	-11.36611	1.70627	0.94655
H	-9.71921	0.32048	0.84450
C	-10.78489	4.06683	1.33152
H	-8.68764	4.46932	1.52096
C	-12.58711	0.81806	0.73911
C	-11.74932	3.06251	1.12292
H	-11.08017	5.10467	1.46703
C	-13.70598	1.84929	0.82443
C	-13.18180	3.14978	1.04774
C	-15.06354	1.65747	0.71696
C	-14.03501	4.26397	1.16071
C	-15.93371	2.77399	0.83240
H	-15.48840	0.67086	0.54729
C	-15.39499	4.07372	1.05407
H	-13.63254	5.26009	1.33008
H	-16.07689	4.91604	1.13858
C	-7.69799	2.02074	1.21971
C	5.61127	0.51872	1.87131

C	-17.32311	2.60194	0.73118
C	6.82265	0.66364	1.97368
C	-18.53475	2.45422	0.64633
C	8.20932	0.82782	2.09074
C	8.77242	2.10069	2.36442
C	9.08834	-0.27513	1.93887
C	10.13285	2.26296	2.47888
H	8.11401	2.95483	2.50249
C	10.44896	-0.11701	2.05580
H	8.67703	-1.25512	1.70955
C	11.00839	1.15732	2.32892
H	10.53749	3.24288	2.71238
H	11.10178	-0.97234	1.91192
C	-19.92460	2.28649	0.55129
C	-20.49088	1.00507	0.33482
C	-20.80065	3.39461	0.67060
C	-21.85344	0.84006	0.24049
H	-19.83647	0.14008	0.25912
C	-22.16383	3.23207	0.58218
H	-20.38448	4.38819	0.81818
C	-22.72583	1.94985	0.36336
H	-22.26421	-0.15453	0.09608
H	-22.81289	4.09932	0.65548

N	12.37579	1.31769	2.44656
N	-24.09734	1.78525	0.27203
C	13.21047	0.23842	2.85199
C	14.37617	-0.04904	2.13140
C	12.88449	-0.52087	3.98378
C	15.20222	-1.08978	2.53395
H	14.62691	0.53791	1.25150
C	13.71134	-1.56293	4.37701
H	11.99267	-0.28360	4.55856
C	14.87501	-1.85683	3.65802
H	16.10169	-1.31727	1.96928
H	13.47168	-2.15422	5.25709
C	12.99680	2.56737	2.16685
C	13.92748	3.09946	3.06771
C	12.70073	3.25453	0.98198
C	14.54877	4.30960	2.79018
H	14.15442	2.56761	3.98815
C	13.32113	4.46586	0.71361
H	11.99672	2.83087	0.27005
C	14.24851	5.00386	1.61252
H	15.26420	4.72542	3.49365
H	13.10410	5.00414	-0.20551
C	-24.98750	2.67230	0.93825

C	-26.08178	3.21107	0.24909
C	-24.78867	2.99119	2.28793
C	-26.95823	4.06365	0.90392
H	-26.23476	2.96715	-0.79909
C	-25.66673	3.84958	2.93582
H	-23.95347	2.55505	2.83032
C	-26.75857	4.39291	2.24928
H	-27.80546	4.49409	0.37616
H	-25.51492	4.09005	3.98405
C	-24.65926	0.72512	-0.49138
C	-25.68137	-0.06193	0.05393
C	-24.21213	0.47970	-1.79688
C	-26.24446	-1.08613	-0.69527
H	-26.02553	0.12557	1.06784
C	-24.77470	-0.54930	-2.53750
H	-23.43559	1.10469	-2.23083
C	-25.79388	-1.34027	-1.99587
H	-27.03156	-1.70055	-0.26796
H	-24.44007	-0.74348	-3.55335
C	15.72908	-2.98562	4.12811
C	14.88818	6.30732	1.27134
C	-26.36575	-2.42955	-2.83854
C	-27.73008	5.31669	2.90234

O	-25.99203	-2.68051	-3.95767
O	-27.33713	-3.09954	-2.22378
O	-27.43267	5.55919	4.17658
O	-28.68388	5.79626	2.34101
O	15.75821	6.71026	2.19356
O	14.64623	6.93262	0.26869
O	16.81318	-3.15791	3.37659
O	15.46935	-3.67119	5.08592
C	0.83663	2.98032	3.21881
H	1.75103	3.56115	3.39100
H	-0.01567	3.66771	3.28487
C	1.01269	3.37146	0.72579
H	1.93203	3.95368	0.86387
H	0.16570	4.06762	0.75880
C	-12.55544	0.13691	-0.64222
H	-11.70336	-0.55056	-0.71053
H	-13.47100	-0.44542	-0.80294
C	-12.71106	-0.23673	1.85468
H	-13.63141	-0.82009	1.72843
H	-11.86429	-0.93311	1.81962
C	16.42484	7.94823	1.96067
H	15.70148	8.76776	1.88787
H	17.08635	8.10310	2.81546

H	17.00735	7.90365	1.03393
C	17.69658	-4.21434	3.74362
H	17.17996	-5.17963	3.70493
H	18.51319	-4.19371	3.01907
H	18.08429	-4.05791	4.75622
C	-28.30311	6.43209	4.89158
H	-29.32052	6.02662	4.91655
H	-27.89957	6.50228	5.90377
H	-28.32578	7.42222	4.42325
C	-27.95056	-4.16348	-2.94672
H	-27.21137	-4.92884	-3.20754
H	-28.71078	-4.58274	-2.28449
H	-28.41396	-3.78796	-3.86564
H	0.74360	2.23680	4.01920
H	-12.46933	0.87489	-1.44852
H	-12.73248	0.23195	2.84565
H	1.04227	2.90974	-0.26822
C	-2.25031	-0.58258	1.16699
C	-2.64748	0.77286	1.35113
C	-1.66782	1.77793	1.57330
C	-0.34038	1.42293	1.60930
C	0.04385	0.06771	1.42447
C	-0.91964	-0.93511	1.20190

H	-3.01564	-1.33580	0.99822
H	-1.98765	2.80811	1.71142
H	-0.62356	-1.97185	1.05994
C	0.87920	2.30896	1.83300
C	1.99813	1.27777	1.74896
C	3.35416	1.46706	1.87091
C	4.22452	0.34996	1.75293
C	3.68647	-0.94767	1.51267
C	2.32793	-1.13535	1.39249
C	1.47456	-0.02086	1.50926
H	3.77881	2.45134	2.05396
H	4.36860	-1.78956	1.42615
H	1.92566	-2.12922	1.21012
C	-4.00653	1.11038	1.31387
C	-5.19836	1.40421	1.28267
C	-6.50614	1.72693	1.24947
C	-9.05738	2.35826	1.18592
C	-10.03823	1.35173	0.97659
C	-9.45364	3.71463	1.36200
C	-11.36611	1.70627	0.94655
H	-9.71921	0.32048	0.84450
C	-10.78489	4.06683	1.33152
H	-8.68764	4.46932	1.52096

C	-12.58711	0.81806	0.73911
C	-11.74932	3.06251	1.12292
H	-11.08017	5.10467	1.46703
C	-13.70598	1.84929	0.82443
C	-13.18180	3.14978	1.04774
C	-15.06354	1.65747	0.71696
C	-14.03501	4.26397	1.16071
C	-15.93371	2.77399	0.83240
H	-15.48840	0.67086	0.54729
C	-15.39499	4.07372	1.05407
H	-13.63254	5.26009	1.33008
H	-16.07689	4.91604	1.13858
C	-7.69799	2.02074	1.21971
C	5.61127	0.51872	1.87131
C	-17.32311	2.60194	0.73118
C	6.82265	0.66364	1.97368
C	-18.53475	2.45422	0.64633
C	8.20932	0.82782	2.09074
C	8.77242	2.10069	2.36442
C	9.08834	-0.27513	1.93887
C	10.13285	2.26296	2.47888
H	8.11401	2.95483	2.50249
C	10.44896	-0.11701	2.05580

H	8.67703	-1.25512	1.70955
C	11.00839	1.15732	2.32892
H	10.53749	3.24288	2.71238
H	11.10178	-0.97234	1.91192
C	-19.92460	2.28649	0.55129
C	-20.49088	1.00507	0.33482
C	-20.80065	3.39461	0.67060
C	-21.85344	0.84006	0.24049
H	-19.83647	0.14008	0.25912
C	-22.16383	3.23207	0.58218
H	-20.38448	4.38819	0.81818
C	-22.72583	1.94985	0.36336
H	-22.26421	-0.15453	0.09608
H	-22.81289	4.09932	0.65548
N	12.37579	1.31769	2.44656
N	-24.09734	1.78525	0.27203
C	13.21047	0.23842	2.85199
C	14.37617	-0.04904	2.13140
C	12.88449	-0.52087	3.98378
C	15.20222	-1.08978	2.53395
H	14.62691	0.53791	1.25150
C	13.71134	-1.56293	4.37701
H	11.99267	-0.28360	4.55856

C	14.87501	-1.85683	3.65802
H	16.10169	-1.31727	1.96928
H	13.47168	-2.15422	5.25709
C	12.99680	2.56737	2.16685
C	13.92748	3.09946	3.06771
C	12.70073	3.25453	0.98198
C	14.54877	4.30960	2.79018
H	14.15442	2.56761	3.98815
C	13.32113	4.46586	0.71361
H	11.99672	2.83087	0.27005
C	14.24851	5.00386	1.61252
H	15.26420	4.72542	3.49365
H	13.10410	5.00414	-0.20551
C	-24.98750	2.67230	0.93825
C	-26.08178	3.21107	0.24909
C	-24.78867	2.99119	2.28793
C	-26.95823	4.06365	0.90392
H	-26.23476	2.96715	-0.79909
C	-25.66673	3.84958	2.93582
H	-23.95347	2.55505	2.83032
C	-26.75857	4.39291	2.24928
H	-27.80546	4.49409	0.37616
H	-25.51492	4.09005	3.98405

C	-24.65926	0.72512	-0.49138
C	-25.68137	-0.06193	0.05393
C	-24.21213	0.47970	-1.79688
C	-26.24446	-1.08613	-0.69527
H	-26.02553	0.12557	1.06784
C	-24.77470	-0.54930	-2.53750
H	-23.43559	1.10469	-2.23083
C	-25.79388	-1.34027	-1.99587
H	-27.03156	-1.70055	-0.26796
H	-24.44007	-0.74348	-3.55335
C	15.72908	-2.98562	4.12811
C	14.88818	6.30732	1.27134
C	-26.36575	-2.42955	-2.83854
C	-27.73008	5.31669	2.90234
O	-25.99203	-2.68051	-3.95767
O	-27.33713	-3.09954	-2.22378
O	-27.43267	5.55919	4.17658
O	-28.68388	5.79626	2.34101
O	15.75821	6.71026	2.19356
O	14.64623	6.93262	0.26869
O	16.81318	-3.15791	3.37659
O	15.46935	-3.67119	5.08592
C	0.83663	2.98032	3.21881

H	1.75103	3.56115	3.39100
H	-0.01567	3.66771	3.28487
C	1.01269	3.37146	0.72579
H	1.93203	3.95368	0.86387
H	0.16570	4.06762	0.75880
C	-12.55544	0.13691	-0.64222
H	-11.70336	-0.55056	-0.71053
H	-13.47100	-0.44542	-0.80294
C	-12.71106	-0.23673	1.85468
H	-13.63141	-0.82009	1.72843
H	-11.86429	-0.93311	1.81962
C	16.42484	7.94823	1.96067
H	15.70148	8.76776	1.88787
H	17.08635	8.10310	2.81546
H	17.00735	7.90365	1.03393
C	17.69658	-4.21434	3.74362
H	17.17996	-5.17963	3.70493
H	18.51319	-4.19371	3.01907
H	18.08429	-4.05791	4.75622
C	-28.30311	6.43209	4.89158
H	-29.32052	6.02662	4.91655
H	-27.89957	6.50228	5.90377
H	-28.32578	7.42222	4.42325

C	-27.95056	-4.16348	-2.94672
H	-27.21137	-4.92884	-3.20754
H	-28.71078	-4.58274	-2.28449
H	-28.41396	-3.78796	-3.86564
H	0.74360	2.23680	4.01920
H	-12.46933	0.87489	-1.44852
H	-12.73248	0.23195	2.84565
H	1.04227	2.90974	-0.26822

Table S15. Atomic coordinates of $\mathbf{2}^{Me2+}$ (triplet) from its DFT geometry-optimized structure.

Atom	**x**	**y**	**z**
C	-2.23359	-0.59597	1.05136
C	-2.62449	0.74645	1.25421
C	-1.64561	1.73502	1.49196
C	-0.31058	1.37266	1.52469
C	0.06695	0.02998	1.32183
C	-0.89497	-0.95702	1.08392
H	-2.99758	-1.34785	0.86890
H	-1.95620	2.76610	1.64665
H	-0.60718	-1.99447	0.92634
C	0.90822	2.25777	1.76421
C	2.03182	1.23047	1.67047
C	3.39076	1.42431	1.80261

C	4.26443	0.31532	1.67528
C	3.73618	-0.97382	1.41516
C	2.37160	-1.16376	1.28384
C	1.51811	-0.06050	1.41140
H	3.80812	2.40898	2.00185
H	4.41897	-1.81468	1.32030
H	1.97558	-2.15722	1.08478
C	-4.00300	1.09932	1.22081
C	-5.18390	1.40014	1.19460
C	-6.50787	1.73740	1.16713
C	-9.06754	2.39105	1.11879
C	-10.04970	1.39808	0.91542
C	-9.45549	3.73762	1.29828
C	-11.38513	1.75996	0.89495
H	-9.74134	0.36385	0.77842
C	-10.79447	4.09825	1.27761
H	-8.68899	4.49296	1.45400
C	-12.60733	0.87006	0.69352
C	-11.75978	3.10661	1.07553
H	-11.07991	5.13885	1.41767
C	-13.72984	1.89850	0.78771
C	-13.21244	3.19485	1.00956
C	-15.09104	1.70095	0.68743

C	-14.06437	4.30008	1.13001
C	-15.96322	2.81152	0.81016
H	-15.51117	0.71192	0.51783
C	-15.43120	4.10634	1.03097
H	-13.66564	5.29790	1.29970
H	-16.11286	4.94849	1.12243
C	-7.68885	2.03817	1.14414
C	5.65660	0.49136	1.80741
C	-17.35809	2.63101	0.71594
C	6.86542	0.64225	1.92287
C	-18.56925	2.47610	0.63731
C	8.24742	0.81203	2.05662
C	8.80080	2.09020	2.34657
C	9.13439	-0.29024	1.90713
C	10.15463	2.25971	2.47554
H	8.13416	2.93743	2.48507
C	10.48822	-0.12970	2.04626
H	8.72804	-1.26805	1.66181
C	11.03876	1.15214	2.33321
H	10.55277	3.23776	2.72644
H	11.14852	-0.97844	1.89932
C	-19.95469	2.30144	0.55078
C	-20.51547	1.01204	0.33496

C	-20.83726	3.40981	0.67824
C	-21.87223	0.83942	0.24539
H	-19.85464	0.15250	0.25827
C	-22.19543	3.24178	0.60366
H	-20.42212	4.40428	0.81983
C	-22.75259	1.95028	0.38163
H	-22.28034	-0.15703	0.10904
H	-22.84934	4.10510	0.67537
N	12.39257	1.31616	2.47028
N	-24.11080	1.77994	0.30109
C	13.23660	0.22864	2.84550
C	14.40420	-0.02353	2.11634
C	12.91017	-0.55993	3.95581
C	15.23403	-1.07206	2.48906
H	14.65092	0.59071	1.25430
C	13.74606	-1.60524	4.32141
H	12.01813	-0.34148	4.53748
C	14.90976	-1.86988	3.59242
H	16.13501	-1.27938	1.91942
H	13.51185	-2.22182	5.18525
C	13.01226	2.58172	2.24550
C	13.91323	3.08750	3.18936
C	12.73993	3.29536	1.07187

C	14.52785	4.31181	2.96508
H	14.11853	2.52980	4.09937
C	13.35991	4.51766	0.85564
H	12.06219	2.88428	0.32794
C	14.25431	5.03471	1.79817
H	15.21869	4.71454	3.69978
H	13.16621	5.08066	-0.05361
C	-25.00897	2.69194	0.93068
C	-26.09177	3.20650	0.20759
C	-24.82113	3.04448	2.27245
C	-26.97079	4.08291	0.82589
H	-26.23100	2.93084	-0.83445
C	-25.70748	3.92166	2.88372
H	-23.99619	2.61818	2.83767
C	-26.78560	4.44756	2.16422
H	-27.80960	4.50170	0.27617
H	-25.57088	4.19133	3.92673
C	-24.67881	0.68565	-0.41591
C	-25.68538	-0.08333	0.17948
C	-24.25022	0.40514	-1.71944
C	-26.25002	-1.13899	-0.52296
H	-26.01194	0.13802	1.19220
C	-24.82082	-0.65168	-2.41400

H	-23.49003	1.02412	-2.18926
C	-25.82063	-1.43058	-1.82287
H	-27.02312	-1.74583	-0.06114
H	-24.50609	-0.87779	-3.42939
C	15.77321	-3.00715	4.03282
C	14.89356	6.35478	1.51229
C	-26.40063	-2.55448	-2.61877
C	-27.76492	5.39452	2.77840
O	-26.04573	-2.83472	-3.73607
O	-27.35007	-3.21083	-1.96110
O	-27.48535	5.66792	4.04814
O	-28.70554	5.86037	2.18605
O	15.72570	6.73960	2.47370
O	14.67746	7.00042	0.51766
O	16.85385	-3.15332	3.27410
O	15.51709	-3.71478	4.97437
C	0.86068	2.91265	3.15735
H	1.77226	3.49514	3.34088
H	0.00530	3.59580	3.23108
C	1.04319	3.33568	0.67249
H	1.95953	3.92085	0.82058
H	0.19288	4.02801	0.70929
C	-12.58388	0.19017	-0.68830

H	-11.72923	-0.49357	-0.76492
H	-13.49808	-0.39605	-0.84502
C	-12.72234	-0.18799	1.80663
H	-13.64083	-0.77598	1.68540
H	-11.87257	-0.88085	1.76728
C	16.38930	7.98970	2.29804
H	15.66066	8.80395	2.22067
H	17.01764	8.12661	3.18029
H	17.00502	7.97363	1.39221
C	17.74703	-4.21282	3.61121
H	17.23602	-5.17985	3.55116
H	18.55953	-4.16829	2.88334
H	18.13793	-4.07730	4.62548
C	-28.36128	6.56438	4.72867
H	-29.38089	6.16459	4.74805
H	-27.97169	6.65723	5.74432
H	-28.36995	7.54191	4.23445
C	-27.97084	-4.30436	-2.63403
H	-27.22994	-5.07068	-2.88636
H	-28.71097	-4.70737	-1.93998
H	-28.45883	-3.96242	-3.55317
H	0.76805	2.15867	3.94819
H	-12.50608	0.92990	-1.49405

H	-12.74029	0.27894	2.79868
H	1.07864	2.88668	-0.32733
C	-2.23359	-0.59597	1.05136
C	-2.62449	0.74645	1.25421
C	-1.64561	1.73502	1.49196
C	-0.31058	1.37266	1.52469
C	0.06695	0.02998	1.32183
C	-0.89497	-0.95702	1.08392
H	-2.99758	-1.34785	0.86890
H	-1.95620	2.76610	1.64665
H	-0.60718	-1.99447	0.92634
C	0.90822	2.25777	1.76421
C	2.03182	1.23047	1.67047
C	3.39076	1.42431	1.80261
C	4.26443	0.31532	1.67528
C	3.73618	-0.97382	1.41516
C	2.37160	-1.16376	1.28384
C	1.51811	-0.06050	1.41140
H	3.80812	2.40898	2.00185
H	4.41897	-1.81468	1.32030
H	1.97558	-2.15722	1.08478
C	-4.00300	1.09932	1.22081
C	-5.18390	1.40014	1.19460

C	-6.50787	1.73740	1.16713
C	-9.06754	2.39105	1.11879
C	-10.04970	1.39808	0.91542
C	-9.45549	3.73762	1.29828
C	-11.38513	1.75996	0.89495
H	-9.74134	0.36385	0.77842
C	-10.79447	4.09825	1.27761
H	-8.68899	4.49296	1.45400
C	-12.60733	0.87006	0.69352
C	-11.75978	3.10661	1.07553
H	-11.07991	5.13885	1.41767
C	-13.72984	1.89850	0.78771
C	-13.21244	3.19485	1.00956
C	-15.09104	1.70095	0.68743
C	-14.06437	4.30008	1.13001
C	-15.96322	2.81152	0.81016
H	-15.51117	0.71192	0.51783
C	-15.43120	4.10634	1.03097
H	-13.66564	5.29790	1.29970
H	-16.11286	4.94849	1.12243
C	-7.68885	2.03817	1.14414
C	5.65660	0.49136	1.80741
C	-17.35809	2.63101	0.71594

C	6.86542	0.64225	1.92287
C	-18.56925	2.47610	0.63731
C	8.24742	0.81203	2.05662
C	8.80080	2.09020	2.34657
C	9.13439	-0.29024	1.90713
C	10.15463	2.25971	2.47554
H	8.13416	2.93743	2.48507
C	10.48822	-0.12970	2.04626
H	8.72804	-1.26805	1.66181
C	11.03876	1.15214	2.33321
H	10.55277	3.23776	2.72644
H	11.14852	-0.97844	1.89932
C	-19.95469	2.30144	0.55078
C	-20.51547	1.01204	0.33496
C	-20.83726	3.40981	0.67824
C	-21.87223	0.83942	0.24539
H	-19.85464	0.15250	0.25827
C	-22.19543	3.24178	0.60366
H	-20.42212	4.40428	0.81983
C	-22.75259	1.95028	0.38163
H	-22.28034	-0.15703	0.10904
H	-22.84934	4.10510	0.67537
N	12.39257	1.31616	2.47028

N	-24.11080	1.77994	0.30109
C	13.23660	0.22864	2.84550
C	14.40420	-0.02353	2.11634
C	12.91017	-0.55993	3.95581
C	15.23403	-1.07206	2.48906
H	14.65092	0.59071	1.25430
C	13.74606	-1.60524	4.32141
H	12.01813	-0.34148	4.53748
C	14.90976	-1.86988	3.59242
H	16.13501	-1.27938	1.91942
H	13.51185	-2.22182	5.18525
C	13.01226	2.58172	2.24550
C	13.91323	3.08750	3.18936
C	12.73993	3.29536	1.07187
C	14.52785	4.31181	2.96508
H	14.11853	2.52980	4.09937
C	13.35991	4.51766	0.85564
H	12.06219	2.88428	0.32794
C	14.25431	5.03471	1.79817
H	15.21869	4.71454	3.69978
H	13.16621	5.08066	-0.05361
C	-25.00897	2.69194	0.93068
C	-26.09177	3.20650	0.20759

C	-24.82113	3.04448	2.27245
C	-26.97079	4.08291	0.82589
H	-26.23100	2.93084	-0.83445
C	-25.70748	3.92166	2.88372
H	-23.99619	2.61818	2.83767
C	-26.78560	4.44756	2.16422
H	-27.80960	4.50170	0.27617
H	-25.57088	4.19133	3.92673
C	-24.67881	0.68565	-0.41591
C	-25.68538	-0.08333	0.17948
C	-24.25022	0.40514	-1.71944
C	-26.25002	-1.13899	-0.52296
H	-26.01194	0.13802	1.19220
C	-24.82082	-0.65168	-2.41400
H	-23.49003	1.02412	-2.18926
C	-25.82063	-1.43058	-1.82287
H	-27.02312	-1.74583	-0.06114
H	-24.50609	-0.87779	-3.42939
C	15.77321	-3.00715	4.03282
C	14.89356	6.35478	1.51229
C	-26.40063	-2.55448	-2.61877
C	-27.76492	5.39452	2.77840
O	-26.04573	-2.83472	-3.73607

O	-27.35007	-3.21083	-1.96110
O	-27.48535	5.66792	4.04814
O	-28.70554	5.86037	2.18605
O	15.72570	6.73960	2.47370
O	14.67746	7.00042	0.51766
O	16.85385	-3.15332	3.27410
O	15.51709	-3.71478	4.97437
C	0.86068	2.91265	3.15735
H	1.77226	3.49514	3.34088
H	0.00530	3.59580	3.23108
C	1.04319	3.33568	0.67249
H	1.95953	3.92085	0.82058
H	0.19288	4.02801	0.70929
C	-12.58388	0.19017	-0.68830
H	-11.72923	-0.49357	-0.76492
H	-13.49808	-0.39605	-0.84502
C	-12.72234	-0.18799	1.80663
H	-13.64083	-0.77598	1.68540
H	-11.87257	-0.88085	1.76728
C	16.38930	7.98970	2.29804
H	15.66066	8.80395	2.22067
H	17.01764	8.12661	3.18029
H	17.00502	7.97363	1.39221

C	17.74703	-4.21282	3.61121
H	17.23602	-5.17985	3.55116
H	18.55953	-4.16829	2.88334
H	18.13793	-4.07730	4.62548
C	-28.36128	6.56438	4.72867
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H	-27.97169	6.65723	5.74432
H	-28.36995	7.54191	4.23445
C	-27.97084	-4.30436	-2.63403
H	-27.22994	-5.07068	-2.88636
H	-28.71097	-4.70737	-1.93998
H	-28.45883	-3.96242	-3.55317
H	0.76805	2.15867	3.94819
H	-12.50608	0.92990	-1.49405
H	-12.74029	0.27894	2.79868
H	1.07864	2.88668	-0.32733

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