Supporting Information

For

Organocatalyzed Atom Transfer Radical Polymerization Using *N*-Aryl Phenoxazines as Photoredox Catalysts

Ryan M. Pearson,[a] Chern-Hooi Lim,[a] Blaine G. McCarthy, [a] Charles B. Musgrave,[a,b,c] Garret M. Miyake[a,c]

[a]Department of Chemistry and Biochemistry, [b]Department of Chemical and Biological Engineering. [c]Materials Science and Engineering Program, University of Colorado Boulder, Boulder, Colorado 80309, USA.

*Corresponding author, E-mail: garret.miyake@colorado.edu

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1. Materials and Methods

Phenoxazine was purchased from Beantown Chemical. 4-biphenyl boronic acid was purchased from TCI America. Glacial acetic acid was purchased from VWR. All other reagents were purchased from Sigma-Aldrich. Chemicals used in polymerizations, including isobutyl methacrylate (BMA), benzyl methacrylate (BnMA), isodecyl methacrylate (IDMA), methyl methacrylate (MMA), diethyl 2-bromo-2-methyl malonate (DBMM), dimethylacetamide (DMA) were purified by vacuum distillation followed by three freeze-pump-thaw cycles and stored under nitrogen atmosphere. Dioxane was purified using an mBraun MB-SPS-800 solvent purification system and kept under nitrogen atmosphere. Dicyclohexylphosphino-2,6-diisopropoxybiphenyl (RuPhos) and chloro-(2-dicyclohexylphosphino-2,6-diisopropoxy-1,1-biphenyl) [2-(2-aminoethyl)phenyl] palladium(II) - methyl-t-butyl ether adduct (RuPhos precatalyst) were stored under nitrogen atmosphere and used as received. Aryl halides used in the catalyst synthesis were degassed and stored under nitrogen. A Vogue Professional Powerful & Double Wide 54 watt UV lamp Light Nail Dryer was used as the UV light source. One sixteen inch strip of double-density white LEDs, purchased from Creative Lighting Solutions (item no. CL-FRS1210-5M-12V-WH), was wrapped inside a 400 mL beaker and used as a visible light source.

Nuclear magnetic resonance spectra were recorded on a Varian 300 MHz NMR Spectrometer for polymerization conversions and using a Varian 400 MHz or Varian 500 MHz NMR Spectrometer for all other characterizations. All ^{1}H NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for residual chloroform (7.26 ppm) or benzene (7.15 ppm) in the deuterated solvent. All ^{13}C NMR spectra are reported in ppm relative to $CDCl_3$ (77.23 ppm) or C_6D_6 (128.62 ppm). Analysis of polymer molecular weights was performed via gel permeation chromatography (GPC) coupled with multi-angle light scattering (MALS), using an Agilent HPLC fitted with one guard column, three PLgel 5 μm MIXED-C gel permeation columns, a Wyatt Technology TrEX differential refractometer, and a Wyatt Technology miniDAWN TREOS light scattering detector, using THF as the eluent at a flow rate of 1.0 mL/min. Ultraviolet-visible spectroscopy was performed on an Cary 5000 spectrophotometer using DMA as the solvent. Emission spectroscopy was performed on a SLM 8000C spectrofluorimeter using DMA as the solvent. Cyclic voltammetry was performed with a CH Instruments electrochemical analyzer with a $Ag/AgNO_3$ (0.01 M in MeCN) reference electrode using DMA as the solvent for the working electrode. Samples were sparged with argon for 5 minutes prior to both emission and electrochemical measurements.

2. Procedures

Synthesis of *N*-aryl phenoxazine catalysts:

10-Phenylphenoxazine (1)

A 50 mL storage flask was charged with a stir bar, flame dried under vacuum and back filled with nitrogen three times. The flask was then charged with phenoxazine (183 mg, 1.0 mmol, 1.00 eq.), NaO^{t}Bu (192.2 mg, 2.0 mmol, 2.00 eq.), and RuPhos (12 mg, 0.03 mmol, 0.03 eq.). The flask was taken into a nitrogen filled glovebox where RuPhos Precat (21mg, 0.03 mmol, 0.03 eq.), 1 mL dry dioxane and bromobenzene (0.11 mL, 2.0 mmol 2.00 eq.) were added. The flask was placed in an oil bath at 130º C while stirring for 48 hours. The flask was then cooled to room temperature, diluted with CH_2Cl_2, and the solution was washed with water three times, brine once, dried over $MgSO_4$ and purified by recrystallization from CH_2Cl_2 layered with hexanes at - 25º C to give 60 mg of yellow crystals, 23% yield. NMR matched that reported previously.[1]

4-Trifluoromethylphenyl -10-phenoxazine (2)

A 100 mL storage flask was charged with a stir bar, flame dried under vacuum and back filled with nitrogen three times. The flask was then charged with phenoxazine (800 mg, 4.37 mmol, 1.00 eq.), NaO^{t}Bu (840 mg, 8.74 mmol, 2.00 eq.), and RuPhos (52.4 mg, 0.13 mmol, 0.03 eq.). The flask was placed into a nitrogen filled glovebox where RuPhos Precat (91.77 mg, 0.13 mmol, 0.03 eq.), and 4 mL dry dioxane and 4-bromobenzotrifluoride (1.22 mL, 8.74 mmol, 2.00 eq.) were added. The flask was placed in an oil bath at 130º C while stirring for 48 hours. The flask was then cooled to room temperature, diluted with CH_2Cl_2, and the solution was washed with water three times, brine once, dried over $MgSO_4$ and purified by recrystallization from CH_2Cl_2 layered with hexanes on top at - 25º C to yield 987 mg of yellow crystals, 69% yield. Final purification was conducted via sublimation at 100 mTorr at 175º C. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.87 (d, *J* = 8.20 Hz, 2H), 7.51 (d, *J* = 8.15 Hz, 2H), 6.73 (dd, *J* = 7.85, 1.75 Hz, 2H), 6.68 (m, 2H), 6.62 (td, *J* = 7.85, 1.75 Hz, 2H), 5.90 (d, *J* = 8.20 Hz , 2H). ^{13}C NMR ($CDCl_3$, 400MHz) δ 144.10, 142.73, 133.89, 131.76, 130.97, 130.64, 128.44, 123.52, 122.09, 115.93, 113.39. ^{19}F NMR ($CDCl_3$, 300MHz) δ 62.55. HRMS (ESI): calculated for M+ $C_{19}H_{12}F_3NO$, 327.0871; observed 327.0869.

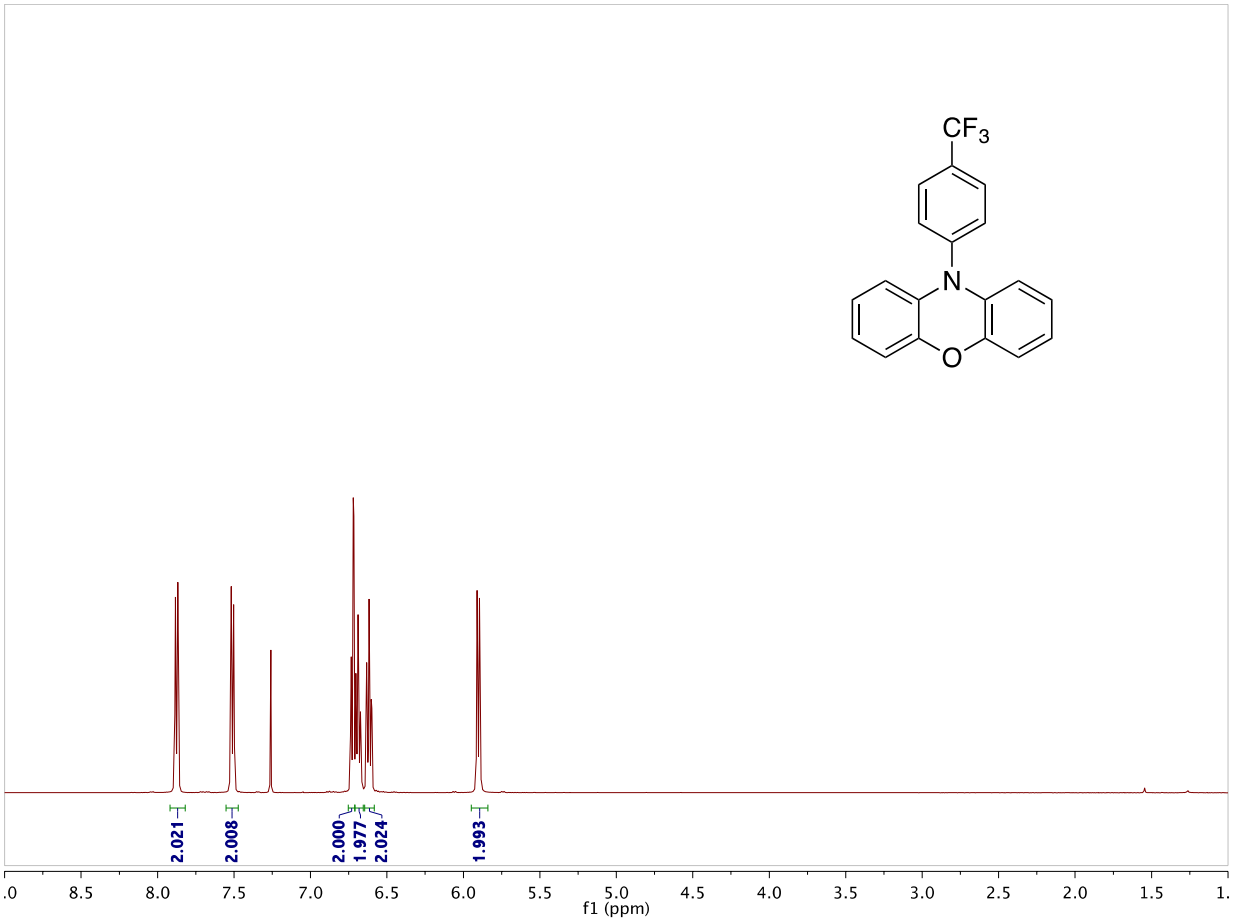


Figure S1. ^{1}H NMR of 4-Trifluoromethylphenyl-10-phenoxazine in $CDCl_3$.

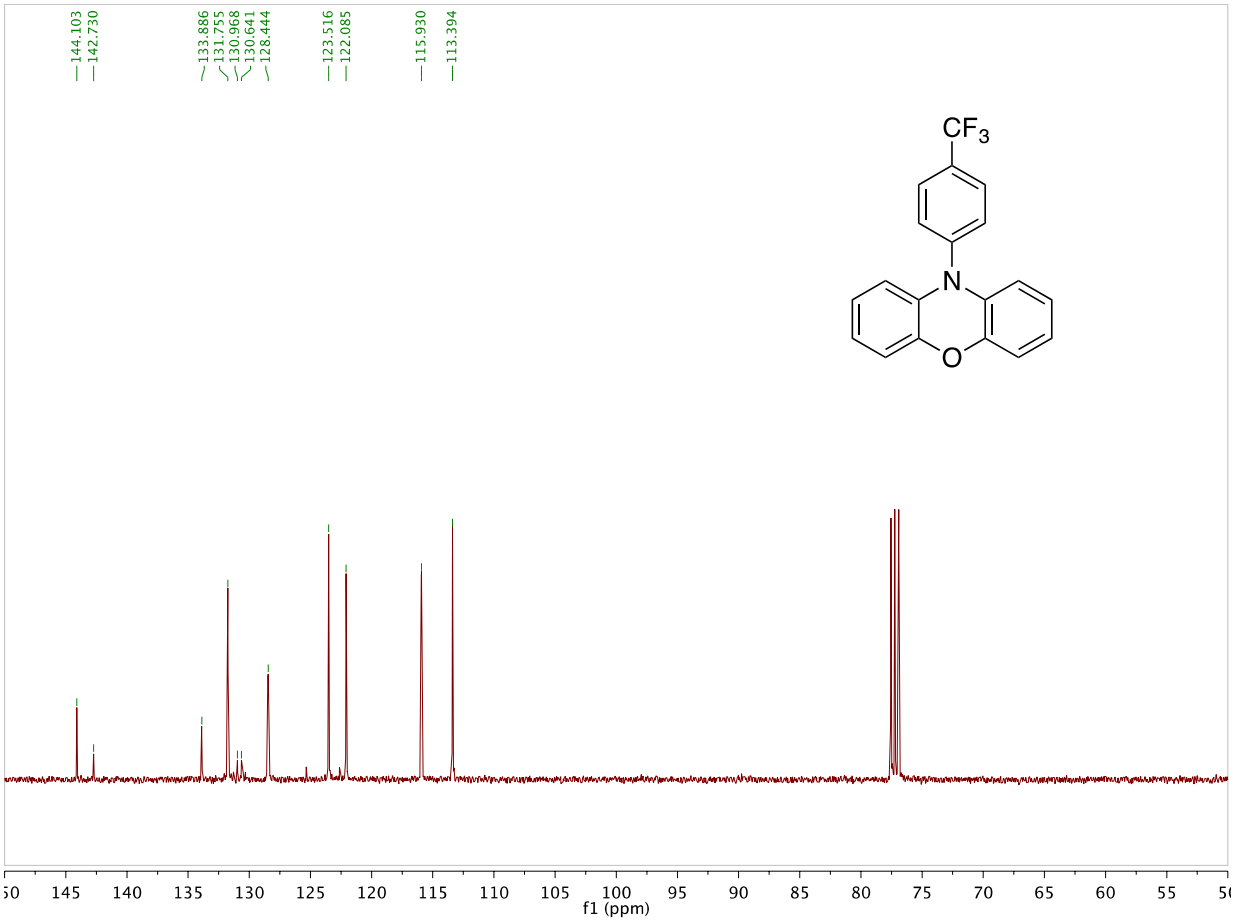


Figure S2. ^{13}C NMR of 4-Trifluoromethylphenyl-10-phenoxazine in $CDCl_3$.

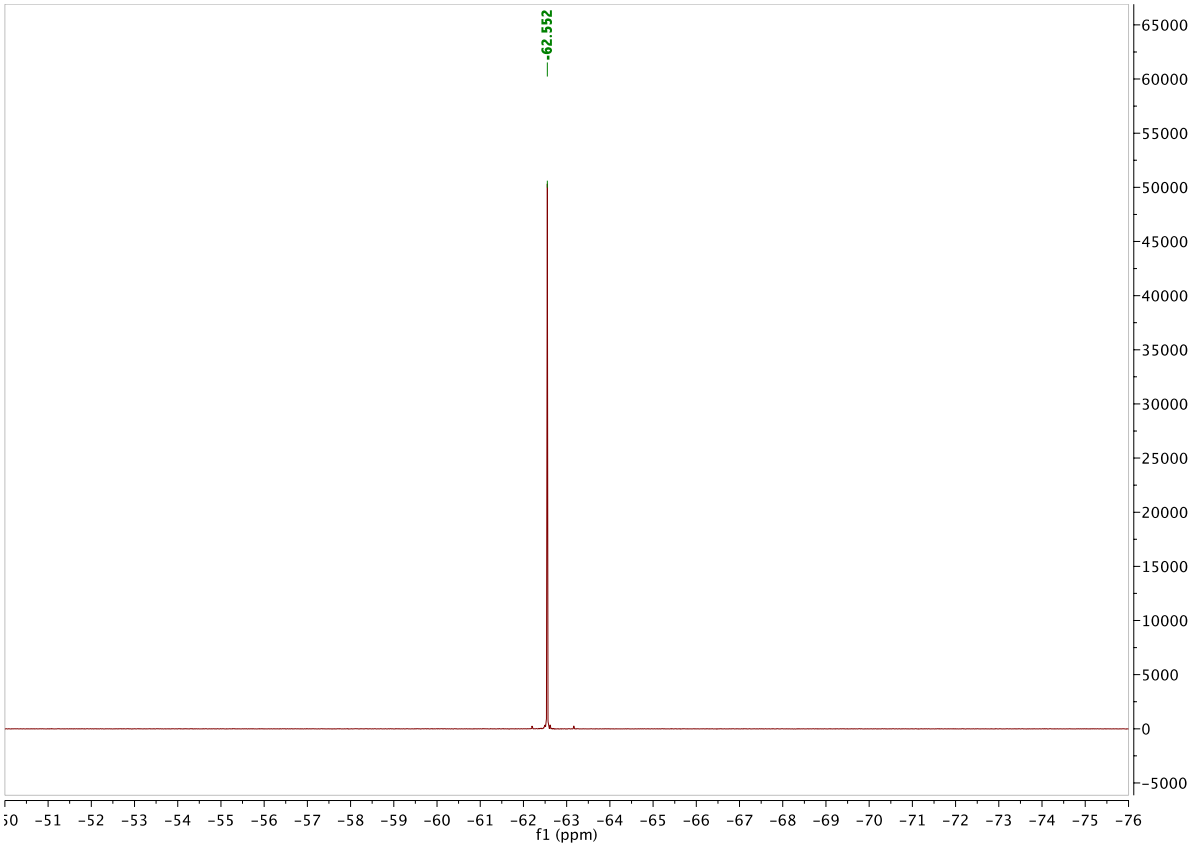


Figure S3. ^{19}F NMR of 4-Trifluoromethylphenyl-10-phenoxazine in $CDCl_3$.

1-Naphthalene-10-phenoxazine (3)

A stir bar was placed into a 100 mL storage flask, flame dried under vacuum and then back filled with nitrogen three times. The flask was then charged with phenoxazine (1.00 g, 5.46 mmol, 1.00 eq.), NaO^tBu (1.054 g, 10.92 mmol, 2.00 eq.), and RuPhos (65.6 mg, 0.16 mmol, 0.03 eq.). The flask was taken into a nitrogen filled glovebox where RuPhos Precat (114.75 mg, 0.16 mmol, 0.03 eq.), 6 mL dry dioxane and 1-bromonaphthalene (1.53 mL, 10.92 mmol, 2.00 eq.) were added. The flask was placed in an oil bath at 130º C while stirring for 48 hours. The flask was then cooled to room temperature, diluted with CH_2Cl_2, and the solution was washed with water three times, brine once, dried over $MgSO_4$ and purified by recrystallization from CH_2Cl_2 layered with hexanes on top at -25º C to yield 790 mg of yellow crystals, 47% yield. Final purification was conducted via sublimation at 100 mTorr at 190º C. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.08 (d, *J* = 8.35 Hz, 1H), 7.99 (dd, *J* = 8.20, 3.95 Hz, 2H), 7.66 (t, *J* = 7.25 Hz, 1H), 7.56 (m, 2H), 7.48 (m, 1H), 6.74 (dd, *J* = 7.90, 1.45 Hz, 2H), 6.63 (t, *J* = 7.85 Hz, 2H), 6.49 (td, *J* = 7.85, 1.45 Hz, 2H), 5.71 (dd, *J* = 7.90, 1.45 Hz, 2H). ^{13}C NMR ($CDCl_3$, 400MHz) δ 144.09, 135.77, 135.24, 134.48, 131.56, 129.35, 129.14, 128.95, 127.50, 127.07, 127.04, 123.57, 123.53, 121.47, 115.58, 113.57. HRMS (ESI): calculated for M+ $C_{22}H_{15}NO$, 309.1154; observed 309.1152.

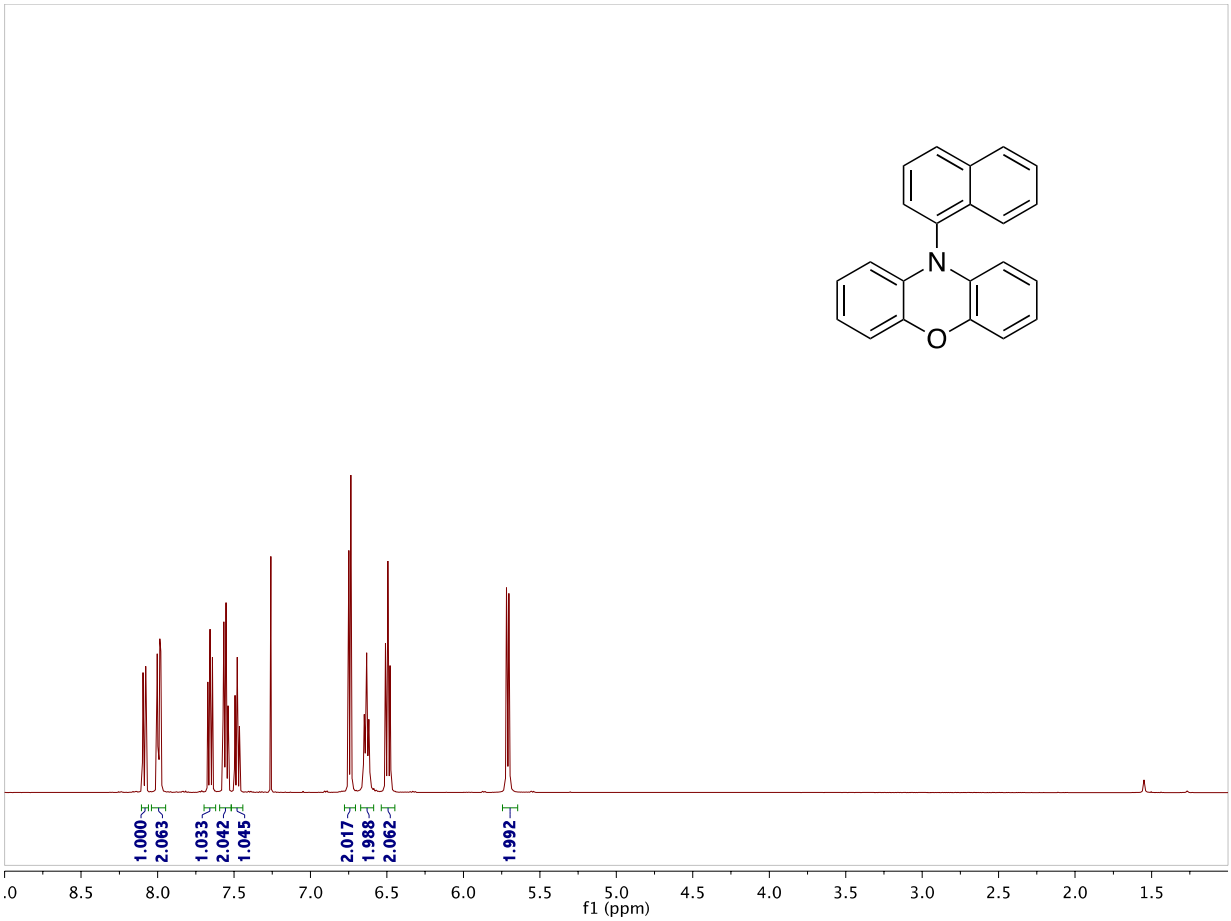


Figure S4. ^{1}H NMR of 1-Naphthalene-10-phenoxazine in $CDCl_3$.

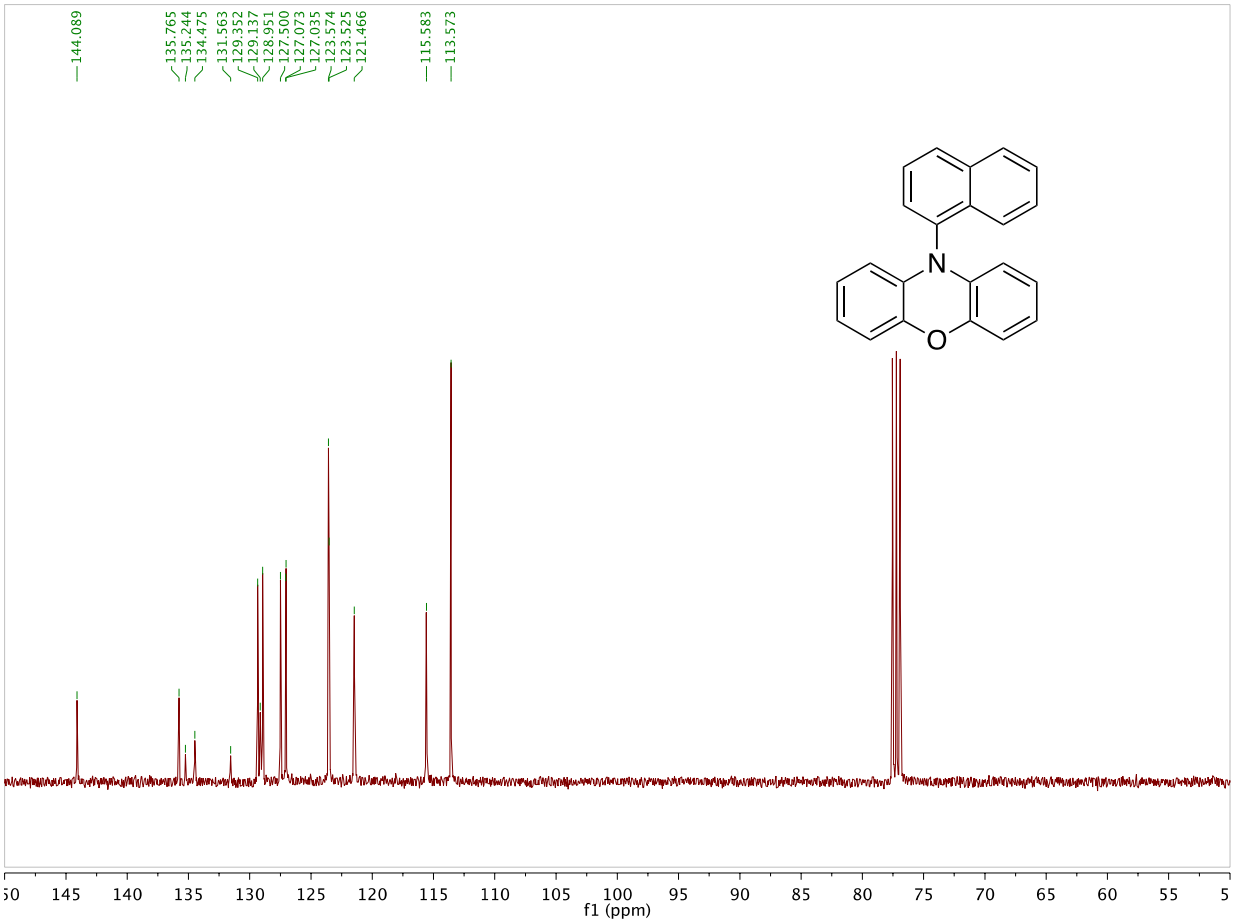


Figure S5. ^{13}C NMR of 1-Naphthalene-10-phenoxazine in $CDCl_3$.

2-Naphthalene-10-phenoxazine (4)

A 100 mL storage flask was charged with a stir bar, flame dried under vacuum then back filled with nitrogen three times. The flask was then charged with phenoxazine (1.00 g, 5.46 mmol, 1.00 eq.), NaO^tBu (1.054 g, 10.92 mmol, 2.00 eq.), and RuPhos (65.6 mg, 0.16 mmol, 0.03 eq.). The flask was taken into a nitrogen filled glovebox where RuPhos Precat (114.75 mg, 0.16 mmol, 0.03 eq.), 6mL dry dioxane and 2-bromonaphthalene (2.26 mg, 10.92 mmol, 2.00 eq.) were added. The flask was placed in an oil bath at 130º C while stirring for 48 hours. The flask was then cooled to room temperature, diluted with CH_2Cl_2, and the solution was washed with water three times, brine, dried over $MgSO_4$ and purified by recrystallization from CH_2Cl_2 at -25º C to yield 890 mg of light yellow, flakey crystals, 53% yield. Final purification was conducted via sublimation at 100 mTorr at 195º C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.08 (d, *J* = 8.60 Hz, 1H), 7.95 (d, *J* = 7.00 Hz, 1H), 7.88 (m, 2H), 7.57 (m, 2H), 7.42 (dd, *J* = 8.64, 2.04 Hz, 1H), 6.73 (dd, *J* = 7.84, 1.56 Hz, 2H), 6.66 (t, *J* = 7.52 ,2H), 6.57 (td, *J* = 8.12, 1.60 Hz, 2H), 5.99 (d, *J* = 7.96, 2H). ^{13}C NMR ($CDCl_3$, 400 MHz) δ 144.42, 136.74, 135.06, 134.78, 133.28, 131.55, 130.29, 128.23, 128.15, 127.12, 126.78, 123.49, 121.66, 115.74, 113.78. HRMS (ESI): calculated for M+ $C_{22}H_{15}NO$, 309.1154; observed 309.1151.

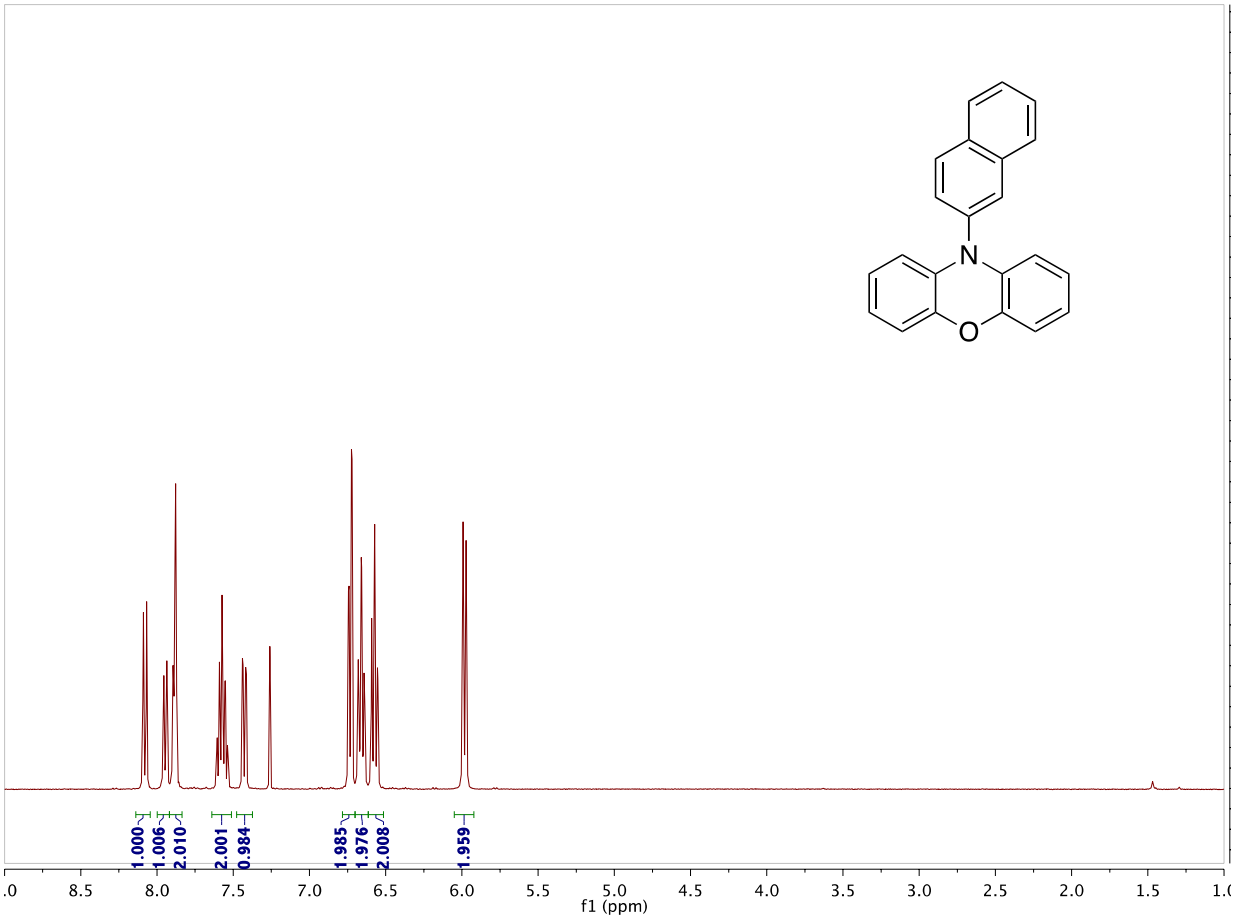


Figure S6. ^{1}H NMR of 2-Naphthalene-10-phenoxazine in $CDCl_3$.

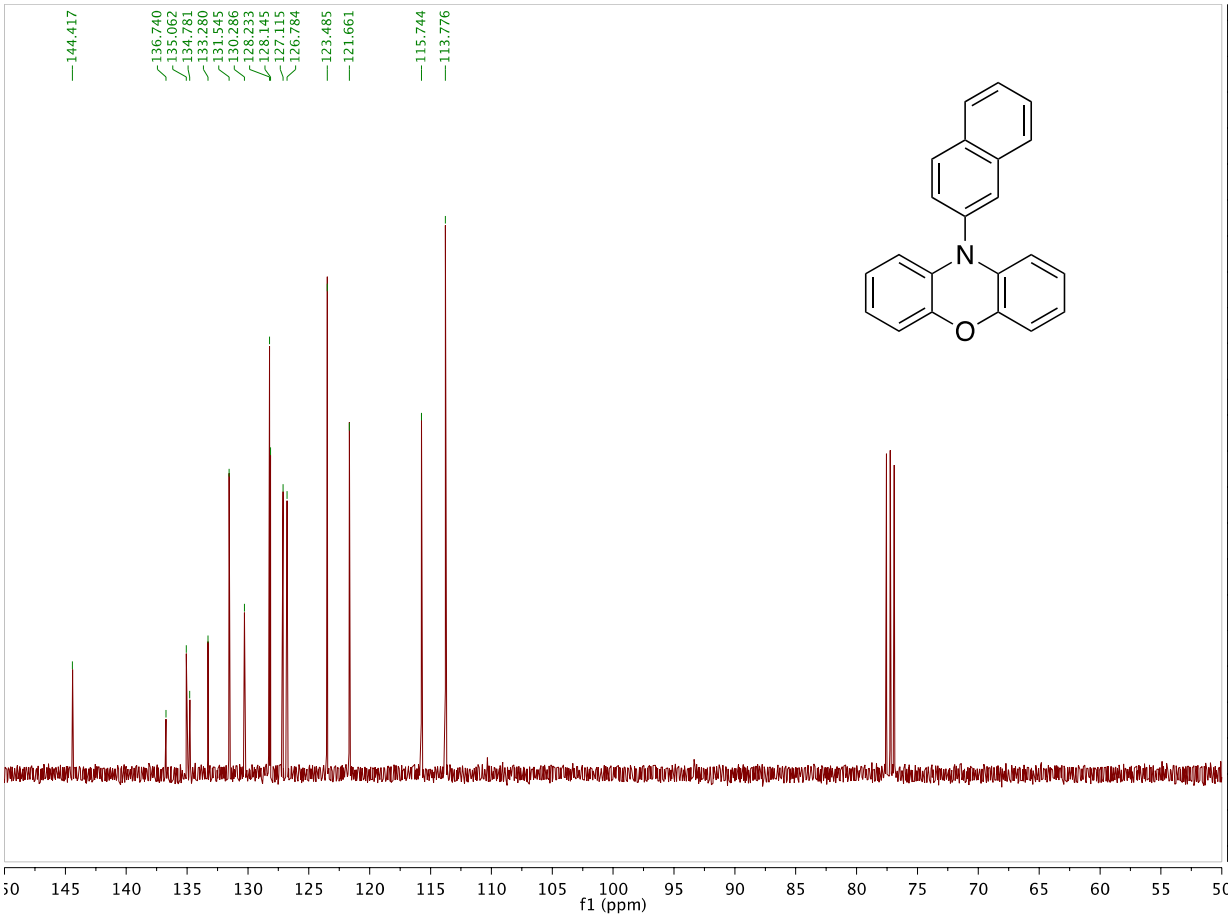


Figure S7. ^{13}C NMR of 2-Naphthalene-10-phenoxazine in $CDCl_3$.

1-Naphthalene-10-phenothiazine

A stir bar was placed in a 50 mL storage flask, flame dried under vacuum and then back filled with nitrogen three times. The flask was then charged with phenothiazine (0.600 g, 3.01 mmol, 1.00 eq.), NaO^tBu (0.578 g, 6.02 mmol, 2.00 eq.), and RuPhos (42.2 mg, 0.09 mmol, 0.03 eq.). The flask was taken into a nitrogen filled glovebox where RuPhos Precat (73.8 mg, 0.09 mmol, 0.03 eq.), 3 mL dry Dioxane and 1-bromonaphthalene (0.84 mg, 6.02 mmol, 2.00 eq.) were added. The flask was placed in an oil bath at 130º C while stirring for 48 hours. The flask was then cooled to room temperature, diluted with CH_2Cl_2, and the solution was washed with water three times, brine once, dried over $MgSO_4$ and purified by recrystallization from CH_2Cl_2 layered with hexanes on top at -25º C to yield 253 mg of a yellowish solid, 26% yield. Final purification was conducted via sublimation at 100 mTorr at 155º C. NMR matched that reported previously.[2]

3,7-Dibromo 1-Naphthalene-10-phenoxazine

A literature procedure was adapted for this synthesis.[3] 1-Naphthalane-10-phenoxazine (800 mg, 2.58 mmol, 1eq.) was dissolved in 80mL of chloroform. 80mL of glacial acetic acid was then added to the stirring mixture. Aluminum foil was thoroughly wrapped around to cover the reaction vial, blocking out light. In the dark, powdered N-Bromosuccinimide (944 mg, 5.30 mmol, 2.05 eq.) was added in small portions over a 20 minute period. After 2 hours at room temperature the reaction mixture was concentrated under vacuum. The resulting solid was washed three times with water, brine, then dried with $MgSO_4$. A light tan powder (1.0 g, 2.14 mmol, 82.8% yield) was collected. This was used for the Suzuki coupling without further purification. ^{1}H NMR (C_6D_6, 500 MHz) δ 7.82 (d, *J* = 8.48 Hz, 1H), 7.57 (dd, *J* = 25.02, 8.3 Hz, 2H), 7.19 (m, 1H), 7.12 (t, *J* = 8.03 Hz, 2H), 6.88 (dd, *J* = 7.32, 0.57 Hz, 3H), 6.84 (d, *J* = 2.19 Hz, 2H), 6.36 (dd, *J* = 8.54, 2.21 Hz, 2H). ^{13}C NMR ($CDCl_3$, 400MHz) δ144.27, 135.82, 134.22, 133.32, 130.91, 129.88, 129.15, 128.87, 127.83, 127.29, 127.06, 126.62, 123.02, 118.86, 114.74, 113.06.

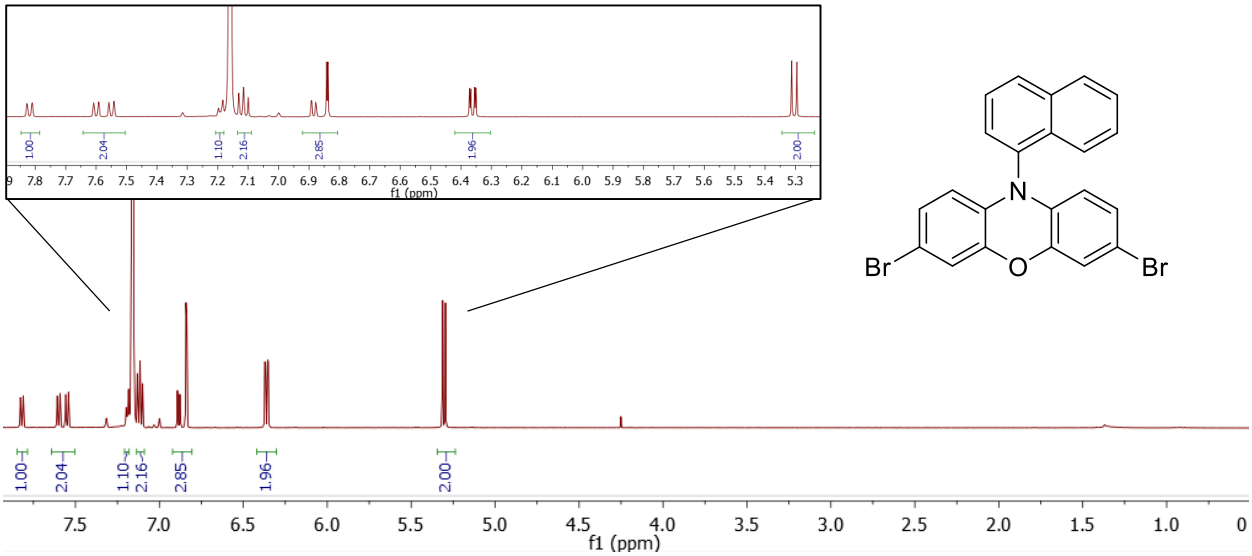


Figure S8. ^{1}H NMR of 3,7- Dibromo 1-Naphthalene-10-phenoxazine in C_6D_6.

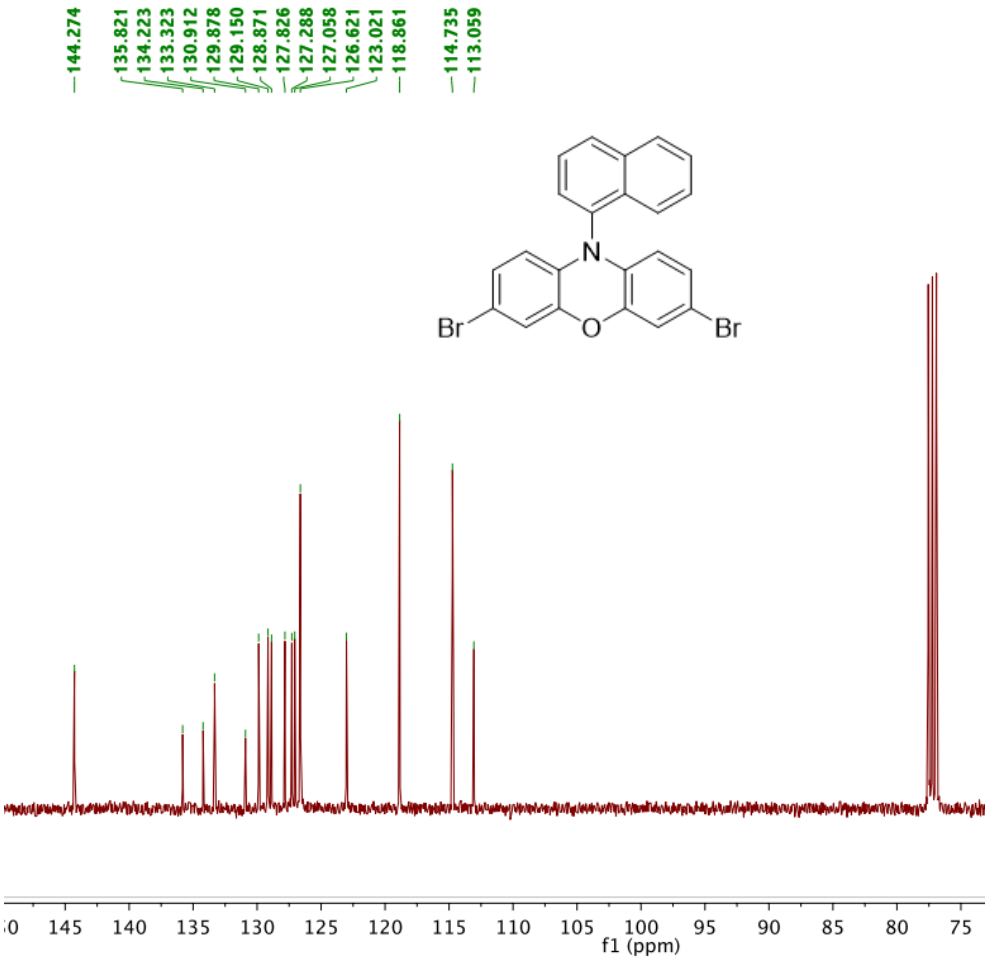


Figure S9. ^{13}C NMR of 3,7- Dibromo 1-Naphthalene-10-phenoxazine in $CDCl_3$.

3,7-Di(4-biphenyl) 1-Naphthalene-10-Phenoxazine (5)

A 200mL schlenk flask was flame dried, filled with nitrogen, and equipped with a stir bar and reflux condenser before 3,7-Dibromo 1-Naphthalene-10-phenoxazine (225 mg, 0.48 mmol, 1 eq.), 4-biphenylboronic acid (381.8 mg, 1.9 mmol, 4 eq.) was added, then dissolved in 20 mL of THF. 6 mL of K_2CO_3 (2M) was syringed into the solution and then heated to 80^{o}C and stirred for 20 minutes. After which, Palladium tetrakis(triphenylphosphine) (93 mg, 15% mol) in a 20mL solution of THF was added then heated to 100^{o}C and left to run for 24 hours. Once complete, the reaction was concentrated under vacuum, dissolved in DCM, and washed with water two times, brine, then dried with $MgSO_4$. A bright yellow powder was collected (270 mg, 0.44 mmol, 91.6% yield) after recrystallization in DCM/Methanol. ^{1}H NMR (C_6D_6, 500 MHz) δ 8.18 (d, *J* = 8.35 Hz, 1H), 7.69 (d, *J* = 8.09 Hz, 2H), 7.66 (dd, *J* = 7.21, 2.22 Hz, 2H), 7.51 (d, *J* = 7.21 Hz, 4H), 7.46 (m, 8H), 7.37 (d, *J* = 2.0 Hz, 2H), 7.25 (m, 8H), 6.73 (dd, *J* = 2.03 Hz, 2H), 5.88 (d, *J* = 8.28 Hz, 2H) . ^{13}C NMR (C_6D_6, 300 MHz) δ 144.49, 140.93, 139.74, 139.02, 135.69, 135.17, 134.49, 133.60, 131.47, 129.06, 128.82, 128.72, 127.52, 127.08, 126.95, 126.86, 126.76, 126.56, 123.38, 122.05, 114.23, 113.98.

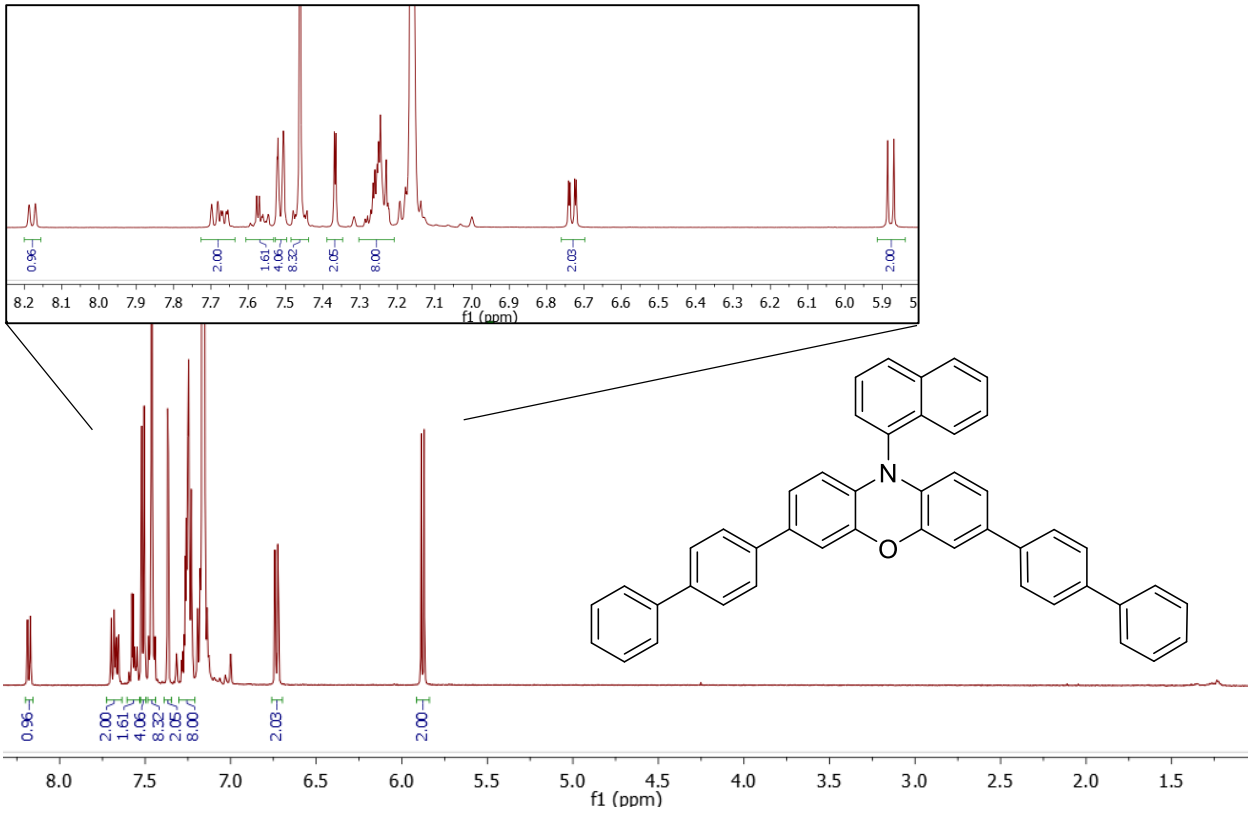


Figure S10. ^{1}H NMR of 3,7- Dibromo 1-Naphthalene-10-phenoxazine in C_6D_6.

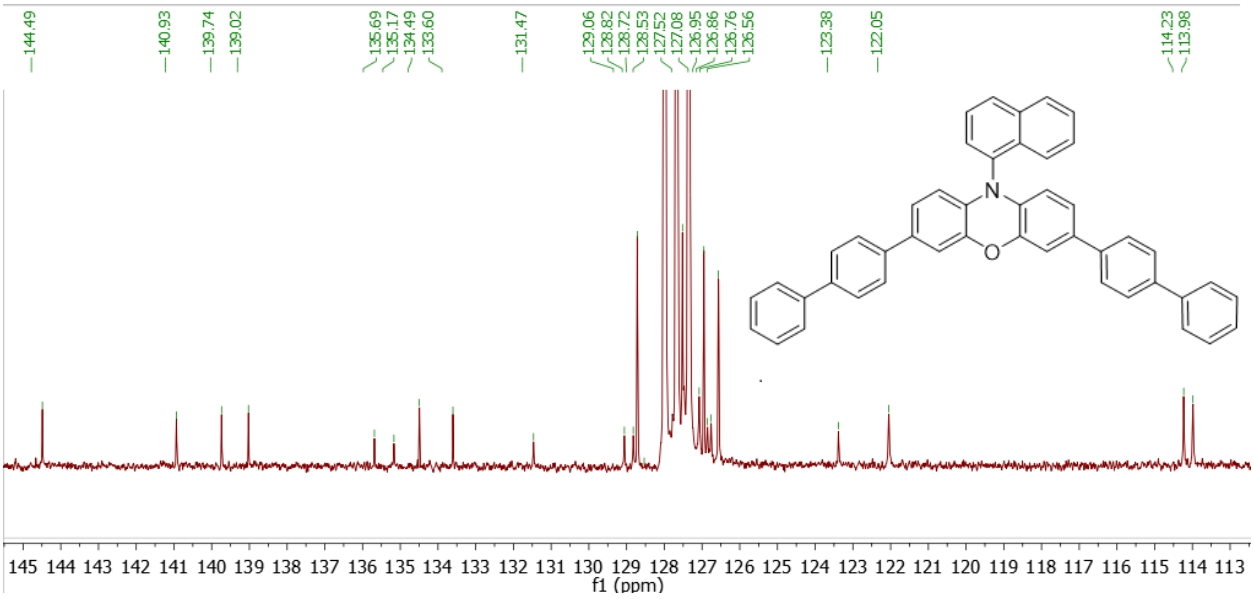


Figure S11. ^{13}C NMR of 3,7- Dibromo 1-Naphthalene-10-phenoxazine in C_6D_6.

Control experiments

Control polymerizations revealed negligible or no polymerization in the absence of any of the components pertinent to the O-ATRP system (light, PC, or initiator) or in the presence of oxygen.

General procedure for O-ATRP of MMA using a UV light source

A 20 mL scintillation vial equipped with a small stirbar was transferred into a nitrogen-atmosphere glove box. To this vial DMA, methyl methacrylate (MMA), photocatalyst from a stock solution in DMA and initiator were added in that order via pipette. The vial was tightly sealed and wrapped in aluminum foil. The vial was transferred out of the glove box, the aluminum foil was removed, then placed under UV irradiation while stirring (Figure S12). Timing of the polymerization started once the vial was placed under irradiation. To analyze the progress of the polymerization at a given time point, aluminum foil was wrapped around the vial, the timer was stopped and the sample was taken back into the glove box where a 0.1 mL aliquot of the reaction was removed via syringe and injected into a vial containing 0.7 mL $CDCl_3$ with 250 ppm butylated hydroxytoluene (BHT) to quench the reaction. The reaction vessel was then transferred back under UV irradiation where the timer was once again started. This aliquot was then analyzed via NMR for conversion. After NMR, the volatiles were removed from the sample, re-dissolved in THF and passed through a syringe filter for analysis by gel permeation chromatography coupled with multi-angle light scattering.

Figure S12. Photograph of the reaction setup for O-ATRP using UV irradiation.

Monomer scope

The polymerization of different monomers - BMA, BnMA and DMA - were carried out using the general polymerization conditions described above. A ratio of [1000]:[10]:[1], [monomer]:[initiator]:[catalyst] was used with 9.35 mmol of monomer used in each trial. An equal volume of DMA to monomer was used. After the polymerization was allowed to run for 8 hours an aliquot was taken for analysis of monomer conversion by ^{1}H NMR, after which, methanol was immediately added to the reaction mixture to precipitate out the polymer. The resulting solid polymer was filtered then dried and used for analysis by gel permeation chromatography coupled with multi-angle light scattering. The results from these polymerizations are given in Table S2.

General procedure for chain extension of poly methyl methacrylate with various monomers by photocatalyzed O-ATRP

Synthesis of PMMA Macroinitiator

Catalyst **3** (23.2 mg, .0748 mmol, 8 eq.) was dissolved in 8.00 mL DMA and stirred with MMA (8.00 mL, 74.8 mmol, 1000 eq.), and DBMM (143 µL, 0.748 mmol, 10 eq.) in a 20 mL scintillation vial in a nitrogen-filled glove box. The reaction mixture was then wrapped in aluminum foil, removed from the glove box and placed into the aforementioned UV apparatus. The reaction ran for 4 hours before the reaction media was poured into 800 mL of stirring room temperature methanol. The resulting polymer was stirred for an hour before being dissolved in a minimal amount of dichloromethane. The polymer was dissolved with dichloromethane and re-precipitated into stirring methanol a total of three times to remove unreacted monomer, initiator or catalyst (M_n = 8.83 kDa, M_w = 9.85 kDa, $Đ$ = 1.12).

Synthesis of Block Copolymers from isolated macroinitiator

Block copolymers were synthesized using a ratio of [1500]:[10]:[1], [monomer]:[initiator]:[catalyst] using 0.100 g of macroinitiator in each trial, and catalyst **3**. Each reaction was set up using the same method as the general polymerization procedure described above. The polymerizations were all run for 10 hours before the reaction media was poured into 100 mL of stirring, room temperature methanol. The resulting polymers were collected via vacuum filtration and dried under vacuum. The results from these polymerizations are given in Table S3.

General procedure for O-ATRP of MMA using a visible light source

A 20 mL scintillation vial equipped with a small stirbar was transferred into a nitrogen-atmosphere glove box. To this vial DMA, methyl methacrylate (MMA), photocatalyst from a stock solution in DMA and initiator were added in that order via pipette. Timing of the polymerization started once the vial was placed into an LED-lined beaker (Figure S13). To analyze the progress of the polymerization at a given time point, a 0.1 mL aliquot of the reaction was removed via syringe and injected into a vial containing 0.7 mL $CDCl_3$ with 250 ppm butylated hydroxytoluene (BHT) to quench the reaction. This aliquot was then analyzed via NMR for conversion. After NMR, the volatiles were removed from the sample, re-dissolved in THF and passed through a syringe filter for analysis by gel permeation chromatography coupled with multi-angle light scattering.

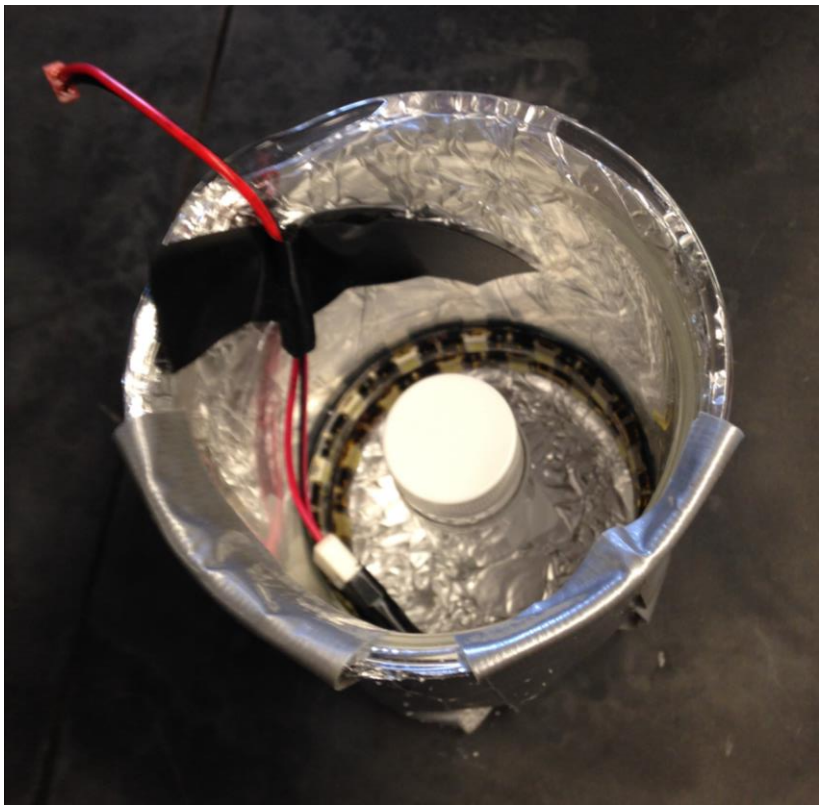


Figure S13. Photograph of the reaction setup for O-ATRP using visible light LED beakers.

3. Characterization of Catalysts' Photoredox Properties

UV-vis absorption spectroscopy

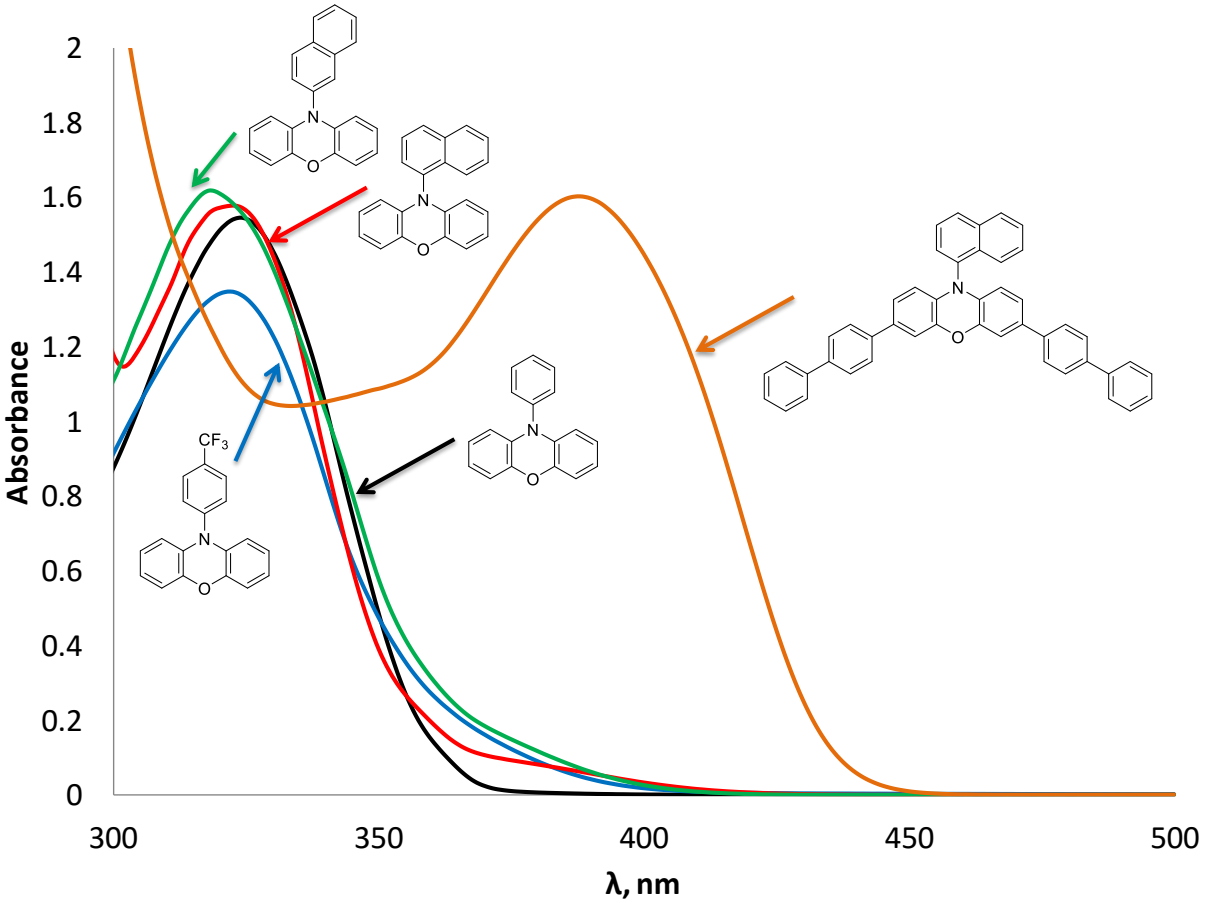


Figure S14. UV-vis absorption spectrums of the phenoxazine photocatalysts. PC **1**-**4** were taken at 0.20 mM and PC **5** was taken at 0.06mM. Solvent = DMA. Path length = 1cm.

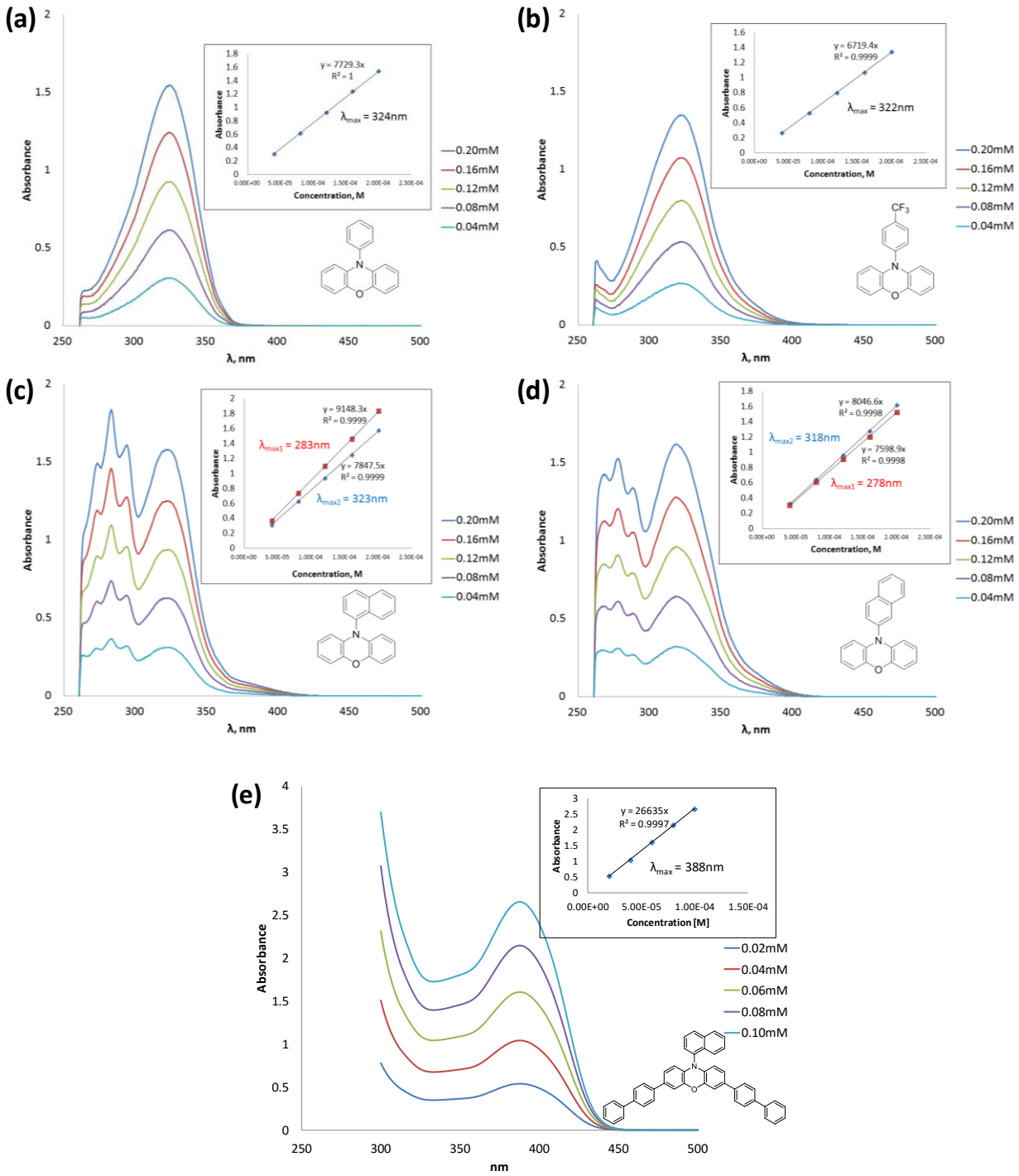


Figure S15. UV-vis absorption of the phenoxazine catalysts taken at different concentrations in DMA. Path length = 1cm.

Fluorescence spectroscopy

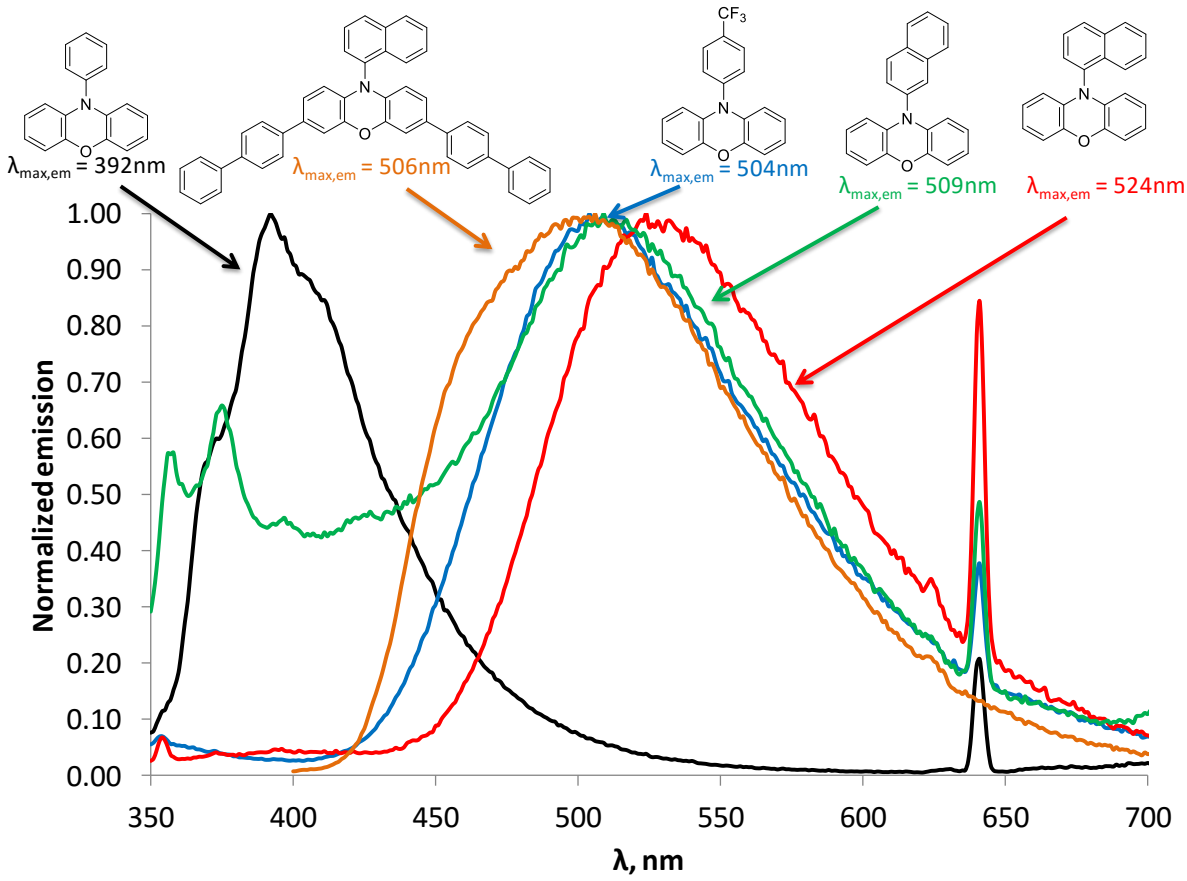


Figure S16. Plot of the normalized emission spectrums of the phenoxazine photocatalysts in DMA. PC **1**-**4** were irradiated with 320 nm light while PC **5** was irradiated with 380nm light.

Cyclic voltammetry

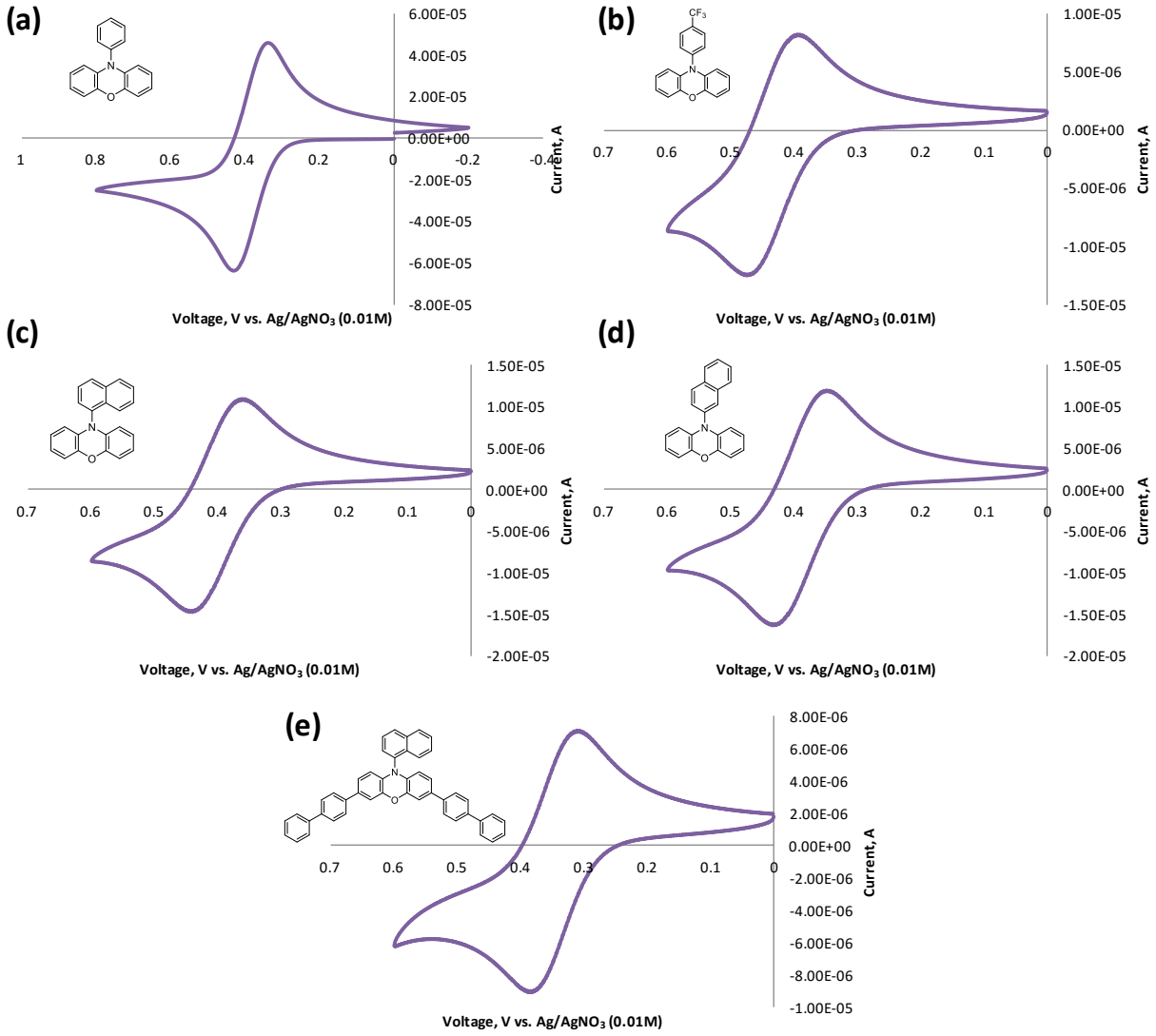


Figure S17. Cyclic voltammograms of the phenoxazine photocatalysts performed in a 3-compartment electrochemical cell. Reference electrode: $Ag/AgNO_3$ (0.01M) in MeCN; electrolyte: 0.1 M NBu_4PF_6; scan rate: 0.10 V/s. DMA is used as the solvent in the working electrode compartment for (b)-(e) while MeCN is used as the solvent in (a). Platinum is used as both the working and counter electrodes.

Experimental and theoretical determination of excited state reduction potentials

Table S1. Calculation of excited state reduction potentials of photocatalysts **1-5**.

PC	abs λ_{max} (nm)[a]	$\varepsilon_{\lambda max}$ ($M^{-1}cm^{-1}$)[b]	em λ_{max} (nm)[c]	E(em λ_{max}) (V vs. SCE)[d]	E(triplet), theo (V vs. SCE)[e]
1	324	7729	392	3.16	2.69
2	322	6719	504	2.46	2.63
3	323	7848	524	2.37	2.39
4	318	8047	509	2.44	2.45
5	388	26635	506	2.45	2.41

PC	$E_{1/2}$ ($PC^{\bullet+}$/PC) (V vs. SCE)[f]	E^0 ($PC^{\bullet+}$/PC), theo (V vs. SCE)[e]	E^{0*} ($PC^{\bullet+}$/PC*) (V vs. SCE)	E^{0*} ($PC^{\bullet+}/^3$PC*), theo (V vs. SCE)[e]
1	0.68	0.58	-2.48[g]	-2.11
2	0.73	0.59	-1.73	-2.03
3	0.70	0.55	-1.67	-1.84
4	0.69	0.55	-1.75	-1.90
5	0.65	0.48	-1.80	-1.93

[a]Maximum absorption wavelength; PC 3 and 4 exhibit another λ_{max} at higher energy wavelengths of 283 nm and 278 nm, respectively. [b]Molar absorptivity at the reported λ_{max}. [c]Maximum emission wavelength when irradiated with 320 nm light (PC **1**-**4**) and 380 nm light (PC **5**). [d]Energy of emitted photons. [e]Theoretical predictions from DFT calculations at uM06/6-311+Gdp/CPCM-H_2O//uM06/6-31+Gdp/CPCM-H_2O level of theory. [f]Obtained from cyclic voltammetry. [g]The E^{0*} of PC **1** is significantly more negative than PC **2**-**5** and deviates from the predicted trend. In the DFT calculations, the triplet excited state was explicitly assumed while the observed emission is likely fluorescence from the relaxed singlet excited state.

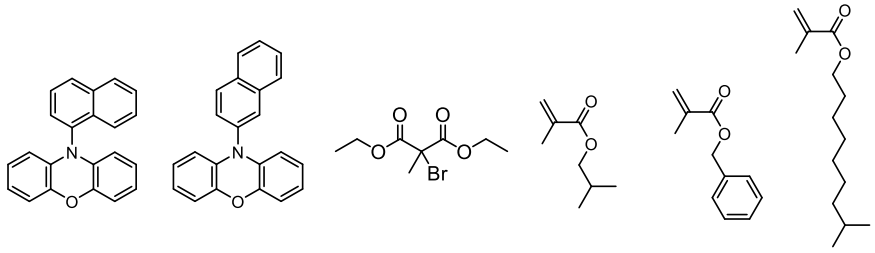
4. Computational Details

Standard reduction potentials (E^0) were calculated following previously reported procedures.[4,5,6,7] A value of -100.5 kcal/mol was assumed for the reduction free energy of the standard hydrogen electrode (SHE) as described in Ref. 4. Thus, $E^0 = (-100.5 - \Delta G_{red})/23.06$ (V vs. SHE); for E^0 ($PC^{\bullet+}/{}^3PC^*$), $\Delta G_{red} = G({}^3PC^*) - G(PC^{\bullet+})$ while for E^0 ($PC^{\bullet+}/PC$), $\Delta G_{red} = G(PC) - G(PC^{\bullet+})$. The Gibbs free energies of ${}^3PC^*$, $PC^{\bullet+}$, and PC (for PC 1-4) were calculated at the unrestricted M06/6-311+G** level of theory in CPCM-H_2O solvent (single point energy) using geometries optimized at unrestricted M06/6-31+G** level of theory in CPCM-H_2O solvent. The triple zeta basis set (6-311+G**) generally improves the E^0 ($PC^{\bullet+}/PC$) by ~0.1V relative to 6-31+G**, while the triplet energy is invariant for these two basis sets. To reference to the Saturated Calomel Electrode (SCE), E^0 (vs. SHE) is converted to E^0 (vs. SCE) using E^0 (vs. SCE) = E^0 (vs. SHE) - 0.24 V. Triplet energies (in eV) of PCs were obtained by [$G({}^3PC^*)$ - G(PC), in kcal/mol]/23.06. Population analysis was performed using electrostatic potential-derived charges with the CHELPG method[8] performed at the unrestricted M06/6-31G** level of theory in CPCM-H_2O solvent.

Geometry optimization of PC **5** (3,7-Di(4-biphenyl) 1-Naphthalene- 10-Phenoxazine) was performed at the unrestricted M06/Lanl2dz level of theory in CPCM-H_2O solvent; the smaller Lanl2dz basis sets was employed for computational efficiency due to its extensive structure. Singlet point calculation at the converged M06/Lanl2dz geometry was then performed at the unrestricted M06/6-311+G** level of theory in CPCM-H_2O solvent.

5. Supplemental Polymerization Data

Table S2. Polymerization Results of O-ATRP of Methacrylates.[a]



PC	Monomer	Time (h)	Conv (%)	M_n (kDa)	M_w (kDa)	$Đ$ (M_w/M_n)	I^* (%)
3	BMA	8	62.0	13.5	16.4	1.22	67.4
3	BnMA	8	46.1	8.2	11.6	1.41	102
3	DMA	8	87.5	20.9	28.3	1.35	42.9
4	BMA	8	62	15.2	17.3	1.14	59.7
4	BnMA	8	77.1	12.5	16.0	1.28	110
4	IDMA	8	83.2	21.7	28.4	1.31	39.6

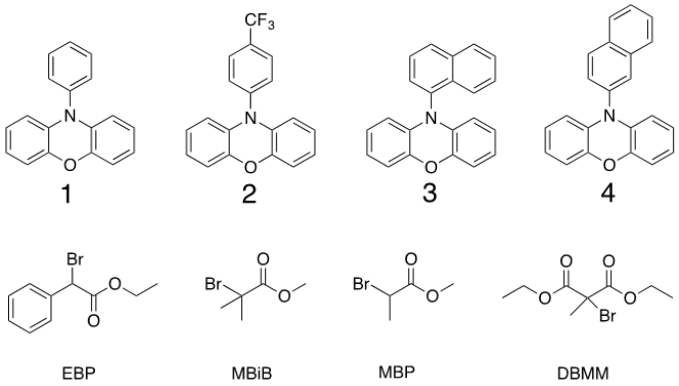
[a]Polymerizations of vinyl monomers were performed at [1000]:[10]:[1] using DBMM as the initiator and the same volume of solvent as that of the monomer added.

Table S3. Polymerization Results of O-ATRP PMMA chain extensions.[a]

PC	Monomer A	Monomer B	Time (h)	M_n(kDa)	M_w(kDa)	$Đ$ (M_w/M_n)
3	MMA	MMA	10	38.8	49.4	1.27
3	MMA	BMA	10	38.8	43.8	1.13
3	MMA	IDMA	10	59.8	77.6	1.29
3	MMA	BnMA	10	46.8	67.1	1.43

[a]Polymerization chain extensions were performed at [1500]:[10]:[1] using a PMMA macroinitiator and the same volume of solvent as that of the monomer added.

Table S4. Polymerization Results of O-ATRP initiator screen for PC **1**-**4**.[a]



PC	Initiator	Time (h)	Conv (%)	M_n(kDa)	M_w(kDa)	Đ (M_w/M_n)	I^* (%)
1	EBP	8	92.2	8.01	14.3	1.79	119
1	DBMM	8	95.6	7.16	10.6	1.48	137
2	EBP	8	61.2	15.4	20.7	1.34	41.2
2	DBMM	8	55.3	6.54	9.48	1.45	85.5
3	EBP	8	66.4	9.29	12.6	1.36	74.2
3	MBiB	8	76.5	9.58	11.8	1.23	81.8
3	MBP	8	70.7	10.9	14.1	1.29	66.4
3	DBMM	8	78.8	8.79	10.8	1.22	92.6
4	EBP	8	59.0	11.3	13.6	1.21	54.7
4	MBiB	8	69.2	11.3	15.0	1.34	63.3
4	MBP	8	31.7	5.80	6.87	1.19	57.6
4	DBMM	8	80.2	10.7	11.9	1.11	77.3

[a]Polymerizations were performed at [1000]:[10]:[1] for [MMA]:[Initiator]:[PC] using the same volume of DMA as that of the monomer added.

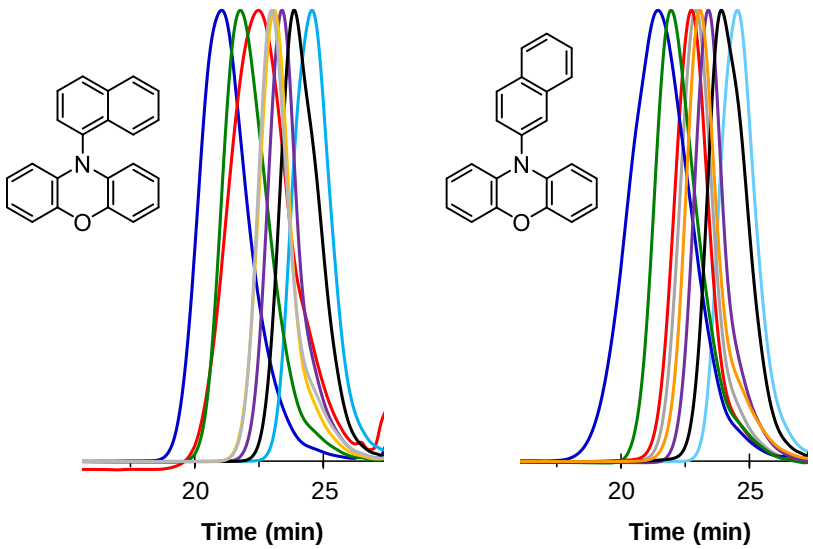


Figure S18. Gel permeation traces of PMMA produced using **3** (left) and **4** (right) reported in Table 2 of the Main Text. Color scheme corresponds to: (left plot) run 5 (light blue), run 6 (gray), run 7 (orange), run 8 (red), run 9 (green), run 10 (blue), run 11 (purple), rune 12 (black); (right plot) run 13 (light blue), run 14 (orange), runt 15 (gray), run 16 (red), run 17 (green), run 18 (blue), run 19 (purple), run 20 (black).

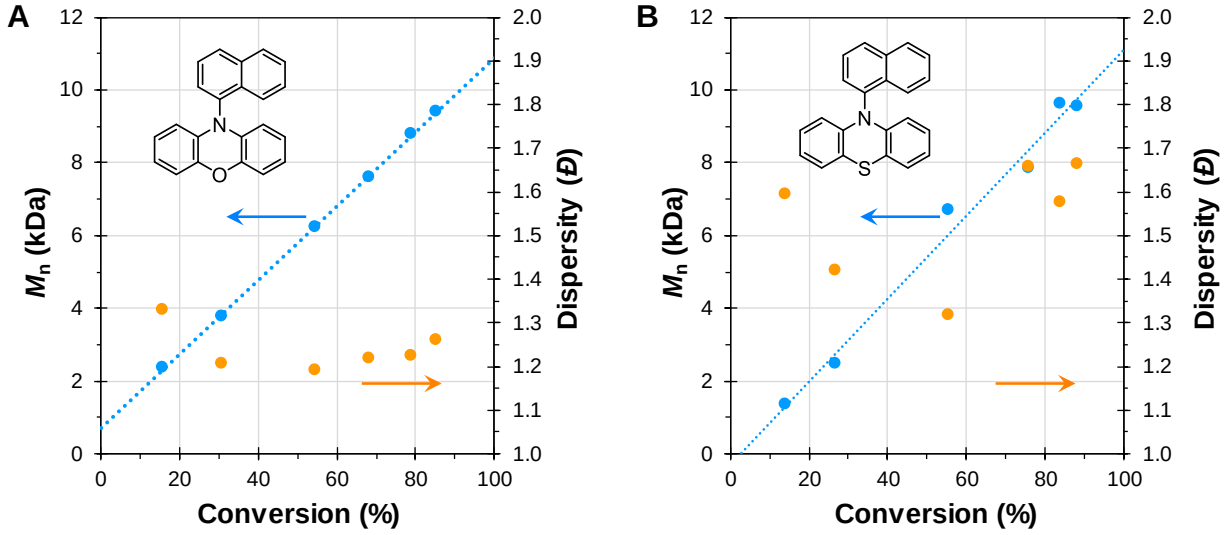


Figure S19. Plots of number average molecular weight (blue) and dispersity (orange) as a function of monomer conversion in the polymerization of methyl methacrylate catalyzed by 1-napthylene-10-phenoxazine (A) and 1-napthylene-10-phenothiazine (B). Conditions: [MMA]:[DBMM]:[PC] = [1000]:[10]:[1]; 9.35 µmoles PC, 1.00 mL dimethylacetamide, and irradiated with 365 nm light.

6. X-ray Crystallography Data

Structures were determined for the compounds listed in Table 1. Single crystals were coated with Paratone-N oil and mounted under a cold stream of dinitrogen gas. Single crystal X-ray diffraction data were acquired on a Bruker Kappa APEX II CCD diffractometer with Mo Kα radiation (λ = 0.71073 Å) and a graphite monochromator. Initial lattice parameters were obtained from a least-squares analysis of more than 100 reflections; these parameters were later refined against all data. None of the crystals showed significant decay during data collection. Data were integrated and corrected for Lorentz and polarization effects using Bruker APEX3 software, and semiempirical absorption corrections were applied using SCALE (Sheldrick, G. M. SADABS – a program for area detector absorption corrections). Space group assignments were based on systematic absences, E statistics, and successful refinement of the structures. Structures were solved using Direct Methods and were refined with the aid of successive Fourier difference maps against all data using the SHELXTL 6.14 software package (Sheldrick, G, M. SHELXTL, v. 6.12; Bruker AXS: Madison, WI, 1999). Thermal parameters for all non-hydrogen atoms were refined anisotropically. All hydrogen atoms were assigned to ideal positions and refined using a riding model with an isotropic thermal parameter 1.2 times that of the attached carbon atom (1.5 times for methyl hydrogens).

In the structure of ‘gm01’, there is a disordered solvate molecule that was found in Fourier difference maps. After numerous attempts to model the disorder failed, SQUEEZE (Spek, A. L. J. Appl. Crystallogr. 2003, 36, 7) was used to remove the remaining disordered components. According to the SQUEEZE output, approximately 4 dichloromethane solvent molecules are present in the void space and were removed. The chemical data presented for ‘gm01’ in Table 1-5 do not include the components removed by SQUEEZE.

1-Naphthalene-10-phenoxazine

Table 1. Crystal data and structure refinement for gm01.

Identification code	gm01	
Empirical formula	C22 H15 N O	
Formula weight	309.35	
Temperature	117(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.8713(6) Å	a= 83.142(4)°.
	b = 9.1631(6) Å	b= 78.687(4)°.
	c = 11.2812(9) Å	g = 71.594(4)°.
Volume	851.59(11) $Å^3$	
Z	2	
Density (calculated)	1.206 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	324	
Crystal size	0.374 x 0.132 x 0.097 mm^3	
Theta range for data collection	1.844 to 27.480°.	
Index ranges	-11<=h<=11, -11<=k<=11, -14<=l<=12	
Reflections collected	13754	
Independent reflections	3908 [R(int) = 0.0632]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7466 and 0.6543	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3908 / 0 / 217	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0569, wR2 = 0.1236	
R indices (all data)	R1 = 0.0976, wR2 = 0.1452	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.714 and -0.316 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for gm01. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	6593(2)	5936(2)	2786(2)	20(1)
O(1)	4626(2)	8354(2)	1482(2)	32(1)
C(1)	7016(3)	7296(2)	2431(2)	18(1)
C(2)	8383(3)	7524(3)	2705(2)	22(1)
C(3)	8730(3)	8902(3)	2356(2)	27(1)
C(4)	7728(3)	10074(3)	1732(2)	27(1)
C(5)	6359(3)	9864(2)	1445(2)	24(1)
C(6)	6018(3)	8490(2)	1783(2)	21(1)
C(7)	4389(3)	6910(2)	1653(2)	21(1)
C(8)	3127(3)	6743(3)	1192(2)	26(1)
C(9)	2788(3)	5348(3)	1372(2)	28(1)
C(10)	3740(3)	4122(3)	1995(2)	25(1)
C(11)	5026(3)	4285(2)	2450(2)	21(1)
C(12)	5354(3)	5691(2)	2301(2)	18(1)
C(13)	7645(3)	4684(2)	3414(2)	18(1)
C(14)	7385(3)	4571(2)	4651(2)	22(1)
C(15)	8427(3)	3356(3)	5281(2)	26(1)
C(16)	9680(3)	2286(3)	4653(2)	24(1)
C(17)	9978(3)	2366(2)	3362(2)	19(1)
C(18)	11261(3)	1279(2)	2679(2)	22(1)
C(19)	11520(3)	1396(2)	1442(2)	23(1)
C(20)	10497(3)	2618(2)	816(2)	22(1)
C(21)	9246(3)	3692(2)	1437(2)	19(1)
C(22)	8944(3)	3600(2)	2728(2)	17(1)

Table 3. Bond lengths [Å] and angles [°] for gm01.

N(1)-C(1)	1.404(3)
N(1)-C(12)	1.407(3)
N(1)-C(13)	1.442(3)
O(1)-C(6)	1.389(3)
O(1)-C(7)	1.390(3)
C(1)-C(2)	1.390(3)
C(1)-C(6)	1.403(3)
C(2)-C(3)	1.387(3)
C(3)-C(4)	1.379(3)
C(4)-C(5)	1.390(3)
C(5)-C(6)	1.379(3)
C(7)-C(8)	1.379(3)
C(7)-C(12)	1.400(3)
C(8)-C(9)	1.386(3)
C(9)-C(10)	1.383(3)
C(10)-C(11)	1.394(3)
C(11)-C(12)	1.392(3)
C(13)-C(14)	1.365(3)
C(13)-C(22)	1.422(3)
C(14)-C(15)	1.421(3)
C(15)-C(16)	1.366(3)
C(16)-C(17)	1.425(3)
C(17)-C(18)	1.416(3)
C(17)-C(22)	1.429(3)
C(18)-C(19)	1.366(3)
C(19)-C(20)	1.413(3)
C(20)-C(21)	1.365(3)
C(21)-C(22)	1.425(3)

C(1)-N(1)-C(12)	118.99(17)
C(1)-N(1)-C(13)	119.37(17)
C(12)-N(1)-C(13)	120.20(16)
C(6)-O(1)-C(7)	117.86(16)
C(2)-C(1)-C(6)	118.03(19)

C(2)-C(1)-N(1)	122.80(19)
C(6)-C(1)-N(1)	119.17(19)
C(3)-C(2)-C(1)	120.6(2)
C(4)-C(3)-C(2)	120.8(2)
C(3)-C(4)-C(5)	119.4(2)
C(6)-C(5)-C(4)	119.9(2)
C(5)-C(6)-O(1)	117.30(19)
C(5)-C(6)-C(1)	121.2(2)
O(1)-C(6)-C(1)	121.44(19)
C(8)-C(7)-O(1)	117.07(19)
C(8)-C(7)-C(12)	121.4(2)
O(1)-C(7)-C(12)	121.50(19)
C(7)-C(8)-C(9)	119.9(2)
C(10)-C(9)-C(8)	119.6(2)
C(9)-C(10)-C(11)	120.4(2)
C(12)-C(11)-C(10)	120.5(2)
C(11)-C(12)-C(7)	118.12(19)
C(11)-C(12)-N(1)	122.76(18)
C(7)-C(12)-N(1)	119.12(18)
C(14)-C(13)-C(22)	121.46(19)
C(14)-C(13)-N(1)	119.5(2)
C(22)-C(13)-N(1)	119.06(19)
C(13)-C(14)-C(15)	120.0(2)
C(16)-C(15)-C(14)	120.2(2)
C(15)-C(16)-C(17)	121.2(2)
C(18)-C(17)-C(16)	122.86(19)
C(18)-C(17)-C(22)	118.5(2)
C(16)-C(17)-C(22)	118.7(2)
C(19)-C(18)-C(17)	121.4(2)
C(18)-C(19)-C(20)	120.1(2)
C(21)-C(20)-C(19)	120.5(2)
C(20)-C(21)-C(22)	120.7(2)
C(13)-C(22)-C(21)	122.67(19)
C(13)-C(22)-C(17)	118.47(19)
C(21)-C(22)-C(17)	118.9(2)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for gm01. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	17(1)	17(1)	24(1)	2(1)	-8(1)	-3(1)
O(1)	22(1)	21(1)	53(1)	11(1)	-17(1)	-4(1)
C(1)	19(1)	19(1)	14(1)	-3(1)	1(1)	-4(1)
C(2)	24(1)	27(1)	17(1)	-1(1)	-6(1)	-8(1)
C(3)	30(2)	33(1)	23(1)	-2(1)	-5(1)	-16(1)
C(4)	35(2)	22(1)	25(1)	-3(1)	1(1)	-13(1)
C(5)	25(1)	18(1)	21(1)	0(1)	2(1)	0(1)
C(6)	16(1)	21(1)	23(1)	-3(1)	-1(1)	-3(1)
C(7)	19(1)	21(1)	22(1)	1(1)	-2(1)	-4(1)
C(8)	19(1)	32(1)	23(1)	6(1)	-8(1)	-5(1)
C(9)	22(1)	44(1)	23(1)	-2(1)	-8(1)	-13(1)
C(10)	27(1)	27(1)	25(1)	-3(1)	-3(1)	-11(1)
C(11)	20(1)	19(1)	21(1)	-1(1)	-5(1)	-3(1)
C(12)	15(1)	22(1)	15(1)	-2(1)	-2(1)	-3(1)
C(13)	16(1)	18(1)	22(1)	2(1)	-7(1)	-4(1)
C(14)	20(1)	24(1)	20(1)	-4(1)	-3(1)	-3(1)
C(15)	26(1)	35(1)	17(1)	1(1)	-6(1)	-8(1)
C(16)	22(1)	29(1)	21(1)	3(1)	-9(1)	-5(1)
C(17)	16(1)	20(1)	24(1)	2(1)	-8(1)	-6(1)
C(18)	19(1)	19(1)	28(1)	2(1)	-8(1)	-4(1)
C(19)	17(1)	23(1)	28(1)	-7(1)	-3(1)	-3(1)
C(20)	25(1)	24(1)	17(1)	-4(1)	-2(1)	-8(1)
C(21)	20(1)	20(1)	20(1)	2(1)	-7(1)	-6(1)
C(22)	16(1)	17(1)	21(1)	0(1)	-6(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for gm01.

	x	y	z	U(eq)
H(2)	9085	6729	3135	27
H(3)	9669	9040	2550	33
H(4)	7971	11017	1499	32
H(5)	5660	10666	1017	28
H(8)	2490	7584	752	31
H(9)	1907	5235	1069	34
H(10)	3515	3162	2113	30
H(11)	5682	3431	2865	25
H(14)	6506	5305	5090	26
H(15)	8253	3287	6141	31
H(16)	10363	1474	5084	29
H(18)	11955	450	3089	27
H(19)	12390	655	1001	28
H(20)	10682	2692	-45	26
H(21)	8569	4509	1005	23

1-Naphthalene-10-phenothiazine

Table 1. Crystal data and structure refinement for gm03.

Identification code	gm03	
Empirical formula	C22 H15 N S	
Formula weight	325.41	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 14.790(5) Å	a= 90°.
	b = 6.904(2) Å	b= 113.094(15)°.
	c = 17.265(6) Å	g = 90°.
Volume	1621.5(10) $Å^3$	
Z	4	
Density (calculated)	1.333 Mg/m^3	
Absorption coefficient	0.201 mm^{-1}	
F(000)	680	
Crystal size	0.202 x 0.200 x 0.063 mm^3	
Theta range for data collection	1.542 to 24.710°.	
Index ranges	-13<=h<=17, -8<=k<=8, -20<=l<=20	
Reflections collected	28247	
Independent reflections	2763 [R(int) = 0.1046]	
Completeness to theta = 24.710°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6585	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2763 / 0 / 217	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0422, wR2 = 0.1143	
R indices (all data)	R1 = 0.0633, wR2 = 0.1254	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.284 and -0.311 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for gm03. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-215(2)	10115(3)	3208(1)	17(1)
C(2)	-763(2)	9721(4)	3691(2)	20(1)
C(3)	-1586(2)	10817(4)	3604(2)	24(1)
C(4)	-1904(2)	12296(4)	3015(2)	25(1)
C(5)	-1365(2)	12699(3)	2535(2)	21(1)
C(6)	-508(2)	11693(3)	2648(1)	18(1)
C(7)	781(2)	10373(3)	2016(2)	18(1)
C(8)	1081(2)	10194(4)	1349(2)	21(1)
C(9)	1590(2)	8574(4)	1279(2)	23(1)
C(10)	1776(2)	7097(4)	1864(2)	23(1)
C(11)	1450(2)	7249(3)	2517(2)	19(1)
C(12)	948(2)	8881(3)	2608(1)	15(1)
C(13)	990(2)	7543(3)	3922(1)	17(1)
C(14)	459(2)	5917(3)	3893(2)	21(1)
C(15)	852(2)	4420(4)	4489(2)	24(1)
C(16)	1780(2)	4569(4)	5092(2)	24(1)
C(17)	2362(2)	6237(3)	5140(2)	20(1)
C(18)	3335(2)	6436(4)	5746(2)	25(1)
C(19)	3872(2)	8066(4)	5792(2)	27(1)
C(20)	3462(2)	9618(4)	5232(2)	24(1)
C(21)	2528(2)	9473(4)	4630(1)	20(1)
C(22)	1957(2)	7781(3)	4558(1)	16(1)
N(1)	634(1)	9030(3)	3287(1)	17(1)
S(1)	256(1)	12566(1)	2155(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for gm03.

C(1)-C(2)	1.398(3)
C(1)-C(6)	1.407(3)
C(1)-N(1)	1.422(3)
C(2)-C(3)	1.390(3)
C(3)-C(4)	1.386(4)
C(4)-C(5)	1.385(3)
C(5)-C(6)	1.391(3)
C(6)-S(1)	1.766(2)
C(7)-C(8)	1.391(3)
C(7)-C(12)	1.403(3)
C(7)-S(1)	1.761(2)
C(8)-C(9)	1.380(3)
C(9)-C(10)	1.385(4)
C(10)-C(11)	1.393(3)
C(11)-C(12)	1.392(3)
C(12)-N(1)	1.425(3)
C(13)-C(14)	1.359(3)
C(13)-C(22)	1.430(3)
C(13)-N(1)	1.443(3)
C(14)-C(15)	1.413(3)
C(15)-C(16)	1.362(4)
C(16)-C(17)	1.421(3)
C(17)-C(18)	1.415(3)
C(17)-C(22)	1.425(3)
C(18)-C(19)	1.362(4)
C(19)-C(20)	1.410(4)
C(20)-C(21)	1.368(3)
C(21)-C(22)	1.418(3)

C(2)-C(1)-C(6)	117.8(2)
C(2)-C(1)-N(1)	122.5(2)
C(6)-C(1)-N(1)	119.7(2)
C(3)-C(2)-C(1)	121.1(2)
C(4)-C(3)-C(2)	120.7(2)

C(5)-C(4)-C(3)	118.5(2)
C(4)-C(5)-C(6)	121.5(2)
C(5)-C(6)-C(1)	120.1(2)
C(5)-C(6)-S(1)	118.82(19)
C(1)-C(6)-S(1)	120.86(18)
C(8)-C(7)-C(12)	121.0(2)
C(8)-C(7)-S(1)	119.34(18)
C(12)-C(7)-S(1)	119.50(18)
C(9)-C(8)-C(7)	120.4(2)
C(8)-C(9)-C(10)	119.4(2)
C(9)-C(10)-C(11)	120.2(2)
C(12)-C(11)-C(10)	121.4(2)
C(11)-C(12)-C(7)	117.5(2)
C(11)-C(12)-N(1)	120.8(2)
C(7)-C(12)-N(1)	121.7(2)
C(14)-C(13)-C(22)	120.8(2)
C(14)-C(13)-N(1)	121.8(2)
C(22)-C(13)-N(1)	117.3(2)
C(13)-C(14)-C(15)	120.7(2)
C(16)-C(15)-C(14)	120.3(2)
C(15)-C(16)-C(17)	120.8(2)
C(18)-C(17)-C(16)	122.6(2)
C(18)-C(17)-C(22)	118.2(2)
C(16)-C(17)-C(22)	119.1(2)
C(19)-C(18)-C(17)	121.6(2)
C(18)-C(19)-C(20)	120.2(2)
C(21)-C(20)-C(19)	120.0(2)
C(20)-C(21)-C(22)	121.1(2)
C(21)-C(22)-C(17)	118.9(2)
C(21)-C(22)-C(13)	122.9(2)
C(17)-C(22)-C(13)	118.2(2)
C(1)-N(1)-C(12)	121.29(18)
C(1)-N(1)-C(13)	119.55(18)
C(12)-N(1)-C(13)	115.79(18)
C(7)-S(1)-C(6)	99.90(11)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for gm03. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	15(1)	18(1)	16(1)	-5(1)	5(1)	-2(1)
C(2)	20(1)	21(1)	19(1)	-4(1)	7(1)	-5(1)
C(3)	21(1)	29(2)	25(1)	-9(1)	12(1)	-4(1)
C(4)	19(1)	30(2)	26(1)	-5(1)	9(1)	3(1)
C(5)	19(1)	20(1)	21(1)	-3(1)	5(1)	2(1)
C(6)	18(1)	19(1)	15(1)	-5(1)	6(1)	-3(1)
C(7)	12(1)	19(1)	20(1)	-2(1)	4(1)	-3(1)
C(8)	20(1)	24(1)	18(1)	2(1)	7(1)	-2(1)
C(9)	22(1)	29(2)	22(1)	-2(1)	13(1)	-1(1)
C(10)	17(1)	28(2)	23(1)	-3(1)	8(1)	2(1)
C(11)	15(1)	22(1)	19(1)	2(1)	5(1)	-1(1)
C(12)	11(1)	19(1)	13(1)	-3(1)	3(1)	-4(1)
C(13)	19(1)	18(1)	15(1)	0(1)	10(1)	3(1)
C(14)	22(1)	23(1)	19(1)	-4(1)	10(1)	-3(1)
C(15)	33(2)	20(1)	24(1)	-4(1)	16(1)	-5(1)
C(16)	34(2)	19(1)	22(1)	4(1)	14(1)	3(1)
C(17)	23(1)	22(1)	17(1)	1(1)	12(1)	6(1)
C(18)	26(1)	28(2)	20(1)	6(1)	9(1)	9(1)
C(19)	17(1)	36(2)	22(1)	2(1)	3(1)	2(1)
C(20)	21(1)	25(1)	24(1)	1(1)	7(1)	-3(1)
C(21)	21(1)	22(1)	16(1)	4(1)	8(1)	3(1)
C(22)	17(1)	19(1)	14(1)	-2(1)	9(1)	2(1)
N(1)	14(1)	21(1)	15(1)	1(1)	6(1)	2(1)
S(1)	24(1)	18(1)	24(1)	2(1)	12(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for gm03.

	x	y	z	U(eq)
H(2)	-569	8688	4085	24
H(3)	-1934	10549	3951	29
H(4)	-2479	13016	2942	30
H(5)	-1586	13686	2119	25
H(8)	934	11193	940	25
H(9)	1812	8474	833	27
H(10)	2125	5977	1819	27
H(11)	1574	6216	2909	23
H(14)	-182	5786	3467	25
H(15)	468	3304	4470	29
H(16)	2040	3546	5485	29
H(18)	3620	5408	6130	30
H(19)	4526	8159	6202	32
H(20)	3833	10763	5274	28
H(21)	2258	10522	4254	23

7. Coordinates of Molecular Structures

All coordinates are reported as XYZ Cartesian coordinates. Energies computed at uM06/6-311+G**/CPCM-H_2O level of theory (reported in parentheses) are arranged in the following order: E_{0K} (not ZPE and thermally corrected), H (298 K) and G (298 K). They are stated in Hartrees units. All energies reported were calculated using the GAUSSIAN 09 computational chemistry package.

10-Phenylphenoxazine (1)

Neutral ground state (-823.3084106, -823.0332097, -823.0941837)

C	-6.47170	-0.93850	0.09685
C	-5.07759	-0.87165	0.05607
C	-4.44481	0.35333	-0.05771
C	-5.17842	1.54709	-0.12655
C	-6.57112	1.46920	-0.08219
C	-7.21247	0.23429	0.02621
C	-3.09640	2.77371	-0.13421
C	-2.40688	1.55352	-0.06602
C	-1.02827	1.51415	0.03982
H	-0.54300	0.54233	0.09116
C	-0.29327	2.70108	0.07204
C	-0.96103	3.91716	0.00237
C	-2.35270	3.95370	-0.09694
H	-6.96420	-1.90316	0.18325
H	-4.46257	-1.76703	0.10549
H	-7.15702	2.38346	-0.13711
H	0.78972	2.66497	0.15026
H	-2.86834	4.90930	-0.15154
H	-8.29845	0.20147	0.05537
H	-0.40651	4.85179	0.02515
N	-4.49249	2.76241	-0.24920
C	-5.21659	3.99274	-0.29382
C	-5.60411	4.61754	0.89017
C	-5.52463	4.55861	-1.52837
C	-6.30658	5.81844	0.83559
H	-5.35138	4.15548	1.84312
C	-6.22626	5.76092	-1.57918
H	-5.21008	4.04985	-2.43758
C	-6.61665	6.38972	-0.39830
H	-6.61211	6.30903	1.75638
H	-6.46797	6.20638	-2.54092
H	-7.16582	7.32715	-0.43861
O	-3.06940	0.34747	-0.12574

Neutral triplet state (-823.2051752, -822.9347994, -822.9954884)

C	-2.05707	3.57872	-0.00028

C	-2.70556	2.35879	-0.00032
C	-1.96995	1.17515	-0.00012
C	-0.52259	1.20062	0.00022
C	0.11706	2.46345	0.00030
C	-0.61945	3.62184	0.00009
C	-0.52268	-1.20060	-0.00015
C	-1.97002	-1.17503	0.00022
C	-2.70571	-2.35862	0.00025
H	-3.79126	-2.28861	0.00047
C	-2.05732	-3.57859	-0.00002
C	-0.61972	-3.62181	-0.00030
C	0.11688	-2.46346	-0.00037
H	-2.63086	4.50094	-0.00056
H	-3.79111	2.28886	-0.00049
H	1.20368	2.50741	0.00057
H	-2.63117	-4.50077	0.00002
H	1.20349	-2.50750	-0.00059
H	-0.10880	4.58093	0.00023
H	-0.10913	-4.58094	-0.00052
N	0.14782	-0.00002	-0.00007
C	1.58549	-0.00006	-0.00002
C	2.26173	-0.00022	1.21413
C	2.26181	0.00009	-1.21413
C	3.65494	-0.00024	1.20946
H	1.69630	-0.00031	2.14382
C	3.65502	0.00004	-1.20937
H	1.69644	0.00022	-2.14385
C	4.34843	-0.00012	0.00007
H	4.19785	-0.00036	2.15092
H	4.19800	0.00014	-2.15079
H	5.43533	-0.00016	0.00011
O	-2.63892	0.00008	0.00039

Cation radical state (-823.1214782, -822.8453124, -822.9040004)

C	-6.45178	-0.91926	0.01108
C	-5.06954	-0.87583	0.03715
C	-4.43447	0.35924	-0.00534
C	-5.17164	1.56228	-0.07584
C	-6.57568	1.49671	-0.10130
C	-7.20084	0.26837	-0.05719
C	-3.10482	2.77640	-0.07523
C	-2.41266	1.54637	-0.00361
C	-1.02520	1.49995	0.04234
H	-0.53698	0.53184	0.09893
C	-0.31368	2.68603	0.01752
C	-0.98637	3.91859	-0.05413

C	-2.36349	3.97013	-0.10110
H	-6.95950	-1.87834	0.04526
H	-4.46181	-1.77389	0.08979
H	-7.15639	2.41236	-0.15291
H	0.77099	2.66276	0.05431
H	-2.88066	4.92287	-0.15642
H	-8.28512	0.22145	-0.07545
H	-0.41754	4.84302	-0.07252
N	-4.48471	2.75939	-0.11793
C	-5.21597	4.00142	-0.21499
C	-5.58720	4.65763	0.95250
C	-5.52580	4.49708	-1.47613
C	-6.29451	5.85184	0.84780
H	-5.32463	4.23571	1.92002
C	-6.23372	5.69182	-1.56569
H	-5.21736	3.95093	-2.36488
C	-6.61627	6.36571	-0.40718
H	-6.59394	6.38014	1.74854
H	-6.48615	6.09493	-2.54242
H	-7.16976	7.29777	-0.48301
O	-3.08191	0.37051	0.02336

4-Trifluoromethylphenyl -10-phenoxazine (2)

Neutral ground state (-1160.343866, -1160.06003, -1160.127372)

C	-6.46905	-0.92247	-0.14086
C	-5.07835	-0.85574	-0.04351
C	-4.44827	0.37238	0.05624
C	-5.18182	1.56704	0.05366
C	-6.57108	1.48956	-0.05123
C	-7.20994	0.25246	-0.14368
C	-3.09698	2.79019	0.05601
C	-2.41196	1.56656	0.05523
C	-1.03266	1.51800	-0.04326
H	-0.55005	0.54360	-0.04334
C	-0.29482	2.69951	-0.13101
C	-0.95859	3.92006	-0.12180
C	-2.35006	3.96500	-0.03129
H	-6.95988	-1.88897	-0.21485
H	-4.46356	-1.75253	-0.03933
H	-7.16022	2.40329	-0.05330
H	0.78829	2.65655	-0.20344
H	-2.86065	4.92467	-0.02079
H	-8.29361	0.21968	-0.21877
H	-0.40108	4.85088	-0.18519
N	-4.49712	2.78878	0.17315
C	-5.21634	4.00657	-0.01739

C	-5.72179	4.68463	1.08590
C	-5.41598	4.49943	-1.30838
C	-6.43414	5.86744	0.90541
H	-5.55734	4.27912	2.08125
C	-6.12213	5.67829	-1.49190
H	-5.01277	3.95207	-2.15794
C	-6.62915	6.35763	-0.38156
H	-6.83208	6.40223	1.76256
H	-6.28065	6.07131	-2.49366
O	-3.07795	0.36893	0.18721
C	-7.38236	7.62869	-0.62022
F	-7.82839	8.19358	0.50842
F	-8.45499	7.43296	-1.41237
F	-6.62144	8.54886	-1.24510

Neutral triplet state (-1160.239871, -1159.961263, -1160.030893)

C	-6.46098	-0.93808	0.00090
C	-5.08239	-0.88036	0.02944
C	-4.43368	0.35467	0.00169
C	-5.18691	1.58342	-0.05943
C	-6.59782	1.49664	-0.09596
C	-7.22405	0.27419	-0.06418
C	-3.11494	2.80465	-0.04234
C	-2.40450	1.53981	-0.01621
C	-1.01079	1.50539	-0.00365
H	-0.52080	0.53429	0.01539
C	-0.28834	2.68141	-0.01291
C	-0.97994	3.94699	-0.03164
C	-2.35140	3.99493	-0.04755
H	-6.96594	-1.89943	0.02566
H	-4.47283	-1.78020	0.07232
H	-7.18702	2.40931	-0.14686
H	0.79729	2.65441	-0.00518
H	-2.86372	4.95427	-0.06366
H	-8.30911	0.22828	-0.08951
H	-0.41083	4.87236	-0.03224
N	-4.48957	2.77057	-0.08440
C	-5.21628	4.00282	-0.18732
C	-5.68299	4.61119	0.97001
C	-5.43711	4.55130	-1.44610
C	-6.39730	5.80343	0.86786
H	-5.49104	4.15222	1.93677
C	-6.14704	5.74065	-1.54617
H	-5.05491	4.04577	-2.32967
C	-6.62373	6.35858	-0.38718
H	-6.77192	6.29133	1.76228

H	-6.32955	6.18633	-2.52097
O	-3.08257	0.37122	0.01253
C	-7.38295	7.63997	-0.54129
F	-7.80205	8.14696	0.62427
F	-8.47384	7.48074	-1.31584
F	-6.63743	8.59026	-1.13797

Cation radical state (-1160.15447, -1159.869849, -1159.936687)

C	-6.45274	-0.91562	0.00179
C	-5.07087	-0.87065	0.02931
C	-4.43728	0.36547	-0.00796
C	-5.17640	1.56784	-0.07170
C	-6.57981	1.50076	-0.10409
C	-7.20313	0.27132	-0.06582
C	-3.10729	2.78423	-0.06603
C	-2.41552	1.55309	-0.00931
C	-1.02769	1.50594	0.02624
H	-0.53945	0.53722	0.06966
C	-0.31635	2.69194	0.00795
C	-0.98937	3.92553	-0.04327
C	-2.36672	3.97810	-0.07999
H	-6.95953	-1.87526	0.03210
H	-4.46180	-1.76798	0.07800
H	-7.16418	2.41401	-0.15700
H	0.76853	2.66833	0.03569
H	-2.88170	4.93285	-0.11783
H	-8.28721	0.22321	-0.08887
H	-0.42060	4.85006	-0.05347
N	-4.48797	2.76532	-0.10430
C	-5.21854	4.00537	-0.19721
C	-5.67648	4.60662	0.96667
C	-5.44374	4.55432	-1.45546
C	-6.38884	5.79796	0.87025
H	-5.48072	4.14698	1.93207
C	-6.15183	5.74376	-1.54432
H	-5.06872	4.05403	-2.34470
C	-6.62111	6.35739	-0.38213
H	-6.75779	6.28207	1.76876
H	-6.33778	6.19233	-2.51692
O	-3.08514	0.37806	0.01549
C	-7.38105	7.64199	-0.52895
F	-7.79457	8.14190	0.64019
F	-8.47182	7.48202	-1.30044
F	-6.63372	8.58973	-1.12352

1-Naphthalene-10-phenoxazine (3)

Neutral ground state (-976.8692387, -976.5445874, -976.6089664)

C	-6.48220	-0.91004	-0.14773
C	-5.09111	-0.84754	-0.05341
C	-4.45366	0.37968	0.00914
C	-5.18084	1.57800	-0.02733
C	-6.57095	1.50380	-0.12522
C	-7.21702	0.26854	-0.18171
C	-3.09227	2.79247	-0.01363
C	-2.41076	1.56697	0.02523
C	-1.02870	1.51448	-0.01862
H	-0.54914	0.53908	0.01548
C	-0.28461	2.69279	-0.09668
C	-0.94526	3.91467	-0.13532
C	-2.33885	3.96366	-0.09684
H	-6.97823	-1.87564	-0.19396
H	-4.48122	-1.74725	-0.02324
H	-7.15206	2.42257	-0.15060
H	0.80037	2.64614	-0.12670
H	-2.85071	4.92261	-0.12632
H	-8.30107	0.23948	-0.25389
H	-0.38299	4.84284	-0.19633
N	-4.49431	2.80040	0.04093
C	-5.20688	4.02223	-0.15494
C	-5.63053	4.74140	0.93586
C	-5.47425	4.47220	-1.47974
C	-6.34581	5.94731	0.76461
H	-5.40809	4.36501	1.93234
C	-6.20350	5.68713	-1.64528
C	-6.62674	6.40649	-0.49843
H	-6.67232	6.50550	1.63800
H	-7.17997	7.33348	-0.63960
O	-3.08280	0.37023	0.13652
C	-6.48699	6.14391	-2.95771
C	-5.05028	3.76057	-2.63024
C	-5.34103	4.23130	-3.88813
H	-5.01211	3.67628	-4.76325
C	-6.06712	5.43272	-4.05511
H	-6.29034	5.79178	-5.05670
H	-7.04491	7.07119	-3.07740
H	-4.49131	2.83453	-2.50749

Neutral triplet state (-976.7761436, -976.4554405, -976.5210735)

C	-6.43760	-1.00121	0.58349
C	-5.04921	-0.89641	0.58096

C	-4.44987	0.31871	0.29202
C	-5.21784	1.46134	0.01326
C	-6.61149	1.32833	-0.02616
C	-7.21480	0.11129	0.26902
C	-3.17356	2.69867	-0.32058
C	-2.45817	1.51954	-0.06980
C	-1.07102	1.49751	-0.10184
H	-0.56662	0.55570	0.09842
C	-0.36575	2.66502	-0.37005
C	-1.06160	3.85414	-0.58451
C	-2.45061	3.87217	-0.55246
H	-6.90590	-1.95536	0.80819
H	-4.41107	-1.75031	0.79258
H	-7.21648	2.18760	-0.30284
H	0.72000	2.64768	-0.39529
H	-2.98842	4.80338	-0.70491
H	-8.29776	0.03204	0.23572
H	-0.52262	4.77907	-0.77064
N	-4.58164	2.67728	-0.27166
C	-5.35019	3.84951	-0.40021
C	-6.09472	4.29961	0.76134
C	-5.39875	4.56358	-1.63787
C	-6.75073	5.49403	0.71991
H	-6.05211	3.70289	1.66978
C	-6.11238	5.81560	-1.66061
C	-6.75779	6.27117	-0.47495
H	-7.26562	5.86577	1.60249
H	-7.29250	7.21897	-0.50414
O	-3.08299	0.34549	0.25726
C	-6.17825	6.53026	-2.86299
C	-4.83200	4.08731	-2.82568
C	-4.90996	4.83603	-4.02759
H	-4.44264	4.44679	-4.92901
C	-5.56847	6.04397	-4.04565
H	-5.62930	6.62770	-4.96105
H	-6.72408	7.47264	-2.88114
H	-4.32605	3.12345	-2.82625

Cation radical state (-976.6811041, -976.3556374, -976.4197774)

C	-6.45142	-0.91807	0.00392
C	-5.07018	-0.87767	0.05999
C	-4.43075	0.35503	0.00810
C	-5.16328	1.55834	-0.09731
C	-6.56615	1.49578	-0.15553
C	-7.19559	0.27005	-0.10420
C	-3.09263	2.76650	-0.09005

C	-2.40576	1.53611	0.01606
C	-1.01878	1.48638	0.07783
H	-0.53461	0.51832	0.16298
C	-0.30343	2.66922	0.03101
C	-0.97113	3.90200	-0.07842
C	-2.34750	3.95680	-0.13944
H	-6.96271	-1.87500	0.04436
H	-4.46638	-1.77610	0.14230
H	-7.14216	2.41249	-0.23662
H	0.78074	2.64363	0.07916
H	-2.86217	4.90914	-0.22282
H	-8.27923	0.22520	-0.14794
H	-0.39874	4.82366	-0.11497
N	-4.47274	2.75407	-0.14690
C	-5.19883	3.99541	-0.27646
C	-5.59106	4.65108	0.86264
C	-5.48089	4.48238	-1.57960
C	-6.30778	5.86142	0.75435
H	-5.34785	4.23121	1.83620
C	-6.20844	5.70634	-1.67054
C	-6.60797	6.37216	-0.48471
H	-6.61834	6.38072	1.65607
H	-7.16234	7.30424	-0.57562
O	-3.07916	0.36350	0.06281
C	-6.51380	6.22476	-2.95389
C	-5.08164	3.82035	-2.76678
C	-5.39521	4.35299	-3.99401
H	-5.08523	3.83828	-4.89967
C	-6.11744	5.56408	-4.09040
H	-6.35666	5.97029	-5.06962
H	-7.07027	7.15778	-3.01844
H	-4.52307	2.88808	-2.70727

2-Naphthalene-10-phenoxazine (4)

Neutral ground state (-976.8676392, -976.5431588, -976.6086008)

C	-6.46217	-0.92603	0.16189
C	-5.06875	-0.86207	0.10323
C	-4.43938	0.35471	-0.08907
C	-5.17422	1.54208	-0.21990
C	-6.56610	1.46793	-0.15308
C	-7.20466	0.24105	0.03281
C	-3.09928	2.77191	-0.22169
C	-2.41049	1.55717	-0.09025
C	-1.04094	1.52477	0.10197
H	-0.55633	0.55605	0.19825
C	-0.31439	2.71569	0.15799

C	-0.98154	3.92725	0.02694
C	-2.36474	3.95632	-0.15747
H	-6.95358	-1.88430	0.30628
H	-4.45275	-1.75321	0.19609
H	-7.15300	2.37736	-0.25621
H	0.76209	2.68691	0.30202
H	-2.87848	4.90878	-0.26213
H	-8.29022	0.20934	0.07513
H	-0.43276	4.86468	0.06709
N	-4.48628	2.74655	-0.43455
C	-5.21511	3.97471	-0.47561
C	-5.59461	4.60439	0.73502
C	-5.53645	4.52998	-1.68781
C	-6.29197	5.78551	0.70184
H	-5.32310	4.13546	1.67943
C	-6.25528	5.75007	-1.75089
C	-6.63987	6.38958	-0.53485
H	-6.58851	6.27661	1.62711
O	-3.06578	0.34949	-0.18911
C	-6.60058	6.35153	-2.98699
C	-7.35757	7.61033	-0.59994
H	-7.65000	8.09555	0.32990
C	-7.67836	8.17103	-1.81294
H	-8.23007	9.10716	-1.85067
C	-7.29648	7.53603	-3.01760
H	-7.55694	7.99044	-3.97036
H	-6.30352	5.85774	-3.91074
H	-5.23561	4.02856	-2.60693

Neutral triplet state (-976.773159, -976.452774, -976.518417)

C	-6.35570	-1.07156	0.42310
C	-5.01033	-0.92681	0.10292
C	-4.46425	0.33955	-0.03861
C	-5.23641	1.49805	0.15081
C	-6.59107	1.33403	0.45491
C	-7.14310	0.06451	0.58922
C	-3.22812	2.79358	-0.18018
C	-2.51446	1.60435	-0.38674
C	-1.13927	1.60887	-0.55003
H	-0.63389	0.66027	-0.71137
C	-0.44165	2.81392	-0.49938
C	-1.12770	4.00084	-0.25470
C	-2.50783	3.99050	-0.08072
H	-6.78381	-2.06379	0.53387
H	-4.36355	-1.78520	-0.05845
H	-7.22383	2.20667	0.57259

H	0.63696	2.81763	-0.62865
H	-3.03959	4.91081	0.14477
H	-8.19943	-0.02927	0.82574
H	-0.58873	4.94128	-0.18071
N	-4.62389	2.75488	-0.04027
C	-5.34076	3.96132	-0.15262
C	-6.21741	4.41336	0.80870
C	-5.16471	4.71840	-1.38856
C	-6.95112	5.59348	0.59712
H	-6.32400	3.87220	1.74612
C	-5.92901	5.87241	-1.63786
C	-6.84412	6.34036	-0.62435
H	-7.61170	5.96548	1.37803
O	-3.15062	0.39496	-0.42637
C	-5.82299	6.60103	-2.84229
C	-7.58275	7.49207	-0.86592
H	-8.27482	7.84563	-0.10265
C	-7.45239	8.21648	-2.08837
H	-8.04502	9.11458	-2.24449
C	-6.58326	7.77277	-3.05821
H	-6.47850	8.31382	-3.99574
H	-5.13556	6.24648	-3.60909
H	-4.49942	4.32918	-2.15737

Cation radical state (-976.6803742, -976.3548851, -976.4193681)

C	-6.46573	-0.89297	-0.05233
C	-5.08382	-0.85432	-0.00746
C	-4.44377	0.37838	-0.04379
C	-5.17555	1.58361	-0.13180
C	-6.57943	1.52313	-0.17208
C	-7.20963	0.29730	-0.13099
C	-3.10499	2.79080	-0.09872
C	-2.41865	1.55907	-0.00484
C	-1.03271	1.50866	0.07297
H	-0.54891	0.53930	0.14441
C	-0.31722	2.69251	0.05934
C	-0.98417	3.92669	-0.03462
C	-2.35968	3.98209	-0.11527
H	-6.97736	-1.85015	-0.02337
H	-4.48017	-1.75444	0.05582
H	-7.15604	2.44077	-0.23220
H	0.76625	2.66609	0.12121
H	-2.87263	4.93580	-0.19057
H	-8.29384	0.25447	-0.16025
H	-0.41206	4.84920	-0.04503
N	-4.48349	2.77785	-0.17557

C	-5.20824	4.02112	-0.29551
C	-5.55742	4.71569	0.88234
C	-5.53592	4.47781	-1.54502
C	-6.25275	5.89363	0.77213
H	-5.27182	4.31033	1.85027
C	-6.25453	5.69024	-1.67552
C	-6.61927	6.40942	-0.49745
H	-6.53364	6.44745	1.66550
O	-3.09190	0.38528	0.00835
C	-6.62313	6.20314	-2.94425
C	-7.34090	7.62171	-0.63210
H	-7.61732	8.16920	0.26701
C	-7.68547	8.09510	-1.87466
H	-8.24000	9.02547	-1.96712
C	-7.32397	7.38012	-3.04050
H	-7.60520	7.76772	-4.01630
H	-6.34193	5.64770	-3.83692
H	-5.25077	3.91214	-2.43094

3,7-Di(4-biphenyl)1-Naphthalene-10-Phenoxazine (5)

Neutral ground state (-1900.582243, -1899.909858, -1900.018478)

C	-6.42073	-0.92021	0.69406
C	-5.01314	-0.81296	0.67314
C	-4.39886	0.41002	0.45459
C	-5.14437	1.58925	0.24065
C	-6.54267	1.48586	0.26106
C	-7.16764	0.25336	0.48509
C	-3.06701	2.82051	-0.07160
C	-2.34293	1.62882	0.14766
C	-0.95980	1.59104	0.07161
H	-0.46754	0.63430	0.22400
C	-0.22235	2.75664	-0.22868
C	-0.93939	3.94667	-0.44826
C	-2.33720	3.97943	-0.37188
H	-4.37634	-1.68419	0.80027
H	-7.14486	2.37708	0.11175
H	-2.86602	4.91385	-0.53538
H	-8.25273	0.22053	0.52147
H	-0.40610	4.87054	-0.65380
N	-4.47293	2.80846	0.01919
C	-5.22693	4.00183	-0.24391
C	-5.60019	4.81778	0.80742
C	-5.59376	4.31557	-1.58956
C	-6.36401	5.99258	0.56712
H	-5.30510	4.54676	1.81727
C	-6.36401	5.50012	-1.82530

C	-6.73751	6.32358	-0.72312
H	-6.65100	6.62277	1.40216
H	-7.32362	7.21886	-0.91572
O	-2.99420	0.42183	0.45179
C	-6.73970	5.82723	-3.16074
C	-5.22191	3.49507	-2.69337
C	-5.60047	3.83889	-3.97946
H	-5.31402	3.21142	-4.81754
C	-6.36706	5.01516	-4.21693
H	-6.65561	5.26957	-5.23180
H	-7.32409	6.72764	-3.33377
H	-4.63593	2.59739	-2.51094
C	1.25441	2.72035	-0.30292
C	1.96220	3.57109	-1.17735
C	2.00396	1.83282	0.49697
C	3.35737	3.53741	-1.24694
H	1.41736	4.25504	-1.82351
C	3.39880	1.79824	0.42589
H	1.49481	1.17385	1.19605
C	4.10659	2.65027	-0.44674
H	3.86924	4.22157	-1.91923
H	3.94209	1.08815	1.04468
C	-7.07907	-2.22466	0.92480
C	-8.34994	-2.50602	0.38081
C	-6.45667	-3.23422	1.68832
C	-8.96779	-3.74132	0.58871
H	-8.85519	-1.76040	-0.22772
C	-7.07291	-4.47135	1.89285
H	-5.48540	-3.04740	2.13975
C	-8.34162	-4.75302	1.34547
H	-9.95536	-3.91527	0.16859
H	-6.55319	-5.23311	2.46888
C	5.58637	2.61362	-0.51698
C	6.26293	2.87328	-1.72737
C	6.35491	2.31562	0.62801
C	7.66176	2.83655	-1.79105
H	5.69402	3.07873	-2.63084
C	7.75357	2.27664	0.56584
H	5.85735	2.13818	1.57846
C	8.41475	2.53739	-0.64469
H	8.16262	3.03166	-2.73457
H	8.32631	2.05138	1.46044
H	9.49884	2.50783	-0.69412
C	-8.99186	-6.06845	1.55254
C	-8.79559	-6.79533	2.74580
C	-9.82024	-6.62812	0.55699

C	-9.40620	-8.04154	2.93663
H	-8.18285	-6.37408	3.53915
C	-10.43301	-7.87321	0.74681
H	-9.96495	-6.10185	-0.38336
C	-10.22851	-8.58706	1.93812
H	-9.24764	-8.58169	3.86520
H	-11.06094	-8.28925	-0.03528
H	-10.70161	-9.55295	2.08599

Neutral triplet state (-1900.48965, -1899.820754, -1899.929948)

C	-6.48008	-1.01747	0.65611
C	-5.07739	-0.88504	0.66947
C	-4.48122	0.33325	0.38026
C	-5.24289	1.48316	0.07595
C	-6.64186	1.34201	0.03141
C	-7.24634	0.11880	0.32488
C	-3.18186	2.72540	-0.27201
C	-2.45089	1.55256	0.00918
C	-1.06257	1.52777	-0.02108
H	-0.56741	0.58066	0.17314
C	-0.33273	2.69198	-0.32173
C	-1.05798	3.87936	-0.56094
C	-2.45228	3.89770	-0.52952
H	-4.42878	-1.73439	0.86331
H	-7.25307	2.19595	-0.24273
H	-2.98598	4.82778	-0.69464
H	-8.33009	0.05450	0.30595
H	-0.52690	4.80909	-0.74246
N	-4.59880	2.70252	-0.22967
C	-5.37286	3.87593	-0.42074
C	-6.15501	4.35677	0.71345
C	-5.38537	4.56545	-1.68113
C	-6.83053	5.54911	0.61809
H	-6.12700	3.79209	1.64156
C	-6.12389	5.80745	-1.76395
C	-6.81786	6.29406	-0.60817
H	-7.37138	5.94010	1.47429
H	-7.36367	7.23207	-0.68125
O	-3.08554	0.35684	0.35547
C	-6.16883	6.49400	-2.99331
C	-4.76705	4.06299	-2.84371
C	-4.82474	4.77994	-4.07645
H	-4.32535	4.37522	-4.95153
C	-5.51052	5.98298	-4.15066
H	-5.55566	6.53657	-5.08359
H	-6.72972	7.42422	-3.05439

H	-4.24699	3.10890	-2.80525
C	1.14411	2.67008	-0.37211
C	1.85367	3.52862	-1.23712
C	1.89007	1.78426	0.43274
C	3.24904	3.49971	-1.29747
H	1.31115	4.21267	-1.88493
C	3.28504	1.75600	0.37201
H	1.37881	1.12112	1.12615
C	3.99529	2.61164	-0.49551
H	3.76312	4.18753	-1.96404
H	3.82673	1.04673	0.99283
C	-7.11750	-2.31847	0.94842
C	-8.32437	-2.69602	0.32407
C	-6.52883	-3.22898	1.85003
C	-8.91241	-3.93584	0.58493
H	-8.79679	-2.02588	-0.38955
C	-7.11899	-4.46733	2.11251
H	-5.60845	-2.96136	2.36305
C	-8.32131	-4.84901	1.48219
H	-9.84943	-4.19089	0.09630
H	-6.62912	-5.15385	2.79826
C	5.47511	2.57542	-0.56070
C	6.15483	2.84071	-1.76808
C	6.23991	2.26967	0.58468
C	7.55366	2.80157	-1.82855
H	5.58873	3.05174	-2.67196
C	7.63856	2.22868	0.52570
H	5.73975	2.08757	1.53282
C	8.30303	2.49468	-0.68191
H	8.05720	3.00075	-2.76973
H	8.20879	1.99734	1.42027
H	9.38713	2.46303	-0.72893
C	-8.93946	-6.16941	1.74653
C	-8.83551	-6.77574	3.01592
C	-9.64036	-6.85410	0.73178
C	-9.41212	-8.02839	3.26237
H	-8.32292	-6.25609	3.82181
C	-10.21736	-8.10689	0.97662
H	-9.71210	-6.41877	-0.26200
C	-10.10511	-8.70071	2.24354
H	-9.32661	-8.47589	4.24796
H	-10.74512	-8.62157	0.17946
H	-10.55075	-9.67223	2.43364

Cation radical state (-1900.396651, -1899.723003, -1899.832029)

C	-6.38694	-0.96130	0.61633

C	-4.98437	-0.87581	0.56192
C	-4.37035	0.34367	0.32502
C	-5.11862	1.53507	0.12923
C	-6.52603	1.45037	0.18102
C	-7.13882	0.23110	0.41733
C	-3.05567	2.75895	-0.16497
C	-2.32675	1.55464	0.02709
C	-0.94304	1.51978	-0.03037
H	-0.45443	0.55951	0.09554
C	-0.21521	2.69841	-0.27524
C	-0.94483	3.90721	-0.46216
C	-2.32804	3.94220	-0.41049
H	-4.35148	-1.74986	0.67236
H	-7.12297	2.34570	0.04636
H	-2.85690	4.87911	-0.54725
H	-8.22105	0.19980	0.47888
H	-0.41258	4.83800	-0.62385
N	-4.44511	2.73096	-0.10387
C	-5.20515	3.94724	-0.32638
C	-5.54747	4.72555	0.76106
C	-5.58444	4.28126	-1.66017
C	-6.30894	5.90789	0.56205
H	-5.23548	4.42714	1.75771
C	-6.35452	5.47532	-1.84451
C	-6.70306	6.26951	-0.71353
H	-6.57752	6.51750	1.41725
H	-7.28874	7.17108	-0.87239
O	-2.98663	0.36119	0.26876
C	-6.75619	5.84187	-3.16130
C	-5.23693	3.49084	-2.79333
C	-5.64173	3.87531	-4.05938
H	-5.37441	3.27137	-4.92026
C	-6.40842	5.05932	-4.24723
H	-6.71688	5.34312	-5.24796
H	-7.34057	6.74843	-3.29507
H	-4.65142	2.58410	-2.66637
C	1.25572	2.68629	-0.32732
C	1.97144	3.69383	-1.01090
C	1.99997	1.66549	0.30407
C	3.36502	3.68191	-1.05767
H	1.44156	4.48757	-1.52881
C	3.39298	1.65592	0.25772
H	1.49199	0.87974	0.85559
C	4.10814	2.66499	-0.42207
H	3.88160	4.48512	-1.57552
H	3.93062	0.84500	0.74076

C	-7.05889	-2.24457	0.87616
C	-8.37981	-2.47995	0.43601
C	-6.40037	-3.28264	1.57070
C	-9.01017	-3.70069	0.67573
H	-8.91681	-1.71479	-0.11714
C	-7.03352	-4.50064	1.81306
H	-5.39161	-3.13246	1.94511
C	-8.35223	-4.73845	1.36913
H	-10.03277	-3.84080	0.33654
H	-6.49169	-5.28319	2.33699
C	5.58771	2.65837	-0.46039
C	6.28608	3.17515	-1.57239
C	6.33396	2.13723	0.61816
C	7.68591	3.17052	-1.60539
H	5.73571	3.55748	-2.42833
C	7.73365	2.13367	0.58669
H	5.82159	1.75878	1.49910
C	8.41676	2.65021	-0.52561
H	8.20501	3.56480	-2.47352
H	8.29006	1.73664	1.43008
H	9.50197	2.64730	-0.55079
C	-9.02123	-6.03383	1.62414
C	-8.71937	-6.78722	2.77859
C	-9.97286	-6.54748	0.71793
C	-9.34808	-8.01507	3.01840
H	-8.01076	-6.40221	3.50758
C	-10.60174	-7.77557	0.95642
H	-10.20343	-6.00061	-0.19289
C	-10.29186	-8.51592	2.10820
H	-9.10774	-8.57644	3.91604
H	-11.32454	-8.15803	0.24237
H	-10.77828	-9.46859	2.29328

10-Phenylphenothiazine

Neutral ground state (-1146.281695, -1146.008636, -1146.06816)

C	-6.58770	-0.89838	0.26473
C	-5.26471	-0.92861	-0.16713
C	-4.57551	0.25460	-0.41864
C	-5.17878	1.50321	-0.19179
C	-6.51014	1.51925	0.24285
C	-7.20663	0.33235	0.45561
C	-3.06001	2.75123	-0.19253
C	-2.25958	1.62020	-0.42455
C	-0.88944	1.64991	-0.17898
H	-0.30341	0.74990	-0.35531
C	-0.27376	2.82088	0.25455

C	-1.05173	3.95609	0.45482
C	-2.42827	3.92162	0.24699
H	-7.12523	-1.82585	0.44251
H	-4.76111	-1.87841	-0.33709
H	-7.01417	2.46673	0.40801
H	0.79872	2.84305	0.42727
H	-3.01213	4.82025	0.42159
H	-8.24191	0.38022	0.78394
H	-0.59290	4.88399	0.78734
S	-2.96786	0.17088	-1.16624
N	-4.45461	2.69640	-0.41565
C	-5.18153	3.93337	-0.44043
C	-5.56411	4.57027	0.74058
C	-5.49587	4.49343	-1.67506
C	-6.26425	5.77135	0.68135
H	-5.30923	4.11882	1.69844
C	-6.19583	5.69740	-1.73158
H	-5.18716	3.97780	-2.58196
C	-6.57958	6.33582	-0.55477
H	-6.56338	6.26815	1.60090
H	-6.44063	6.13572	-2.69583
H	-7.12665	7.27429	-0.59867

Neutral triplet state (-1146.183574, -1145.913724, -1145.975536)

C	-6.68778	-0.87930	0.21538
C	-5.33056	-0.94291	0.32643
C	-4.51964	0.21660	0.12819
C	-5.18749	1.50169	-0.13396
C	-6.58268	1.51430	-0.30501
C	-7.33526	0.36606	-0.14736
C	-3.04356	2.72514	-0.08668
C	-2.22553	1.56860	-0.23730
C	-0.82772	1.69243	-0.28023
H	-0.23165	0.78921	-0.40095
C	-0.21492	2.92170	-0.15040
C	-1.01423	4.07030	0.02024
C	-2.38736	3.97490	0.04993
H	-7.29105	-1.76448	0.40284
H	-4.83726	-1.88632	0.56110
H	-7.08776	2.45193	-0.52646
H	0.86844	2.99836	-0.16612
H	-2.98012	4.87567	0.17987
H	-8.41225	0.40049	-0.28274
H	-0.54930	5.04640	0.13232
S	-2.88711	-0.02934	-0.41565
N	-4.43176	2.66544	-0.11815

C	-5.15236	3.91040	-0.18928
C	-5.68536	4.45541	0.97341
C	-5.31555	4.53322	-1.42165
C	-6.39376	5.65187	0.89947
H	-5.54105	3.94086	1.92144
C	-6.02956	5.72702	-1.48914
H	-4.88628	4.07948	-2.31289
C	-6.56729	6.28523	-0.33059
H	-6.81058	6.08855	1.80333
H	-6.16672	6.21980	-2.44821
H	-7.12401	7.21724	-0.38591

Cation radical state (-1146.094901, -1145.821109, -1145.881181)

C	-6.70948	-0.88018	-0.02749
C	-5.33437	-0.95929	0.01234
C	-4.55431	0.20578	-0.01625
C	-5.16662	1.48158	-0.08401
C	-6.57648	1.53393	-0.12494
C	-7.32658	0.37835	-0.09738
C	-3.03936	2.73200	-0.08445
C	-2.22145	1.57704	-0.02506
C	-0.82370	1.69308	-0.00884
H	-0.22080	0.78916	0.03377
C	-0.22611	2.93416	-0.04877
C	-1.02693	4.08512	-0.10237
C	-2.40136	3.99114	-0.11951
H	-7.30797	-1.78555	-0.00611
H	-4.83671	-1.92456	0.06582
H	-7.07803	2.49392	-0.17981
H	0.85606	3.01769	-0.03780
H	-2.99759	4.89605	-0.16085
H	-8.40941	0.45111	-0.13029
H	-0.56476	5.06728	-0.13257
S	-2.83943	-0.04103	0.03502
N	-4.42570	2.65582	-0.11132
C	-5.15968	3.90248	-0.18134
C	-5.54235	4.52670	0.99937
C	-5.45901	4.43635	-1.42896
C	-6.24854	5.72404	0.92400
H	-5.28873	4.07693	1.95694
C	-6.16513	5.63411	-1.49172
H	-5.14201	3.91662	-2.33068
C	-6.55830	6.27531	-0.31820
H	-6.55606	6.22550	1.83741
H	-6.40760	6.06563	-2.45886

H -7.11062 7.20965 -0.37179

1-Naphthalene-10-phenothiazine

Neutral ground state (-1299.842414, -1299.519779, -1299.585155)

C -6.60246 -0.89676 0.20226
C -5.28644 -0.91235 -0.25127
C -4.59130 0.27856 -0.44503
C -5.18098 1.51503 -0.13413
C -6.50458 1.51677 0.32276
C -7.20849 0.32511 0.47579
C -3.05244 2.75886 -0.12750
C -2.26255 1.64062 -0.44045
C -0.88409 1.66252 -0.24442
H -0.30359 0.77285 -0.48145
C -0.25364 2.81589 0.21446
C -1.02320 3.94071 0.49283
C -2.40652 3.91104 0.33746
H -7.14510 -1.82898 0.33357
H -4.79422 -1.85448 -0.48527
H -6.99227 2.45896 0.55538
H 0.82468 2.83274 0.34679
H -2.98904 4.79603 0.57596
H -8.23793 0.36088 0.82346
H -0.55177 4.85414 0.84697
N -4.45330 2.71434 -0.28990
C -5.17356 3.94572 -0.39415
C -5.58174 4.62856 0.72724
C -5.45870 4.44405 -1.69707
C -6.29727 5.83965 0.60942
H -5.34726 4.22096 1.70945
C -6.18360 5.66857 -1.80897
C -6.59170 6.34629 -0.63278
H -6.61215 6.36557 1.50681
H -7.14393 7.27917 -0.73337
C -6.47701 6.17626 -3.10017
C -5.05162 3.77324 -2.87823
C -5.35190 4.29378 -4.11425
H -5.03473 3.77093 -5.01333
C -6.07163 5.50559 -4.22813
H -6.30151 5.90475 -5.21296
H -7.03105 7.11028 -3.17876
H -4.49624 2.84082 -2.79019
S -2.99575 0.22430 -1.22228

Neutral triplet state (-1299.747767, -1299.429582, -1299.497632)

C -6.58547 -0.97915 0.48492

C	-5.26734	-1.00394	0.03702
C	-4.60388	0.17930	-0.27675
C	-5.23192	1.42295	-0.09377
C	-6.56385	1.43416	0.33775
C	-7.23216	0.24518	0.61703
C	-3.13560	2.70921	-0.24635
C	-2.31536	1.59596	-0.48074
C	-0.93307	1.68824	-0.33327
H	-0.32345	0.80414	-0.50986
C	-0.33824	2.90000	0.00621
C	-1.14357	4.01375	0.22534
C	-2.52759	3.91764	0.11621
H	-7.10146	-1.90784	0.71290
H	-4.75004	-1.95156	-0.10060
H	-7.08982	2.37869	0.44605
H	0.74198	2.96910	0.10044
H	-3.14441	4.79237	0.30951
H	-8.26790	0.28584	0.94455
H	-0.69852	4.96761	0.49699
N	-4.54048	2.62047	-0.37652
C	-5.27076	3.83636	-0.46081
C	-5.77627	4.46490	0.74751
C	-5.41954	4.45508	-1.73164
C	-6.41362	5.66120	0.67179
H	-5.60168	3.96831	1.70012
C	-6.10486	5.72401	-1.79424
C	-6.59925	6.30266	-0.60115
H	-6.78015	6.14867	1.57139
H	-7.12145	7.25587	-0.65607
C	-6.26534	6.33849	-3.04286
C	-4.94211	3.88227	-2.91588
C	-5.11379	4.53740	-4.17670
H	-4.72427	4.06789	-5.07615
C	-5.76263	5.73827	-4.23891
H	-5.90249	6.24584	-5.18981
H	-6.78615	7.29318	-3.09516
H	-4.44179	2.91604	-2.87217
S	-3.02226	0.08240	-1.07977

Cation radical state (-1299.654881, -1299.331714, -1299.397442)

C	-6.70545	-0.87476	-0.04831
C	-5.33271	-0.95500	0.04079
C	-4.54937	0.20807	0.00746
C	-5.15699	1.48196	-0.11212
C	-6.56413	1.53551	-0.20332
C	-7.31734	0.38222	-0.17243

C	-3.02757	2.72876	-0.10808
C	-2.21417	1.57517	0.00948
C	-0.81620	1.68914	0.04248
H	-0.21660	0.78665	0.13348
C	-0.21505	2.92596	-0.04393
C	-1.01196	4.07518	-0.16262
C	-2.38616	3.98312	-0.19319
H	-7.30624	-1.77852	-0.02429
H	-4.83956	-1.91931	0.13636
H	-7.05992	2.49562	-0.29943
H	0.86705	3.00787	-0.02075
H	-2.98044	4.88607	-0.28283
H	-8.39816	0.45524	-0.24586
H	-0.54675	5.05380	-0.23376
N	-4.41436	2.65590	-0.14849
C	-5.14496	3.90168	-0.25089
C	-5.52091	4.54120	0.90219
C	-5.44643	4.41213	-1.54020
C	-6.23616	5.75502	0.82456
H	-5.26433	4.10573	1.86558
C	-6.16998	5.64043	-1.60278
C	-6.55126	6.28863	-0.40119
H	-6.53330	6.25937	1.73935
H	-7.10419	7.22359	-0.46865
C	-6.49095	6.17936	-2.87397
C	-5.06817	3.76600	-2.74290
C	-5.39714	4.31743	-3.95754
H	-5.10362	3.81451	-4.87527
C	-6.11447	5.53369	-4.02562
H	-6.36651	5.95539	-4.99507
H	-7.04457	7.11540	-2.91676
H	-4.51373	2.83007	-2.70250
S	-2.83779	-0.03733	0.12756

10-Phenylphenoxazine (from X-ray crystal analysis)

Doi: 10.1039/C4RA09593F

Neutral ground state structure

O	7.49400	11.36400	10.45100
N	7.49400	8.56300	10.45100
C	5.12200	8.63800	11.02300
C	9.86500	8.63800	9.87800
H	5.07600	7.70900	11.02700
H	9.91100	7.70900	9.87400
C	4.00000	9.37300	11.31400
C	10.98700	9.37300	9.58700

H	3.20400	8.93700	11.51900
H	11.78400	8.93700	9.38200
C	4.04500	10.74000	11.30600
C	10.94200	10.74000	9.59500
H	3.28200	11.23300	11.50300
H	11.70600	11.23300	9.39800
C	5.21700	11.37900	11.00700
C	9.77000	11.37900	9.89500
H	5.24900	12.30800	10.99800
H	9.73900	12.30800	9.90300
C	6.34000	10.65900	10.71900
C	8.64700	10.65900	10.18200
C	6.31800	9.25900	10.72400
C	8.67000	9.25900	10.17700
C	7.49400	7.12800	10.45100
C	7.72900	6.45800	11.61600
C	7.25800	6.45800	9.28500
H	7.89200	6.92400	12.40400
H	7.09500	6.92400	8.49800
C	7.72300	5.08000	11.60800
C	7.26400	5.08000	9.29300
H	7.87400	4.61200	12.39700
H	7.11300	4.61200	8.50400
C	7.49400	4.39900	10.45100
H	7.49400	3.47000	10.45100

10-Phenylphenothiazine (from X-ray crystal analysis)

Doi: 10.1107/S0108270185007144

Neutral ground state structure 1

S	18.09300	9.94900	14.26700
N	15.27100	10.89100	13.71900
C	17.18900	11.12700	15.22800
C	17.76200	11.63600	16.36000
C	17.05000	12.47900	17.20300
C	15.74900	12.81200	16.85100
C	15.18100	12.32400	15.71200
C	15.85900	11.45500	14.86600
C	17.40500	10.27600	12.69000
C	18.17800	10.06000	11.54600
C	17.63600	10.11300	10.30000
C	16.28200	10.39800	10.16200
C	15.50900	10.66600	11.28400
C	16.05100	10.63000	12.55700
C	13.83800	11.10100	13.53900
C	12.95900	10.13000	13.97200
C	11.59800	10.29600	13.80700

C	11.11000	11.46400	13.22500
C	11.99100	12.44600	12.81100
C	13.35900	12.27400	12.96400
H	18.62200	11.36100	16.61600
H	17.42000	12.87100	18.01800
H	15.24700	13.42300	17.39200
H	14.22200	12.56500	15.44600
H	19.04000	9.82600	11.73100
H	18.15300	9.93300	9.52600
H	15.87400	10.32600	9.26700
H	14.57600	10.84500	11.15900
H	13.29100	9.36700	14.38400
H	10.97300	9.60000	14.11200
H	10.24800	11.59400	13.10500
H	11.61900	13.29600	12.47900
H	14.01100	12.97700	12.68300

Neutral ground state structure 2

S	13.38200	10.31300	6.29200
N	13.07100	7.28600	6.66400
C	13.08200	9.45400	7.80000
C	12.89900	10.20500	8.94100
C	12.41500	9.63300	10.10400
C	12.20300	8.27200	10.12500
C	12.45400	7.49000	9.01700
C	12.90100	8.05800	7.81000
C	14.09200	9.04400	5.30600
C	14.84000	9.43400	4.18100
C	15.35000	8.48400	3.32600
C	15.17300	7.14600	3.59800
C	14.44000	6.75200	4.71700
C	13.87900	7.69200	5.57000
C	12.73500	5.87600	6.72800
C	11.54800	5.45400	6.17300
C	11.20600	4.10600	6.24600
C	12.05100	3.20500	6.84800
C	13.25200	3.63300	7.38400
C	13.59300	4.97800	7.32700
H	13.11900	11.07900	8.95400
H	12.31000	10.19000	10.87300
H	11.86700	7.85800	10.90000
H	12.29000	6.55600	8.98200
H	14.99800	10.39200	4.04200
H	15.76900	8.71100	2.58600
H	15.49000	6.44000	2.99400
H	14.32400	5.83100	4.81700

H	10.96100	6.07800	5.75600
H	10.41800	3.78300	5.81100
H	11.85200	2.26100	6.81800
H	13.86400	3.00700	7.78400
H	14.34400	5.28800	7.71600

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