Electronic Supplementary Information

Systematic investigation of phthalocyanines, naphthalocyanines, and their aza-analogues. Effect of the isosteric aza-replacement in the core.

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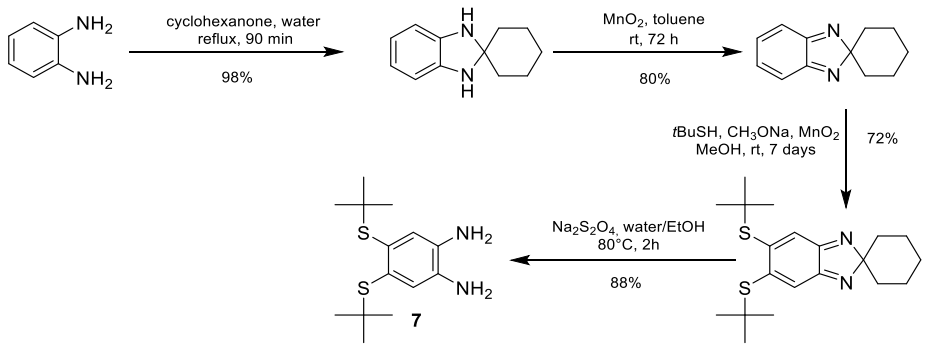
CONTENT

GENERAL

All of the organic solvents were of analytical grade. Anhydrous butanol was stored over magnesium butoxide and distilled prior to use. All chemicals for the syntheses were obtained from established suppliers (Aldrich, Acros, Merck, and TCI Europe) and were used as received. TLC was performed using Merck aluminum sheets with silica gel 60 F254. Merck Kieselgel 60 (0.040–0.063 mm) was used for column chromatography. A CEM Discover and Explorer 24 Automated Microwave Synthesis Workstation with a 24-position reaction deck (CEM Corporation, Matthews, North Carolina, USA) was used for the reactions under microwave irradiation. Reaction temperatures during microwave heating were controlled by external infrared sensor. Melting points were measured on an Electrothermal IA9200 Series Digital Melting Point apparatus. Infrared spectra were measured on a Nicolet 6700 (ATR mode). ^{1}H and ^{13}C NMR spectra were recorded on a Varian Mercury Vx BB 300 NMR or VNMR 500 spectrometers. The reported chemical shifts are given relative to $Si(CH_3)_4$ and are referenced to the signal of the solvent. Elemental analysis was carried out using an Automatic Microanalyser EA1110CE. The UV/Vis spectra were recorded using a Shimadzu UV-2600 spectrophotometer. Matrix-assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectra were recorded in the positive reflectron mode on an AB Sciex 4800 MALDI TOF/TOF mass spectrometer using *trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile as the matrix. The instrument was calibrated externally with a five-point calibration using Peptide Calibration Mix 1 (LaserBio Labs, Sophia- Antipolis, France).

SYNTHESIS OF PRECURSORS



Scheme S1. Synthesis of compound **7**.

2H-benzimidazole-2-spirocyclohexane. This compound was synthesized starting from benzene-1,2-diamine following the original two step procedure (Scheme S1) published by Garner *et al*.[1] with almost identical yield.

5,6-Bis(tert-butylsulfanyl)-2H-benzimidazol-2-spirocyclohexane. The procedure was adopted from lit.[2] but with small modifications that substantially increased the yield. Sodium methoxide (31.5 g, 583 mmol) was dissolved in anhydrous methanol (600 mL) and 2-methylpropane-2-thiol (52.6 g, 65.7 mL, 583 mmol) was added. Then, 2*H*-benzimidazole-2-spirocyclohexane (10.9 g, 58.5 mmol) was added followed by MnO_2 (50.4 g, 583 mmol) and the reaction was stirred for 7 days at rt. Then, the suspension was filtered, the solvent evaporated and water was

added. The mixture was washed three times with chloroform and the organic phase was collected and dried (Na_2SO_4). The product was purified by column chromatography on silica with toluene/acetone 30:1 ($R_f = 0.25$) to yield yellow solid (15.3 g, 72 %). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.34 (s, 2H), 2.02-1.88 (m, 4H), 1.81-1.60 (m, 6H), 1.51 (s, 18H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 157.5, 134.3, 126.0, 107.1, 48.6, 33.2, 30.6, 25.5, 24.7 ppm. The analytical data corresponded well with those published for this compound earlier.[2]

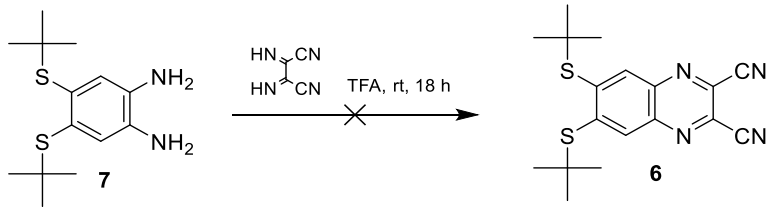
Synthesis of 4,5-bis(*tert*-butylsulfanyl)benzene-1,2-diamine (7). The procedure was adopted from the literature[3] with minor modifications. Sodium dithionite (contains 85 % of the material, 23.7 g, 0.116 mol) was dissolved in water (240 mL) and mixed with a solution of 5,6-bis(*tert*-butylsulfanyl)-2*H*-benzimidazol-2-spirocyclohexane (7.0 g, 19 mmol) in ethanol (240 mL). The reaction mixture was heated at 80°C for 2 h, and then, the ethanol was evaporated under reduced pressure. The aqueous phase was washed three times with ethyl acetate, and the organic layer was dried (Na_2SO_4). The crude product was purified by column chromatography on silica with ethyl acetate/hexane (2:1) to obtain an off-white solid (4.83 g, 88 %). M.p. 158.3-159.1°C (lit.[3] 159.5-160.5°C). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.06 (s, 2H), 3.50 (s, 4H), 1.24 (s, 18H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 134.8, 130.5, 126.8, 47.1, 31.0 ppm. IR (ATR): ν 3417, 3330, 3236, 2974, 2959, 2922, 2898, 2863, 1615, 1561, 1479, 1391, 1362, 1280, 1221, 1166, 966, 889 cm^{-1}. The analytical data corresponded well with those published for this compound previously.[3]

Synthesis of 6,7-bis(*tert*-butylsulfanyl)-1,4-dihydroquinoxaline-2,3-dione (8). Compound **7** (4.8 g, 16.9 mmol) was dissolved in diethyloxalate (100 mL) at 160°C. The product that precipitated from the reaction after several minutes was dissolved by the addition of ethanol (40 mL), and the reaction ran with a reflux condenser for the next 2.5 h at the same temperature. Then, the ethanol was distilled off by removing the condenser, and the reaction was cooled overnight in the freezer. The precipitated product **8** was collected, and the residue that remained in the solvent was purified by column chromatography on silica with ethyl acetate/acetic acid (20:1) as an eluent. Both fractions were combined to obtain a light brown solid (5.0 g, 88 %). The sample was sufficiently pure for the subsequent reactions. The analytical sample was crystallized twice from EtOH/water to obtain light yellow crystals. M.p. dec. from 324°C. ^{1}H NMR (300 MHz, CD_3SOCD_3): δ 11.93 (s, 2H), 7.45 (s, 2H), 1.23 (s, 18H) ppm. ^{13}C NMR (75 MHz, CD_3SOCD_3): δ 155.1, 132.8, 126.0, 123.8, 47.5, 30.9 ppm. IR (ATR): ν 3172, 3058, 2962, 2921, 1696, 1607, 1474, 1456, 1439, 1392, 1363, 1274, 1163, 1106, 990 cm^{-1}. Calcd. for $C_{16}H_{22}N_2O_2S_2$: C 56.77, H 6.55, N 8.28; found: C 56.80, H 6.63, N 8.24 %.

Synthesis of 6,7-bis(*tert*-butylsulfanyl)-2,3-dichloroquinoxaline (9). Compound **8** (3.9 g, 11.5 mmol) was dissolved in THF (300 mL). $SOCl_2$ (8.52 mL, 120 mmol) and DMF (0.85 mL, 11 mmol) were added, and the mixture was heated at reflux for 3 h. Then, the solvents were removed, and the solid was washed with water, dried and purified by column chromatography on silica with toluene/hexane (1:1) as an eluent to obtain a yellow solid (3.35 g, 77 %). M.p. 133.4-134.5°C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.15 (s, 2H), 1.48 (s, 18H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 145.3, 144.0, 139.0, 131.7, 48.6, 30.9 ppm. IR (ATR): ν 2965, 2924, 1582, 1438, 1396, 1362, 1253, 1203, 1140, 1076, 1001, 977, 901, 866 cm^{-1}. Calcd. for $C_{16}H_{20}Cl_2N_2S_2$: C 51.19, H 5.37, N 7.46; found: C 51.16, H 5.46, N 7.27 %.

ALTERNATIVE ATTEMPTS TO SYNTHESIS OF COMPOUND 6

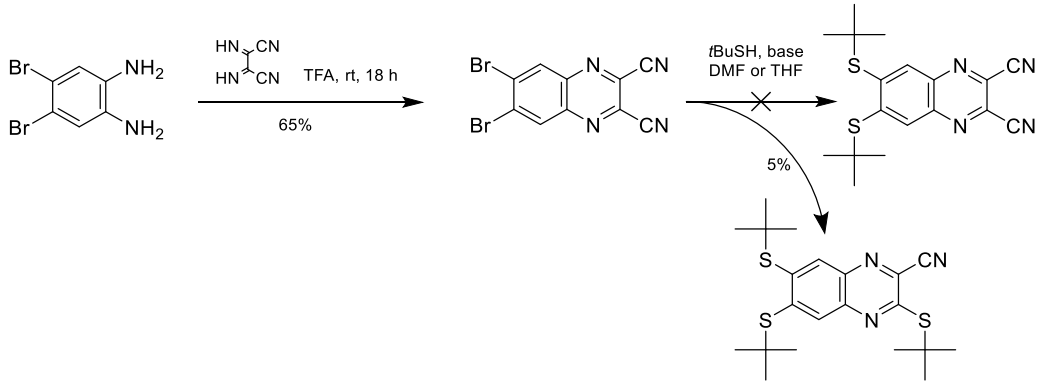
Condensation of compound 7 and diiminosuccinonitrile.



Scheme S2. Alternative attempt to synthesize compound **6** directly from **7**.

This attempt (Scheme S2) was based on known formation of quinoxaline-2,3-dicarbonitriles by reaction of different benzene-1,2-diamines with diiminosuccinonitrile.[4] Compound **7** (60 mg, 0.16 mmol) was homogenized with diiminosuccinonitrile[5] (30 mg, 0.28 mmol) and transferred into the round-bottom flask with trifluoroacetic acid (TFA, 5 mL) that was subsequently filled with argon. The reaction ran at rt for 18 h and then was poured to water. TLC analysis of the precipitate did not show any product with expected R_f in chloroform or toluene as mobile phases.

Nucleophilic substitution of 6,7-dibromoquinoxaline-2,3-dicarbonitrile.



Scheme S3. Alternative attempt to synthesize compound **6** based on nucleophilic substitution in 6,7-dibromoquinoxaline-2,3-dicarbonitrile.

6,7-Dibromoquinoxaline-2,3-dicarbonitrile. 4,5-Dibromobenzene-1,2-diamine[6] (1.68 g, 6.3 mmol) was homogenized with diiminosuccinonitrile[5] (1.00 g, 9.4 mmol) and transferred into the round-bottom flask with TFA (30 mL) that was subsequently filled with argon. The reaction ran at rt for 18 h and then was poured to water. The precipitate was collected, washed with water and purified by column chromatography on silica with toluene to obtain light yellow solid (1.4 g, 65 %). M.p. 300-303°C (dec.). ^{1}H NMR (300 MHz, CD_3SOCD_3): δ 8.85 (s) ppm. ^{13}C NMR (75 MHz, CD_3SOCD_3): δ 139.7, 133.6, 132.7, 132.0, 114.5 ppm.

Nucleophilic substitution of 6,7-dibromoquinoxaline-2,3-dicarbonitrile (Scheme S3). 6,7-Dibromoquinoxaline-2,3-dicarbonitrile (0.1 g, 0.296 mmol) was dissolved in DMF and 2-methylpropane-2-thiol (66 μL, 0.585 mmol) was added. Anhydrous K_2CO_3 (0.12 g, 0.868 mmol) was subsequently added. The reaction was stirred at rt for 1 hour, then poured into a water and washed three times with chloroform. The TLC (toluene) of the organic layer indicated

large number of products. The most intense spot was isolated by column chromatography on silica (toluene) and a yellow product was obtained (5 mg, 5 %). The product was characterized to be 3,6,7-tris(*tert*-butylsulfanyl)quinoxaline-2-carbonitrile. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.18 (s, 1 H), 8.08 (s, 1 H), 1.74 (s, 9H), 1.54 (s, 9H), 1.48 (s, 9H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 30.1, 30.9, 31.0, 48.5, 48.8, 50.9, 114.8, 128.8, 130.2, 135.0, 136.8, 140.3, 140.9, 148.1, 158.5 ppm.

SYNTHESIS OF MACROCYCLES

Synthesis of 2,3,9,10,16,17,23,24-octakis(*tert*-butylsulfanyl)tetrapyrazinoporphyrazinato zinc(II) (TPyzPz). Compound **1** (100 mg, 0.33 mmol) and anhydrous $Zn(CH_3COO)_2$ (61 mg, 0.33 mmol) were weighed in a flask that was subsequently filled with argon. Anhydrous pyridine (1 mL) was added, and the mixture was heated at reflux for 12 h. Pyridine was evaporated, and a mixture of water/methanol/acetic acid (10:10:1) (100 mL) was added. The precipitate was collected, washed with the same mixture, water, and methanol and then air-dried. The solid was extracted using chloroform, filtered, evaporated and purified by column chromatography on silica with toluene/chloroform/THF (20:10:1) as an eluent. The pure fractions were evaporated, and the solid was washed with methanol to obtain a green solid (64 mg, 63 %). ^{1}H NMR (300 MHz, $CDCl_3/C_6D_5N$ 3:1): δ 2.24 (s, 72H) ppm. ^{13}C NMR (75 MHz, $CDCl_3/C_6D_5N$ 3:1): δ 158.5, 151.5, 144.5, 51.5, 30.8 ppm. The analytical data corresponded well with those published for this compound prepared by an alternative procedure.[7]

Synthesis of 2,3,9,10,16,17,23,24-octakis(*tert*-butylsulfanyl)phthalocyaninato zinc(II) (Pc). The same procedure that was used to synthesize **TPyzPz** was used to synthesize **Pc** but starting from compound **4** (100 mg, 0.33 mmol). Yield: 54 mg (51 %). ^{1}H NMR (300 MHz, $CDCl_3/C_6D_5N$ 3:1): δ 9.91 (s, 8H), 1.78 (s, 72H) ppm. ^{13}C NMR (75 MHz, $CDCl_3/C_6D_5N$ 3:1): δ 154.2, 141.7, 137.7, 130.8, 48.9, 31.7 ppm. The analytical data corresponded well with those published for this compound prepared by an alternative procedure.[7]

Synthesis of 2,3,11,12,20,21,29,30-octakis(*tert*-butylsulfanyl)tetra[6,7]quinoxalinoporphyrazinato zinc(II) (6,7-TQPz). Compound **3** (100 mg, 0.28 mmol) and anhydrous $Zn(CH_3COO)_2$ (51 mg, 0.28 mmol), were weighed into a flask that was subsequently filled with argon. Anhydrous pyridine (1 mL) was added, and the mixture was heated at reflux for 12 h. The reaction mixture was poured into water/methanol/acetic acid (10:1:1 mixture, 100 mL) and stirred for 30 min. The precipitate was collected, washed with water, methanol, and acetone and air dried. The crude product was adsorbed to silica (0.5 g) and washed with methanol until the passing solution was colorless. Then, the silica was dried carefully, and the product was further purified by column chromatography on silica with toluene/pyridine (20:1) as an eluent. After the evaporation of the pure fractions from chromatography, the solid was washed thoroughly with acetone to obtain a dark green solid (45 mg, 43 %). ^{1}H NMR (300 MHz, $CDCl_3/C_6D_5N$ 3:1): δ 9.66 (s, 8H), 2.06 (s, 72H) ppm. ^{13}C NMR (75 MHz, $CDCl_3/C_6D_5N$ 3:1): δ 156.8, 153.3, 139.2, 136.9, 121.4, 50.5, 30.6 ppm. The

analytical data corresponded well with those published for this compound prepared by an alternative procedure.[8]

SYNTHETIC PROTOCOLS USED FOR ASSESSMENT OF REACTIVITY IN CYCLOTETRAMERIZATION.

Reaction with lithium butoxide. Corresponding starting material, aromatic dicarbonitrile (0.33 mmol) was dissolved in anhydrous butanol (2 mL) freshly distilled from magnesium and heated to reflux. A piece of metal lithium (0.33 mmol) was put inside through the condenser and the reflux continued for next 3 h. Afterwards, anhydrous $Zn(CH_3COO)_2$ (303 mg, 1.65 mmol) was added and the mixture was heated at reflux for 1 h. The reaction was cooled down to rt and poured into a mixture of water/methanol/acetic acid 10:10:1 (100 mL). The precipitate was collected, washed with the same mixture of solvents, water and air-dried. The purification followed the procedures mentioned for particular compound in the manuscript or ESI.

Reaction with magnesium butoxide. Magnesium (55 mg, 2.30 mmol) was added to anhydrous butanol (2 mL) freshly distilled from magnesium and heated to reflux with a small crystal of iodine. Magnesium butoxide formed after 2 h and starting material, aromatic dicarbonitrile (0.33 mmol), was added. The reaction was heated to reflux for 12 h, cooled down to rt and poured into a mixture of water/methanol/acetic acid 10:10:1 (100 mL). The precipitate was collected, washed with the same mixture, water and air-dried. The solid was extracted using chloroform, filtered, evaporated and dissolved in chloroform (50 mL). *p*-Toluenesulfonic acid (156 mg, 0.82 mmol) dissolved in THF (20 mL) was added and the mixture was stirred at rt for 2 h. After evaporation of the solvents, the metal-free derivative was washed with water and air-dried. All product was subsequently dissolved in pyridine (25 mL), anhydrous $Zn(CH_3COO)_2$ (151 mg, 0.82 mmol) was added and the mixture was heated at reflux for 1 h. Pyridine was evaporated and a mixture of water/methanol/acetic acid 10:10:1 (100 mL) was added. The purification followed the procedures mentioned for particular compound in the manuscript or ESI.

Reaction with zinc acetate in pyridine. Starting materials, aromatic dicarbonitrile (0.33 mmol) and anhydrous $Zn(CH_3COO)_2$ (61 mg, 0.33 mmol), were weighted into the flask that was subsequently filled with argon. Anhydrous pyridine (1 mL) was added and the mixture was heated to reflux for 12 h. Pyridine was evaporated and a mixture of water/methanol/acetic acid 10:10:1 (100 mL) was added. The purification followed the procedures mentioned for particular compound in the manuscript or ESI. Alternatively, the reaction was performed also under microwave irradiation in a closed vessel with the same amounts of reactants, reaction time 12 h and temperature 170 °C.

Reaction with zinc acetate in DMF. The same procedure as above (*Reaction with zinc acetate in pyridine)* was used but with refluxing anhydrous DMF (1 mL).

NMR SPECTRA

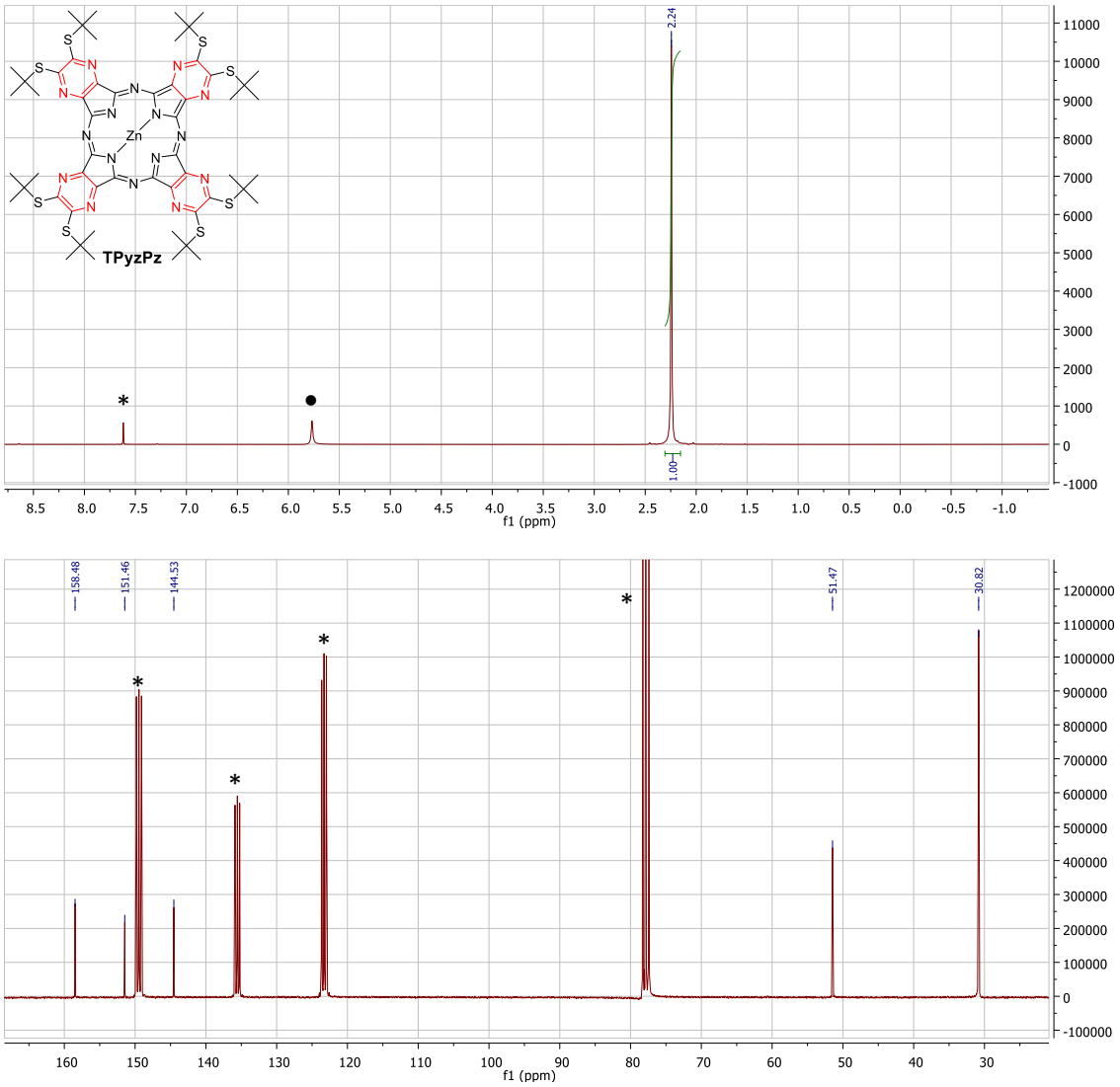


Figure S1. ^{1}H (300 MHz) and ^{13}C NMR (75 MHz) spectra of **TPyzPz** in $CDCl_3/C_6D_5N$ 3:1. Asterisk indicates solvent signal, dot indicates signal of water.

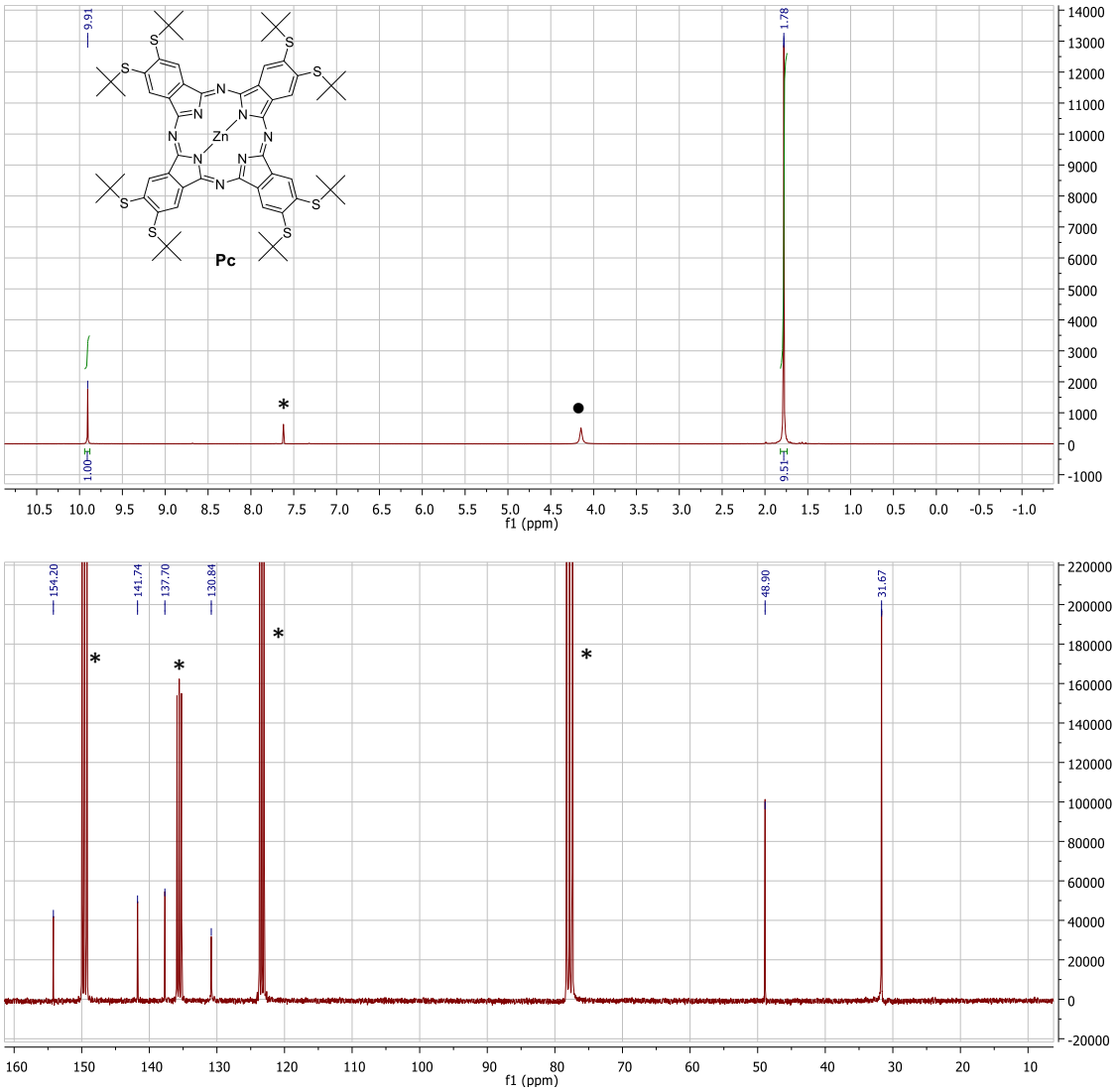


Figure S2. ^{1}H (300 MHz) and ^{13}C NMR (75 MHz) spectra of **Pc** in $CDCl_3/C_6D_5N$ 3:1. Asterisk indicates solvent signal, dot indicates signal of water.

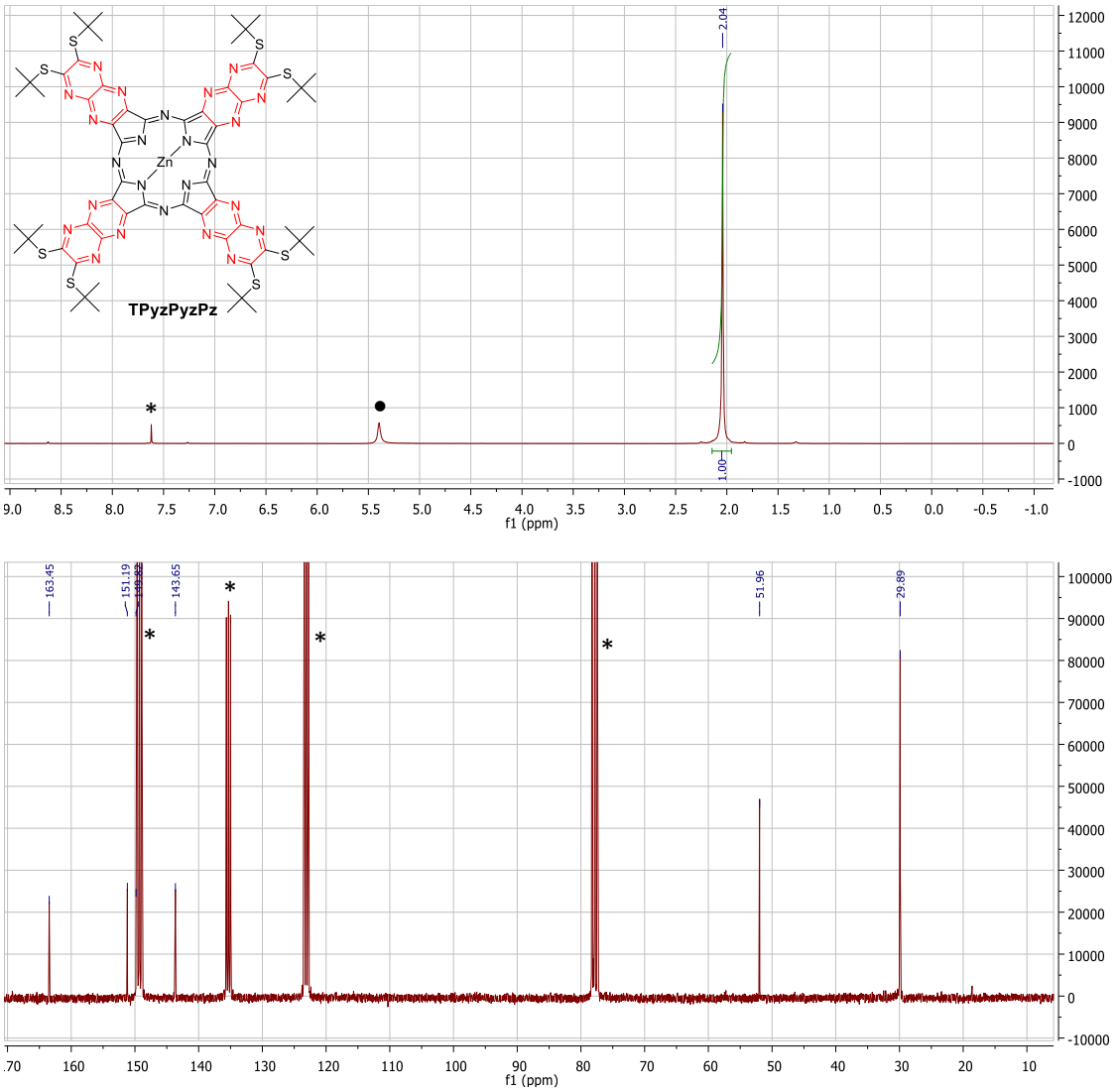


Figure S3. ^{1}H (300 MHz) and ^{13}C NMR (75 MHz) spectra of **TPyzPyzPz** in $CDCl_3/C_6D_5N$ 3:1. Asterisk indicates solvent signal, dot indicates signal of water.

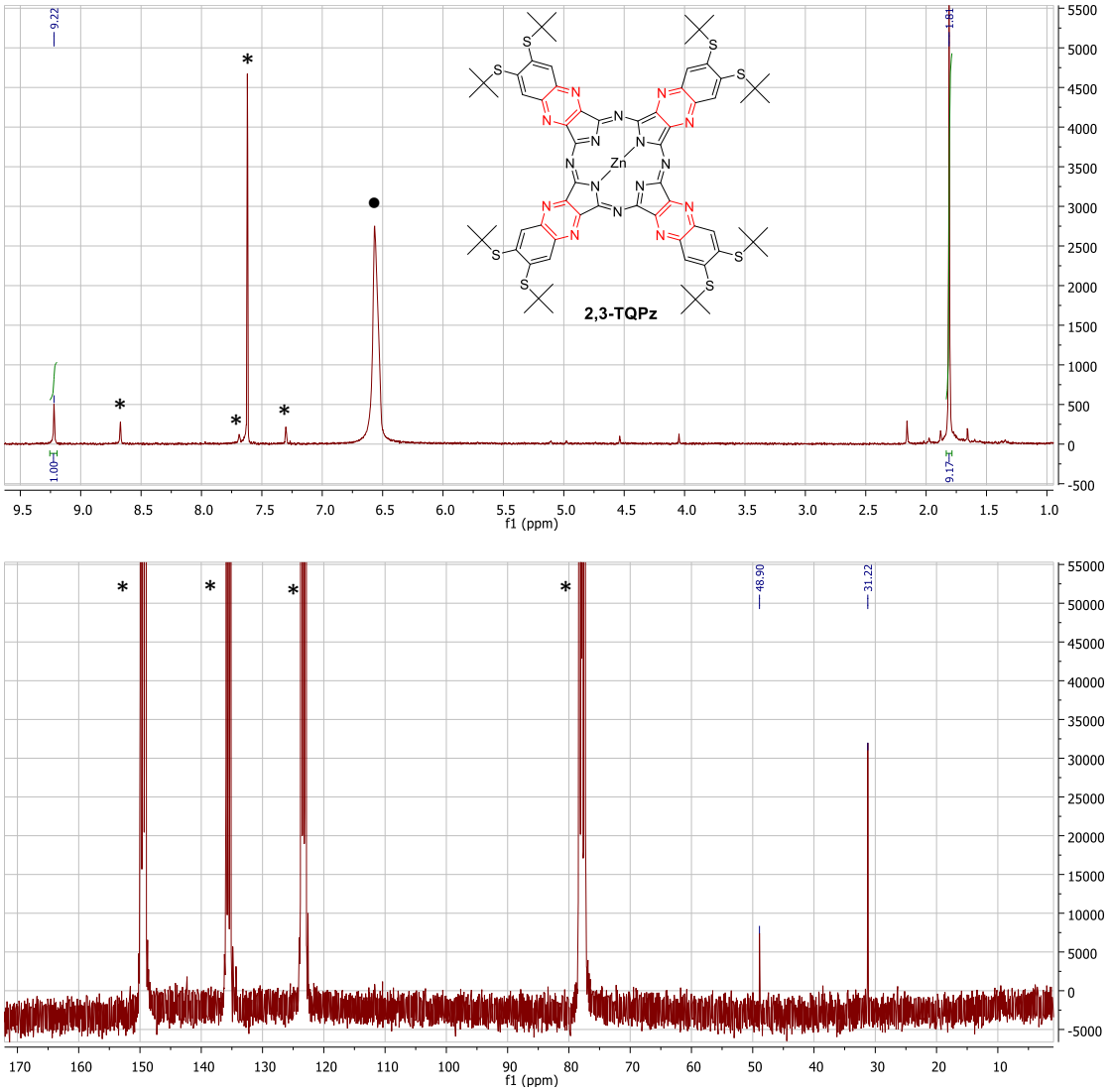


Figure S4. ^{1}H (300 MHz) and ^{13}C NMR (75 MHz) spectra of **2,3-TQPz** in $CDCl_3/C_6D_5N$ 3:1. Asterisk indicates solvent signal, dot indicates signal of water.

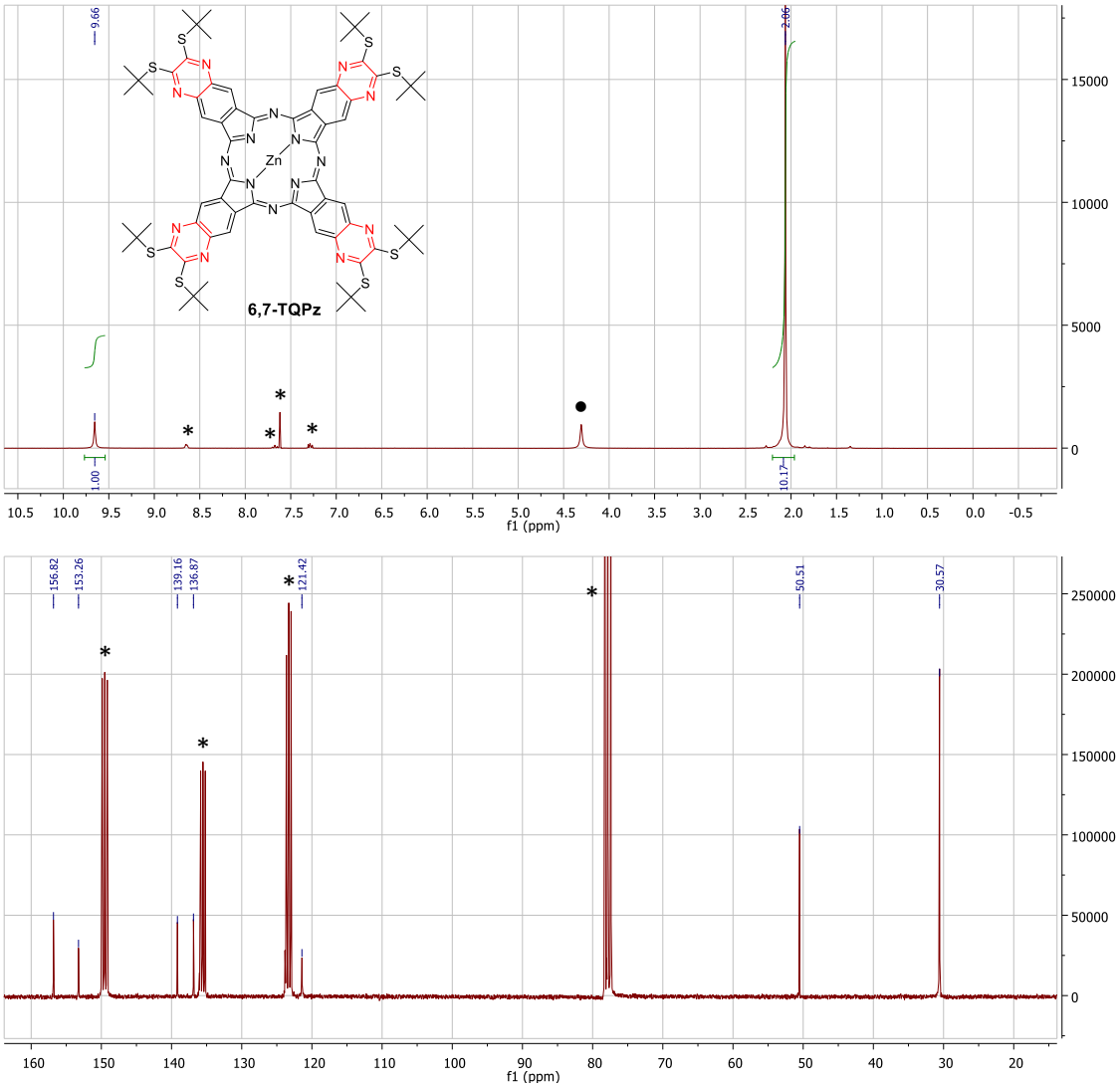


Figure S5. ^{1}H (300 MHz) and ^{13}C NMR (75 MHz) spectra of **6,7-TQPz** in $CDCl_3/C_6D_5N$ 3:1. Asterisk indicates solvent signal, dot indicates signal of water.

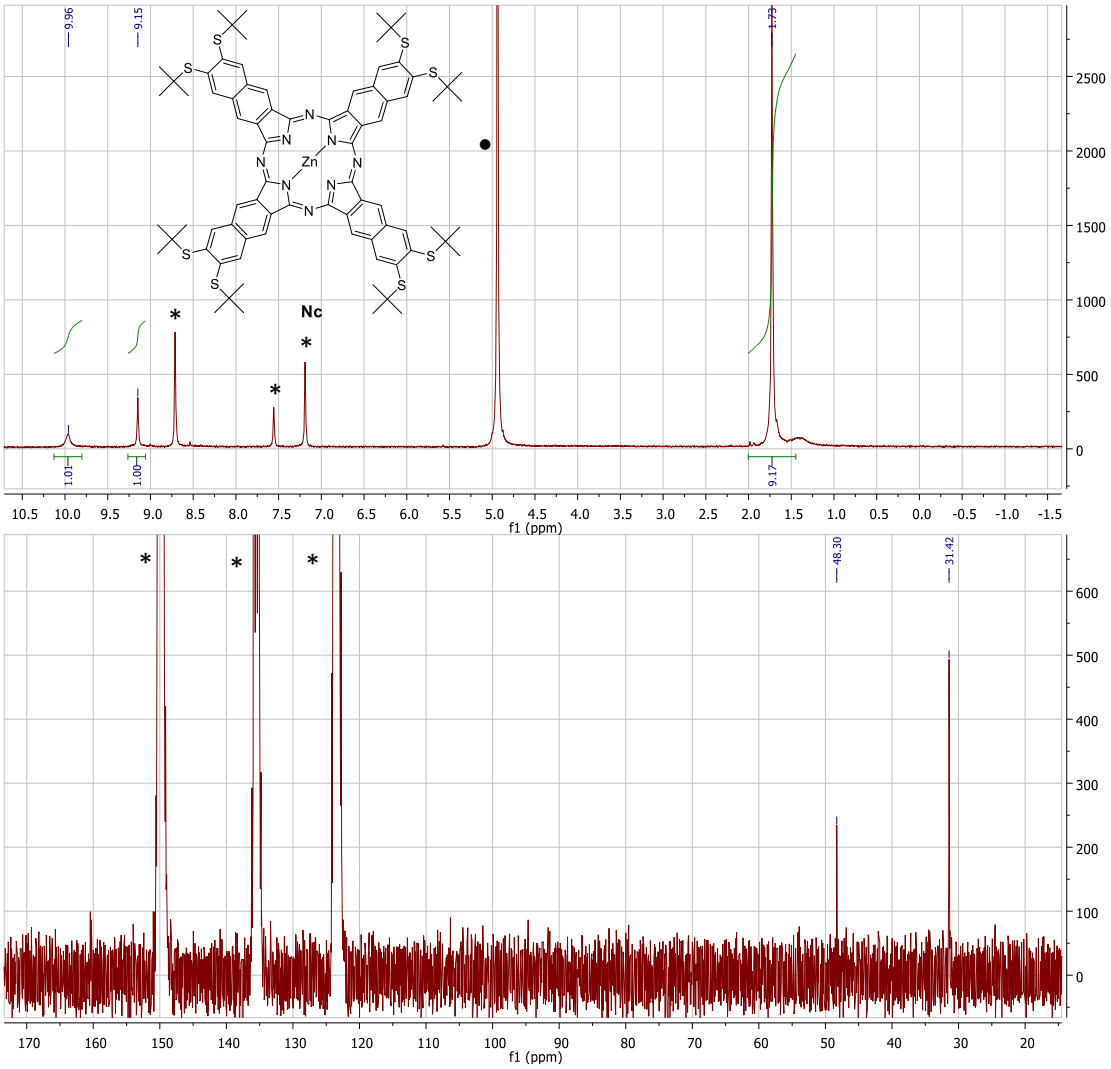


Figure S6. ^{1}H (300 MHz) and ^{13}C NMR (75 MHz) spectra of **Nc** in C_6D_5N. Asterisk indicates solvent signal, dot indicates signal of water.

ABSORPTION SPECTRA, MCD SPECTRA

UV-vis-NIR data were obtained on a Jasco V-670 or Shimadzu UV-2600 spectrophotometer. Magnetic circular dichroism (MCD) data were recorded using an OLIS DCM 17 CD spectropolarimeter using a permanent 1.4 T DeSa magnet. The spectra were recorded twice for each sample, first with a parallel field and then with an antiparallel field. Their intensities were expressed by molar ellipticity per T.

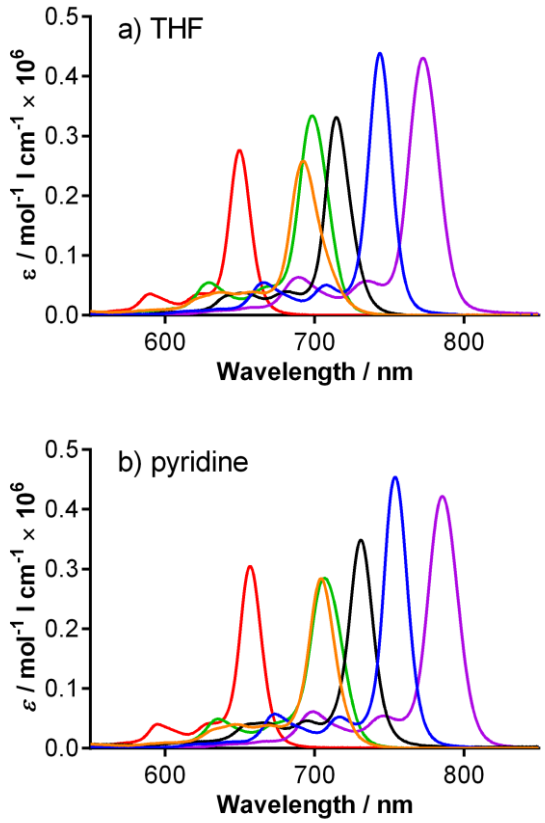


Figure S7. Absorption spectra of **TPyzPz** (red), **TPyzPyzPz** (orange), **Pc** (green), **2,3-TQPz** (black), **6,7-TQPz** (blue) and **Nc** (magenta) in THF (a) and pyridine (b).

SOLUBILITY

Experimental: A sample (approximately 5 mg) was suspended in the solvent (typically 1-2 mL) at room temperature to obtain a concentrated solution with an undissolved portion of solid. This suspension was stirred for 5 h, sonicated for 10 min and stirred for another 12 h at room temperature. The supernatant was collected and centrifuged (16,800 g, 21°C, 15 min), and the supernatant was collected again. The centrifugation was repeated (at least once more) to obtain a homogenous solution without the remaining undissolved solid. The solution (10 μL) was diluted in pyridine to obtain a concentration in a range of 0.5-1.5 μM, and the absorption spectra were measured. Pyridine was chosen to ensure the monomeric character of the studied compounds. Concentration (c) of a saturated solution was calculated using Eq. S1:

$$c = \frac{A}{\varepsilon} \times dilution \qquad \text{(Eq. S1)}$$

where A is absorbance of the solution and ε is the extinction coefficient in pyridine. The data presented are the means of three independent experiments.

Discussion: In general, unsubstituted Pcs and their derivatives are known for low solubility in organic solvents that is usually improved by peripheral substitution. First, solubility of two representative compounds was studied in solvents of different polarity. The solubility increased with less polar character of the solvent due to the hydrophobic nature of both **TPyzPz** and **Pc**, as is clear from Figure S8 and Table S1. The unusually high solubility of **Pc** in pyridine that does not fit to the observed polarity dependence can be explained by the strong coordinating character of this solvent. Coordination apparently broke the intermolecular forces and increased the solubility. Interestingly, unsubstituted ZnPc was reported to dissolved well in rather more polar coordinating solvents DMAC, DMSO, THF (<1 mmol kg^{-1}), NMP (6.9 mmol kg^{-1}) while being insoluble in benzene or toluene.[9] Apparently, the coordination character plays much more important role in solubility of flat unsubstituted ZnPc. In case of Pcs substituted with bulky substituents that are the primary cause of decreased self-association in the solid state, the solubility follows rather the hydrophilic/phobic nature of the macrocycle and the solvent.

Table S1. Solubility (mM) of **Pc** and **TPyzPz** in different solvents.[a]

Solvent	**Pc**	**TPyzPz**	Polarity index
toluene	4.38 (± 0.10)	4.74 (± 0.09)	2.4
benzene	4.31 (± 0.14)	2.15 (± 0.21)	2.7
THF	1.11 (± 0.03)	0.54 (± 0.04)	4
1,4-dioxane	0.51 (± 0.01)	0.74 (± 0.02)	4.8
acetone	0.06 (± 0.01)	0.17 (± 0.02)	5.1
pyridine	2.91 (± 0.08)	0.72 (± 0.02)	5.3
DMF	0.51 (± 0.01)	0.10 (± 0.02)	6.4

[a]Expressed as mean (± standard deviation) of three measurements.

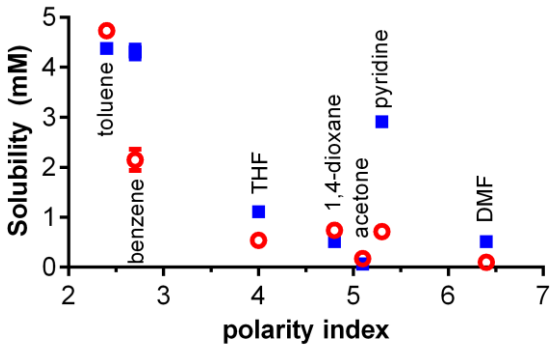


Figure S8. Solubility of **TPyzPz** (red dot) and **Pc** (blue square) in different solvents. Mean (± standard deviation) of three independent measurements.

Based on the above-mentioned observations, toluene was selected as the solvent for solubility determination of the whole series of studied compounds, because it assured high solubility. It is also a non-coordinating solvent that did not influence solubility by different levels of coordination. The results are summarized in Table S2. Unexpectedly, **2,3-TQPz** was found to be fully insoluble in toluene. For this reason, its solubility was determined also in the coordinating solvents THF and pyridine (Table S2). However, even in these solvents the solubility of **2,3-TQPz** was of several orders of magnitude lower than for **Pc** or **TPyzPz** in the same solvents (compare with data in Table S1). Two important facts can be revealed from data in Table S2, when omitting **2,3-TQPz**: a) enlarged macrocycles suffer from much lower solubility in comparison with lower homologues, and b) aza-replacement increases the solubility. The latter fact was well documented, particularly for enlarged macrocycles **6,7-TQPz** and **TPyzPyzPz** with a comparable solubility (~ 2.5 mM) that exceeds that of **Nc** (0.1 mM) by more than 1 order of magnitude. The differences were less pronounced between **Pc** and **TPyzPz** (both ~ 4.5 mM) that, in general, behaved very similarly (Figure S8, Table S2). The first fact is supported by similarly decreasing solubility after enlargement of the macrocycle system for magnesium complexes of octapyridinated porphyrazine, TPyzPz and 6,7-TQPz where the highest solubility is reported to be in order of ~10^{-3}, ~10^{-4} and ~10^{-5} M, respectively.[10]

Table S2. Solubility of the studied compounds in toluene.

Compound	Solubility (mM)	Solubility (mg mL^{-1})
Nc	0.10	0.15
6,7-TQPz	2.16	3.21
TPyzPyzPz	2.44	3.65
2,3-TQPz	-[a]	-
Pc	4.38	5.62
TPyzPz	4.74	6.10

[a]insoluble in toluene, solubility of **2,3-TQPz** in THF: 2.8 μM, in pyridine: 130 μM.

AGGREGATION

The solution (100 μM) of the appropriate compound in toluene was prepared and absorption spectrum was measured (Figure S9). The solution was then diluted twice with toluene and absorption spectrum was taken again. The diluting procedure was repeated several times until the signal of absorption spectra was detectable (usually up to 0.2 μM). Absorption spectra of more concentrated solutions were taken using quartz optical cell with 1 mm pathlength while samples of lower concentrations using quartz optical cell with 10 mm pathlength. Dimerization constant (K_D) was estimated (where possible) from dependence of ε on concentration (Figure S9 insets) using nonlinear regression in Prism 6 for Windows (v 6.04, GraphPad Software, Inc.).

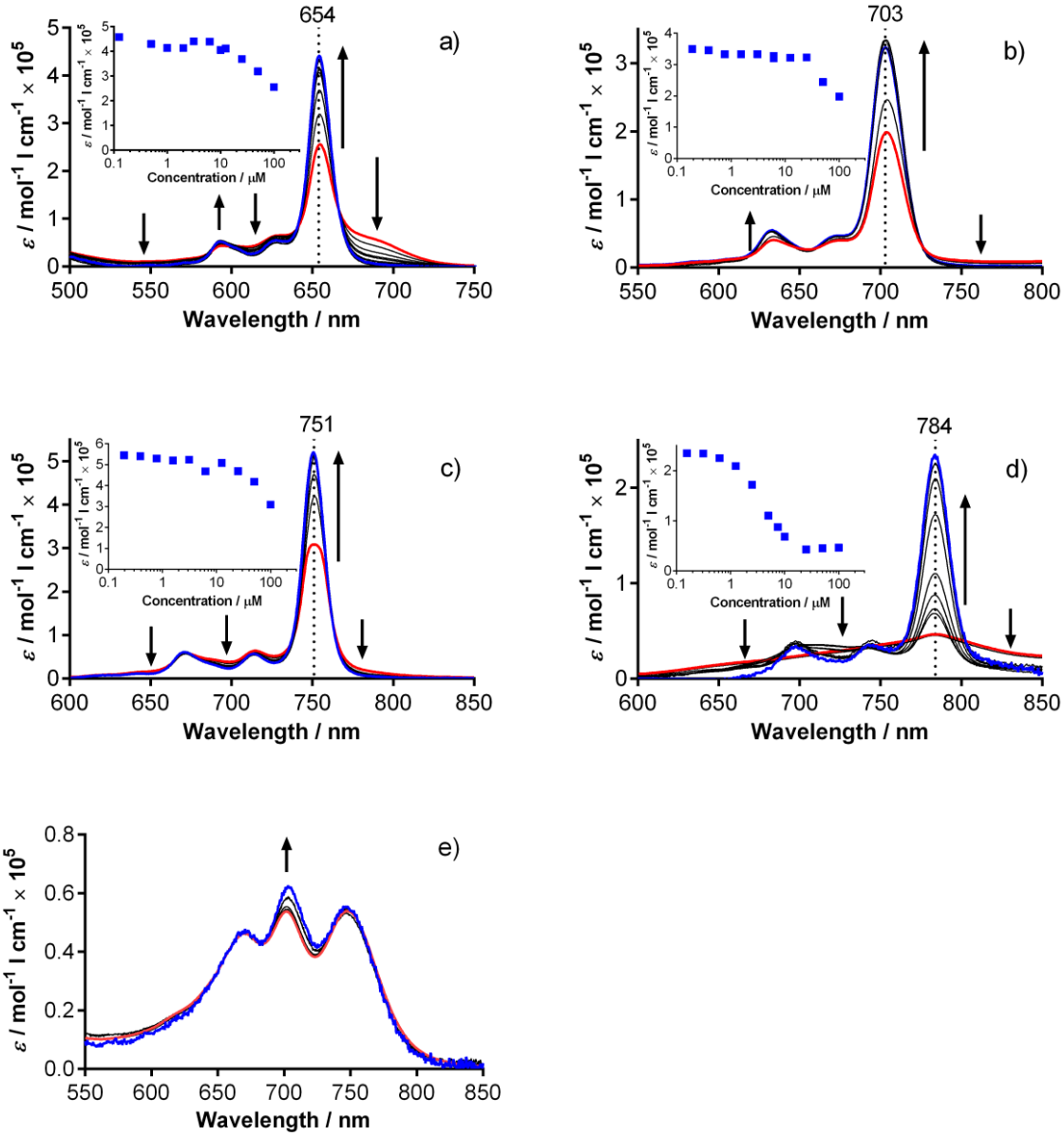


Figure S9. Changes in absorption spectra of studied compounds (**TPyzPz** (a), **Pc** (b), **6,7-TQPz** (c), **Nc** (d), **TPyzPyzPz** (e)) in toluene with dilution from 100 μM (red spectrum) to approximately 0.2 μM (blue spectrum). Insets: dependence of ε at Q-band maximum (dotted line in spectra) on concentration.

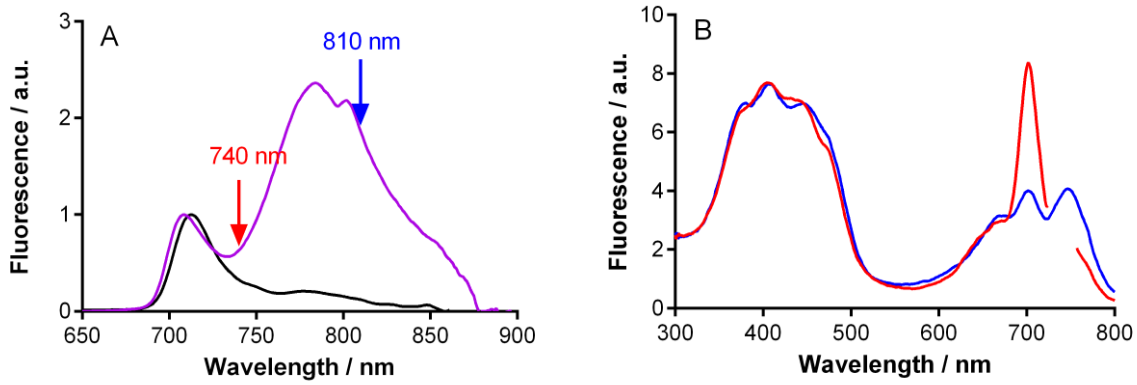


Figure S10. A) Normalized emission spectra (λ_{exc} = 410 nm) of **TPyzPyzPz** in toluene (magenta) and pyridine (black) The spectra were normalized to the same fluorescence intensity of monomeric species. B) Excitation spectra of **TPyzPyzPz** in toluene with λ_{em} = 810 nm (blue, major contribution from J-dimer) and λ_{em} = 740 nm (red, more contribution from monomer). The excitation spectra were normalized to the same signal intensity in B-band. The part of the red excitation spectrum corresponding to scattered light (λ_{em} = 740 nm) was removed.

PHOTOPHYSICAL MEASUREMENTS

All samples were re-purified using preparative TLC for the photophysical measurements (both Φ_F and Φ_Δ) to ensure that they were highly pure. The fluorescence spectra were obtained using an AMINCO Bowman Series 2 luminescence spectrometer. All emission spectra were corrected for the instrument response. The fluorescence quantum yields (Φ_F) were determined in THF or pyridine *via* the comparative method[11] using unsubstituted zinc phthalocyanine (ZnPc, Sigma-Aldrich) as a reference (Φ_F = 0.32 in THF[12], Φ_F = 0.28 in pyridine[12]). Both the reference and sample were excited at 370 nm. The absorbance at the excitation wavelength was held below 0.015, and the absorbance at the Q-band maximum was held below 0.05 to limit the inner filter effect. All experiments were performed in triplicate with the data representing the mean (estimated error ± 15 %).

The quantum yields of the singlet oxygen (Φ_Δ) were determined in THF or pyridine according to a previously published procedure[11] using the decomposition of a chemical trap 1,3-diphenylisobenzofuran (DPBF) with ZnPc as a reference (Φ_Δ = 0.53 in THF[13], Φ_Δ = 0.61 in pyridine[14]). All experiments were performed in triplicate, and the data presented herein represent the mean of the three experiments (estimated error: ± 10 %).

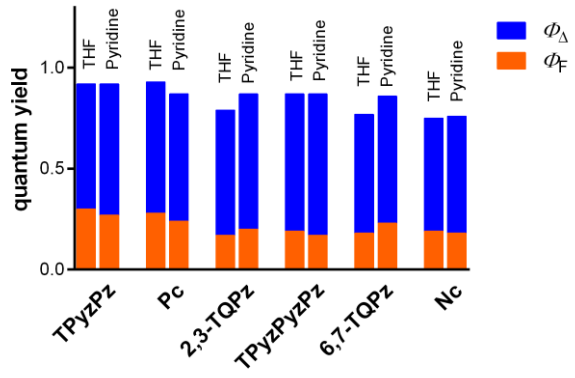


Figure S11. Quantum yields of fluorescence and singlet oxygen of studied compounds in THF and pyridine.

PHOTOSTABILITY

The 2.5 mL of solution of the corresponding dye in pyridine (c ≅ 2 μM) was stirred at rt and irradiated in 10 mm × 10 mm quartz cell for total time of 30 minutes using a halogen lamp (EMOS, 400 W). In case when the photodecomposition was too slow, the irradiation continued for longer time to see the progress in spectra. Absorption spectra were collected typically in 5 min periods. Incident light was filtered through a water filter (6 cm) to remove heat. A decomposition of a sample was expressed as a relative decrease of its absorbance at Q-band maximum (707 nm for **Pc**, 657 nm for **TPyzPz**, 705 nm for **TPyzPyzPz**, 754 nm for **6,7-TQPz**, 731 nm for **2,3-TQPz**, 786 nm for **Nc**, and 674 nm for ZnPc). Unsubstituted ZnPc was added to the series as a reference. All experiments were performed three times, and the data represent a mean of these three experiments. A control experiment involved measurement of the same samples in the dark. No spectral changes were observed without irradiation.

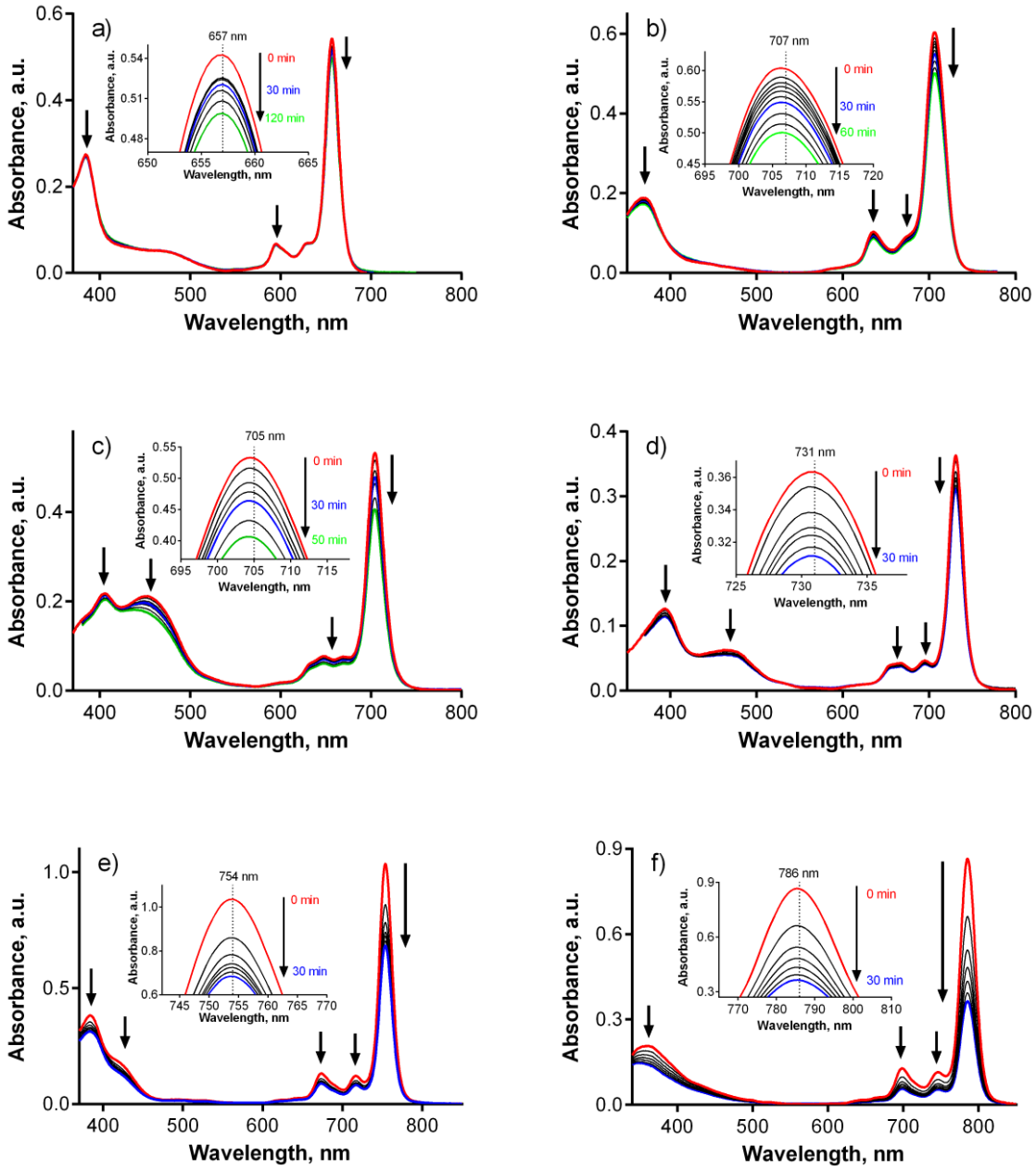


Figure S12. Spectral changes of the target compounds upon irradiation of the pyridine solution by halogen lamp (400 W). Red line – before irradiation, blue line – 30 min of irradiation. Insets: enlarged area of the Q-band. **TPyzPz** (a), **Pc** (b), **TPyzPyzPz** (c), **2,3-TQPz** (d), **6,7-TQPz** (e), **Nc** (f).

ELECTROCHEMISTRY AND SPECTROELECTROCHEMISTRY

The electrochemical measurements (cyclic voltammetry, square wave voltammetry) were performed at room temperature (25 °C) using an Autolab PGSTAT30 potentiostat. Measurements were carried out with a three electrode setup consisting of a glassy carbon electrode (working electrode), a platinum wire (counter electrode), and a $Ag/AgNO_3$ non-aqueous electrode (reference electrode). The cell was degassed under an argon atmosphere, solution of appropriate compound (typically 1×10^{-3} M) in anhydrous solvent (THF or pyridine) containing 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) as a supporting electrolyte was added and purged by argon for 5 minutes to remove dissolved oxygen. Different scan rates were applied at cyclic voltammetry measurement (50 mV/s, 100 mV/s and 200 mV/s) for each sample and solvent. Half-wave potentials ($E_{1/2}$) were calculated from square wave voltammetry (sweep width 25.05 mV, step potential 19.5 mV) and are referenced to a saturated calomel electrode (SCE) with ferrocene as the internal standard (half-wave potential $E_{1/2}(Fc/Fc^+) = +0.38$ V vs. SCE[15]).

Spectroelectrochemical data were collected on a JASCO-720 spectrophotometer at room temperature, and the experiments were conducted using a CHI-620C electrochemical analyzer using a custom-made 1 mm cell, and a Pt mesh-working electrode. Measurements were conducted in 0.3 M tetrabutylammonium perchlorate (TBAP) in pyridine.

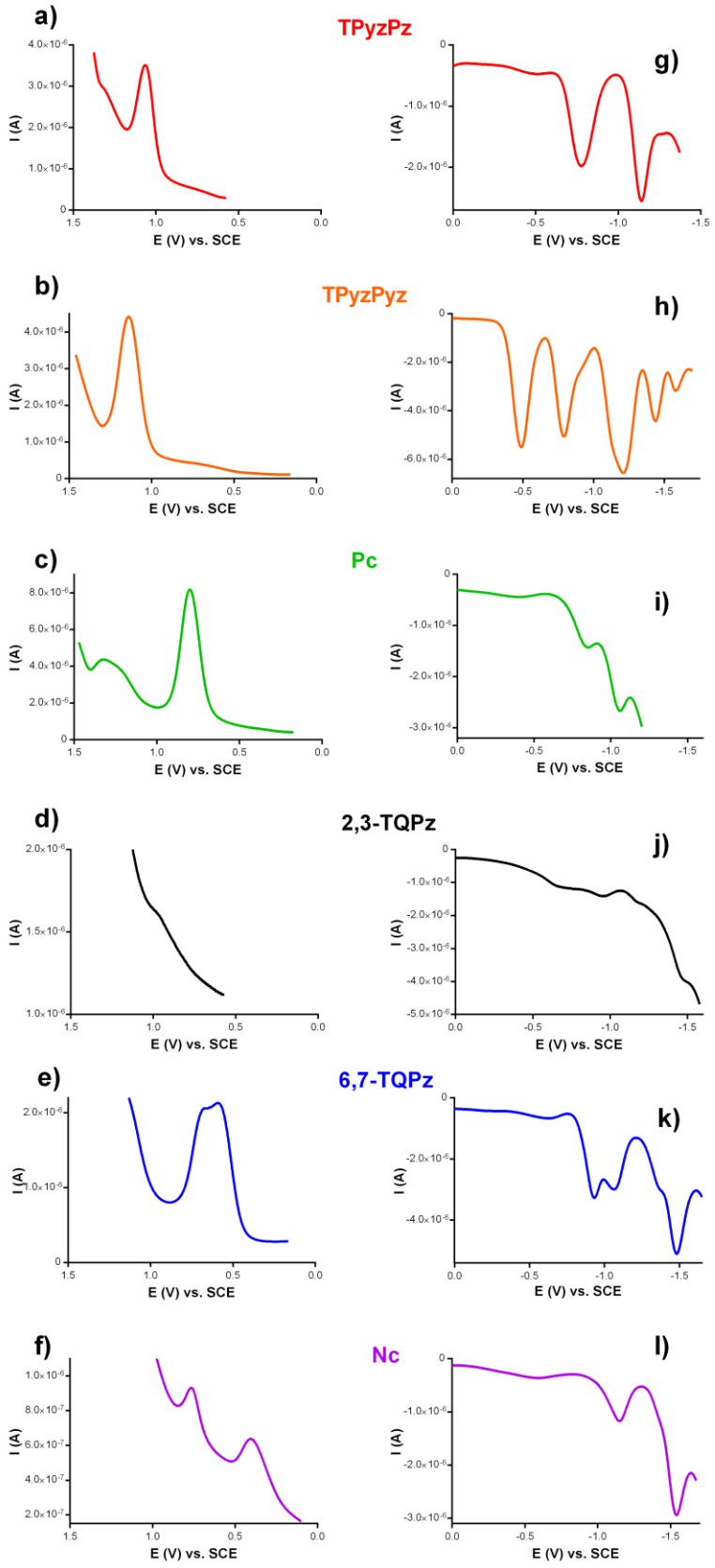


Figure S13. Square wave voltammograms of studied compounds in THF at 25 °C (a-f oxidation processes; g-l reduction processes). Sweep width 25.05 mV, step potential 19.5 mV.

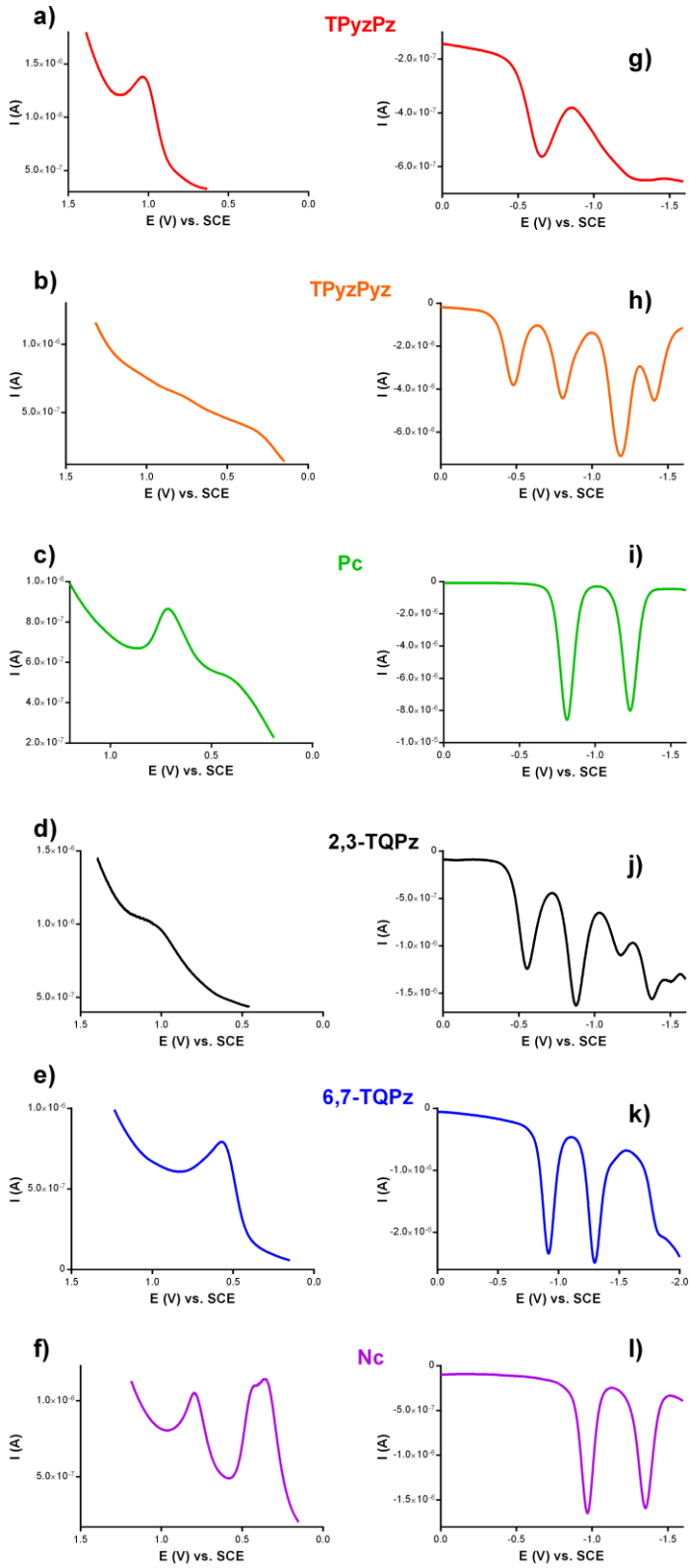


Figure S14. Square wave voltammograms of studied compounds in pyridine at 25 °C (a-f oxidation processes; g-l reduction processes). Sweep width 25.05 mV, step potential 19.5 mV. E_{ox}^{1} of TPyzPyz mentioned in Table 3 was determined directly from appropriate cyclic voltammogram due to low quality of square wave voltammogram b).

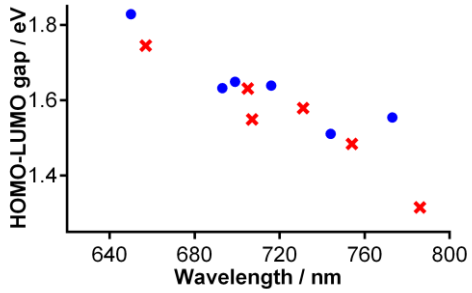


Figure S15. Dependence of HOMO-LUMO gap determined from electrochemical measurements on wavelength of maximum in Q-band in the studied compounds (**TPyzPz**, **Pc**, **TPyzPyzPz**, **2,3-TQPz**, **6,7-TQPz**, **Nc**) in THF (blue dot) and pyridine (red cross).

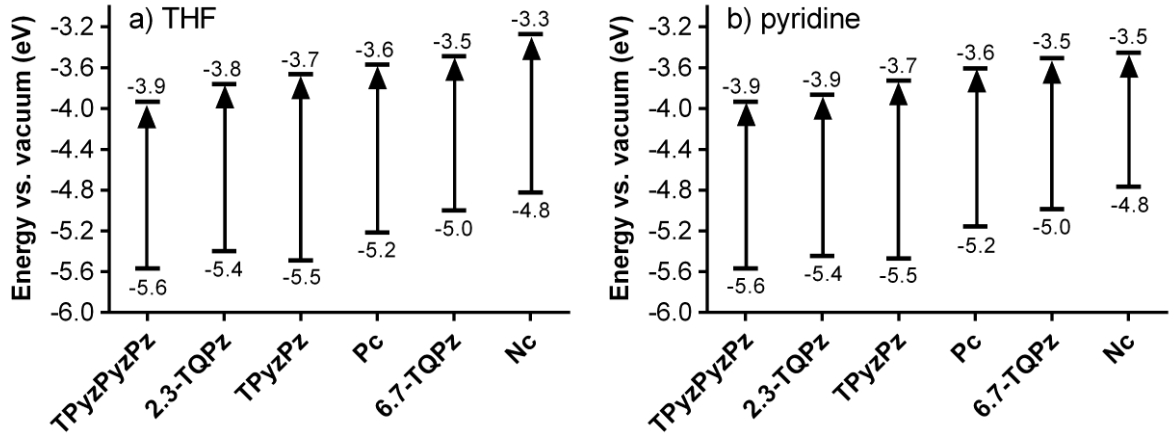


Figure S16. Positions of HOMO-LUMO (eV) of studied compounds in THF (a) and pyridine (b) calculated from experimental electrochemical data.

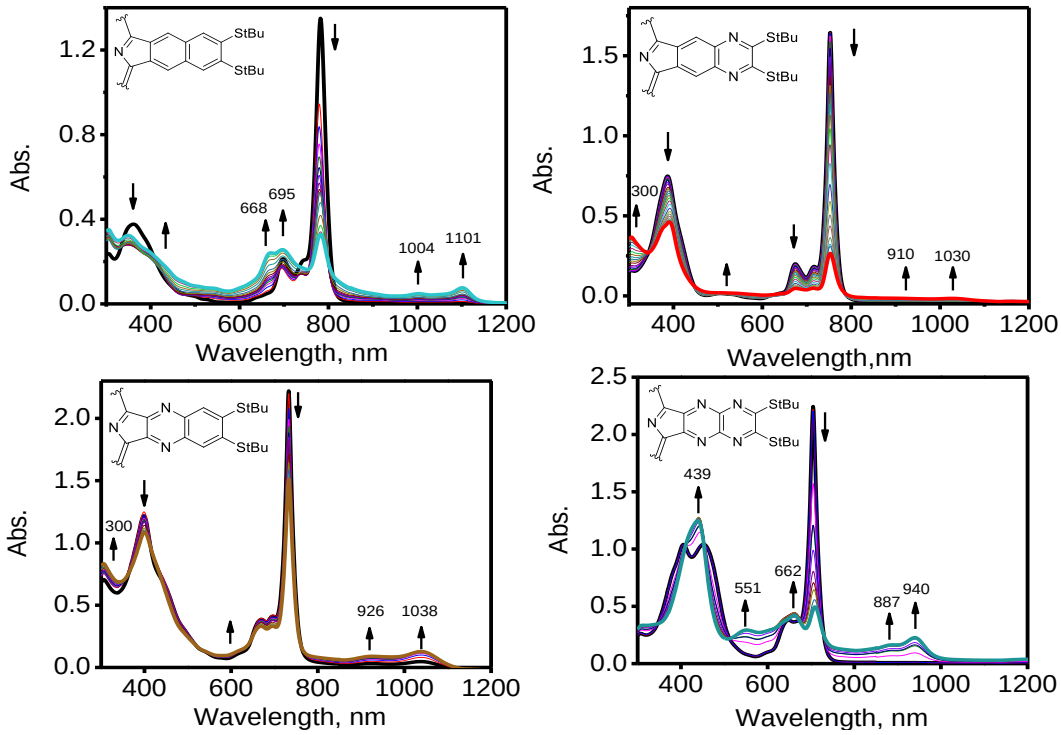


Figure S17. Spectroelectrochemical transformation of the neutral **Nc**, **2,3-TQPz**, **6,7-TQPz**, and **TPyzPyzPz** complexes during the first reductions in pyridine/TBAP system.

THEORETICAL CALCULATIONS

The starting geometries of all compounds were optimized in D_{4h} symmetry using the B3LYP exchange-correlation functional[16, 17] coupled with the 6-31G(d) basis set for all atoms.[18] Energy minima in optimized geometries were confirmed by frequency calculations. In all cases, *tert*-butyl groups were replaced with methyl substituents in order to reduce a computational cost. Pyridine was used as a solvent in all of the single point DFT-PCM and TDDFT-DCM calculations; solvent effects were calculated using the polarized continuum model (PCM).[19] The first 70 states of each compound were calculated in all TDDFT-PCM calculations. All DFT calculations were conducted using the Gaussian 09 software package,[20] and the QMForge program[21] was used for the molecular orbital analysis.

Table S3. TDDFT-PCM predicted excited state energies (E), oscillator strengths (f), and expansion coefficients for target compounds.

Excited state	E, nm (cm^{-1})	f	Expansion Coefficients
Pc			
	693(14430)	1.0068	243 → 244(0.57476), 243 → 245(-0.40016)
2	693(14430)	1.0068	243 → 244(0.40016), 243 → 245(0.57476)
8	484(20661)	0.4999	239 → 244(0.67669), 242 → 244(-0.19075)
9	484(20661)	0.4999	239 → 245(0.67669), 242 → 245(0.19075)
28	328(30487)	0.8907	233 → 245(-0.43949), 234 → 244(-0.26238), 243 → 249(0.45902)
29	328(30487)	0.8907	233 → 244(-0.43949), 234 → 245(0.26238), 243 → 250(0.45902)
TPyzPz			
1	621(16103)	0.8599	231 → 245(0.11185), 243 → 244(0.69051)
2	621(16103)	0.86	231 → 244(-0.11185), 243 → 245(0.69051)
8	502(19920)	0.6176	239 → 245(0.68723), 242 → 245(0.13355)
9	502(19920)	0.6177	239 → 244(0.68723), 242 → 244(-0.13355)
36	351(28490)	1.5941	231 → 244(0.46891), 234 → 245(-0.23877,) 239 → 248(-0.19294), 240 → 246(-0.29719), 240 → 247(0.21456), 242 → 248(0.19520)
36	351(28490)	1.5941	231 → 245(0.46891), 234 → 244(0.23876), 239 → 249(0.19294), 241 → 246(-0.29719), 241 → 247(-0.21456), 242 → 249(0.19520)

Nc

1	799(12515)	1.2592	295 → 296(0.60192), 295 → 297(-0.36597)
2	799(12515)	1.2592	295 → 296(0.36597), 295 → 297(0.60192)
15	448(22321)	0.6819	288 → 296(0.13073), 288 → 297(0.55160), 291 → 297(0.35800), 295 → 301(-0.18884)
16	448(22321)	0.6819	288 → 296(0.55160), 288 → 297(-0.13073), 291 → 296(-0.35800), 295 → 300(-0.18884)
28	338(29585)	1.9099	285 → 297(0.43461), 288 → 300(-0.20471), 289 → 298(0.33666), 289 → 299(-0.24351), 291 → 300(-0.20656), 293 → 298(-0.15406)
29	338(29585)	1.9099	285 → 296(0.43461), 288 → 301(0.20471), 290 → 298(0.33666), 290 → 299(0.24351), 291 → 301(-0.20656), 292 → 298(-0.15406)

TPyzPyzPz

1	674(14836)	0.965	295 → 296(0.49906), 295 → 297(0.48447)
2	674(14836)	0.965	295 → 296(-0.48447), 295 → 297(0.49906)
11	484(20661)	1.3128	291 → 297(0.49741), 294 → 297(-0.10826), 295 → 301(0.45721)
12	484(20661)	1.3128	291 → 296(0.49741), 294 → 296(0.10826), 295 → 300(0.45721)
32	393(25445)	0.7871	283 → 297(-0.19979), 287 → 296(-0.18980), 287 → 297(0.54832), 293 → 298(0.22595), 293 → 299(0.14803)
33	393(25445)	0.7871	283 → 2969(0.19979), 287 → 296(0.54832), 287 → 297(0.18980), 292 → 298(0.22595), 292 → 299(-0.14803)

2,3-TQPz

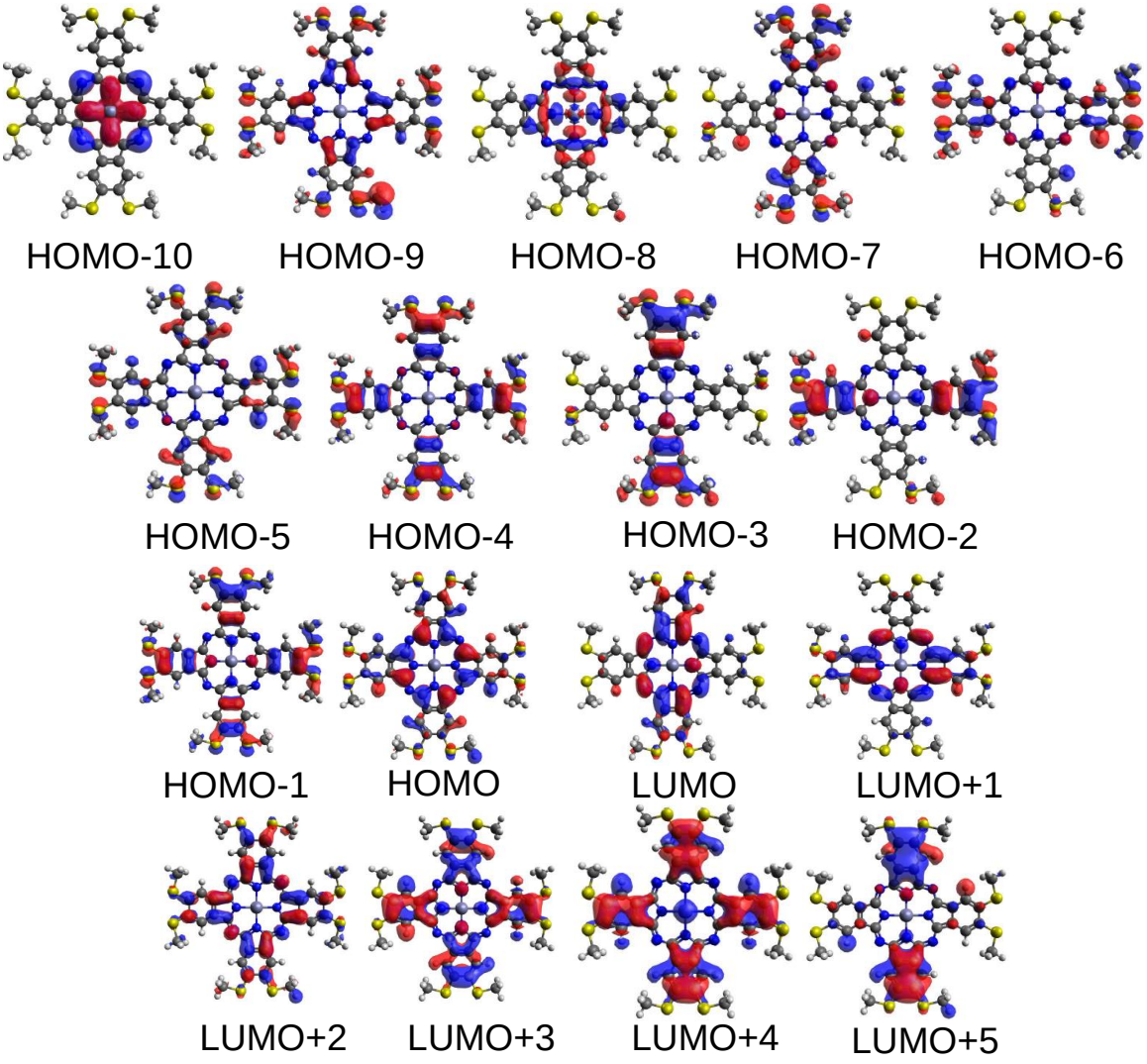
1	716(13966)	1.0524	295 → 296(0.33959), 295 → 297(0.61196)
2	716(13966)	1.0524	295 → 296(0.61196), 295 → 297(-0.33959)
8	503(19880)	0.7062	291 → 296(0.67048), 291 → 297(0.14454), 294 → 296(-0.13812)
9	503(19880)	0.7062	291 → 296(-0.14454), 291 → 297(0.67048), 294 → 297(0.13812)
30	390(25641)	1.114	282 → 296(-0.16727), 287 → 297(-0.12534), 291 → 301(0.14181), 292 → 298(0.25724), 292 → 299(0.14379), 293 → 298(0.46234), 293 → 299(-0.25843), 294 → 301(-0.15677)

31	390(25641)	1.114	282 → 297(-0.16727), 287 → 296(0.12534), 291 → 300(-0.14181), 292 → 298(0.46234), 292 → 299(0.25843), 293 → 298(-0.25724), 293 → 299(0.14379), 294 → 300(-0.15677)
6,7-TQPz			
1	743(13458)	1.1882	295 → 296(0.39106), 295 → 297(0.58354)
2	743(13458)	1.1882	295 → 296(0.58354), 295 → 297(-0.39106)
12	438(22831)	0.7186	291 → 296(0.68469), 294 → 296(-0.14245)
13	438(22831)	0.7186	291 → 297(0.68469), 294 → 297(0.14245)
27	354(28248)	1.4196	282 → 296(0.36260), 282 → 297(0.15187), 286 → 296(-0.13515), 286 → 297(0.32268), 291 → 301(0.16227), 292 → 298(0.11511) 293 → 298(0.27483), 293 → 299(-0.22106), 294 → 301(-0.16591)
28	354(28248)	1.4196	282 → 296(-0.15187), 282 → 297(0.36260), 286 → 296(-0.32268), 286 → 297(-0.13515), 291 → 300(-0.16227), 292 → 298(0.27483), 292 → 299(0.22106), 293 → 298(-0.11511), 294 → 300(-0.16591)

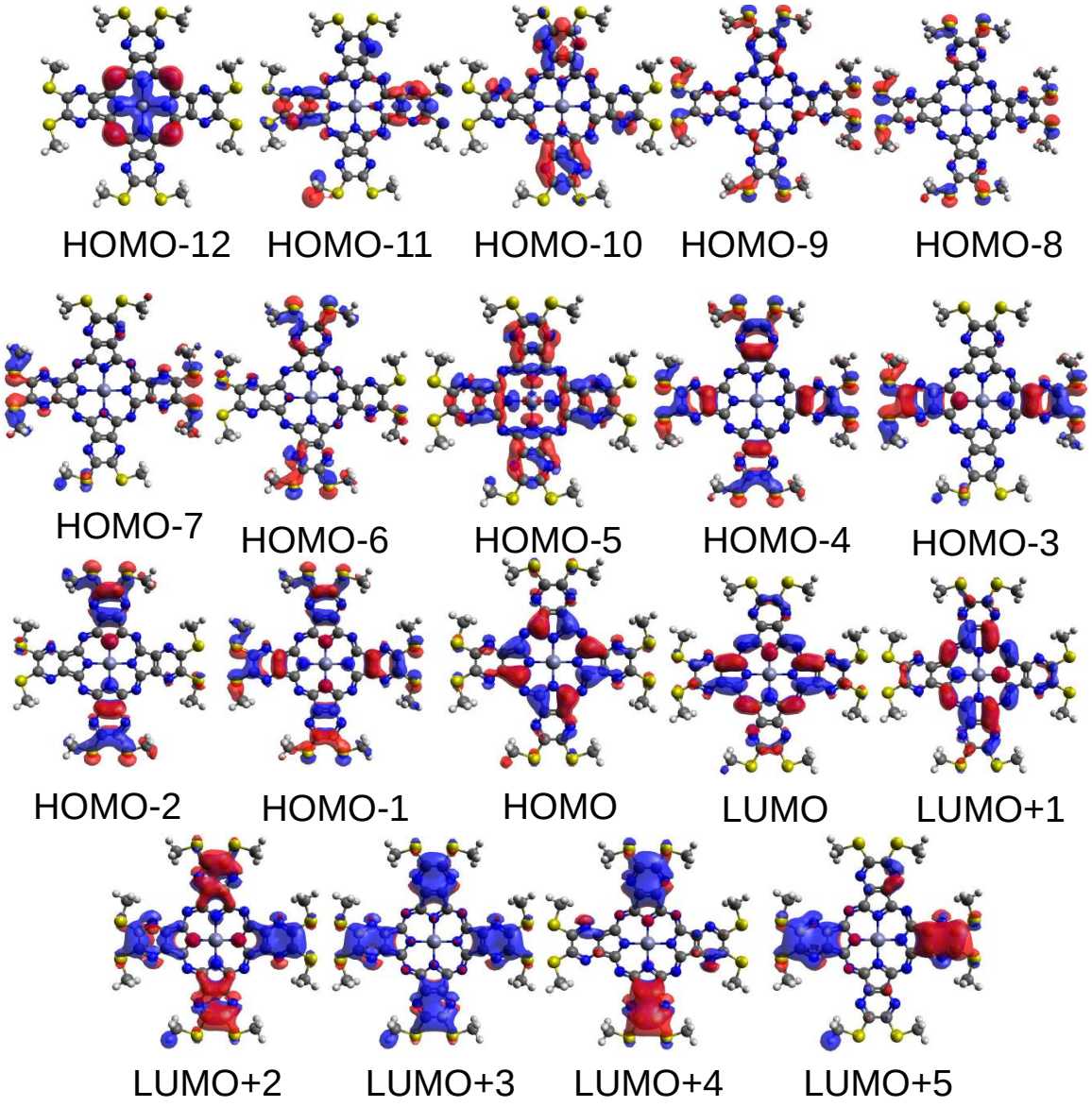
DFT-PCM predicted frontier orbitals for target compounds

Figure S18. DFT-PCM predicted frontier orbitals for target compounds.

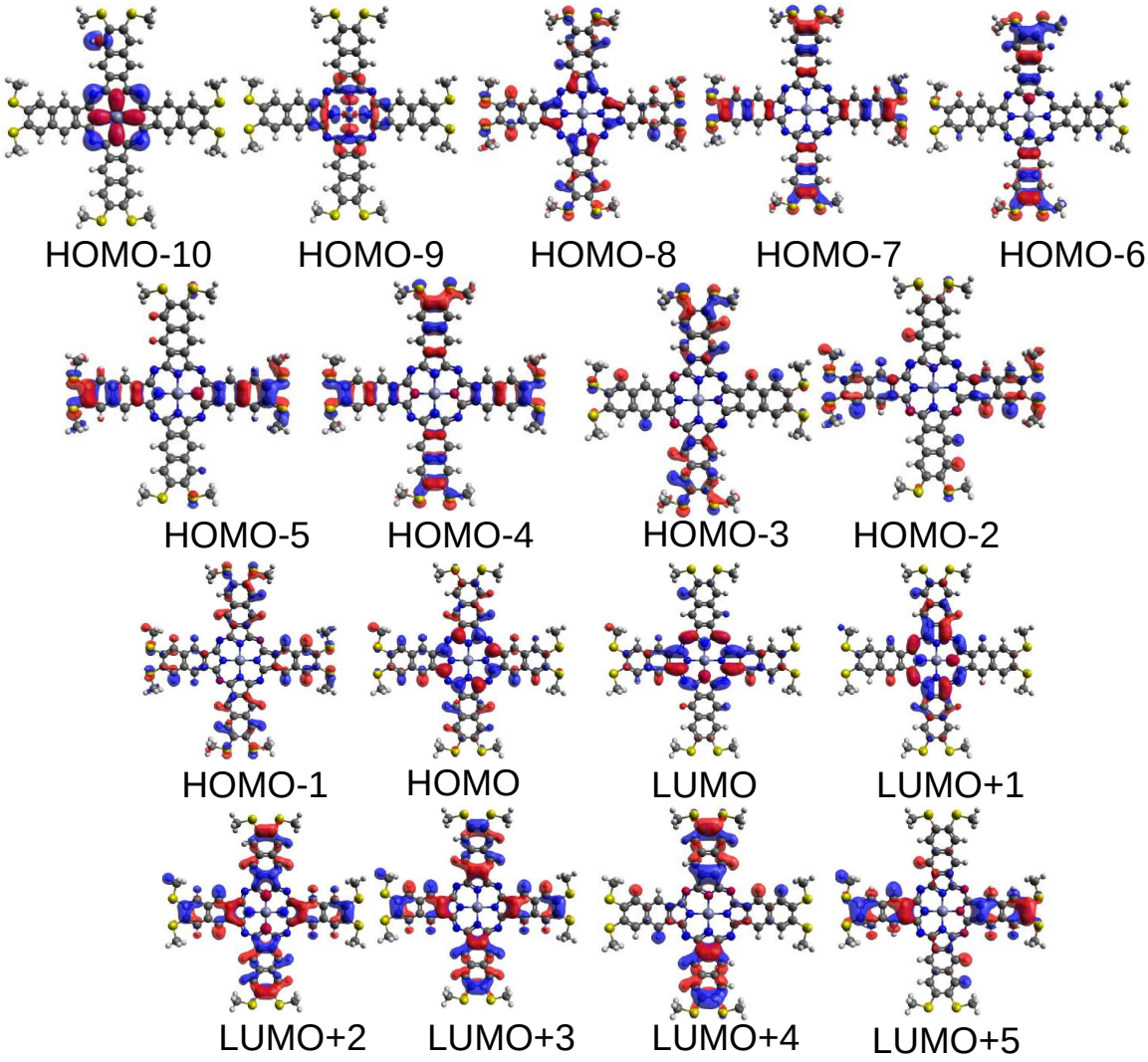
Molecular Orbitals for **Pc**:



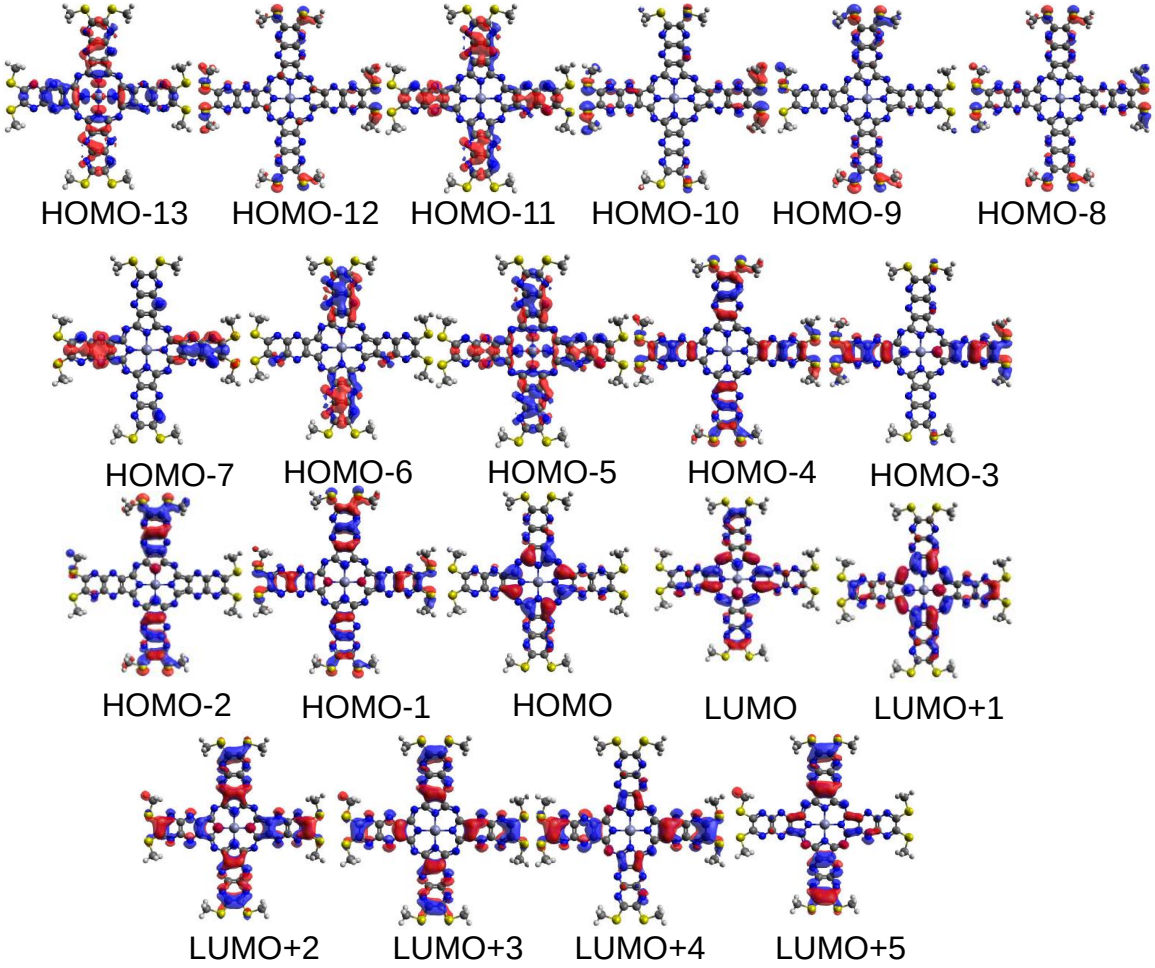
Molecular Orbitals for **TPyzPz**:



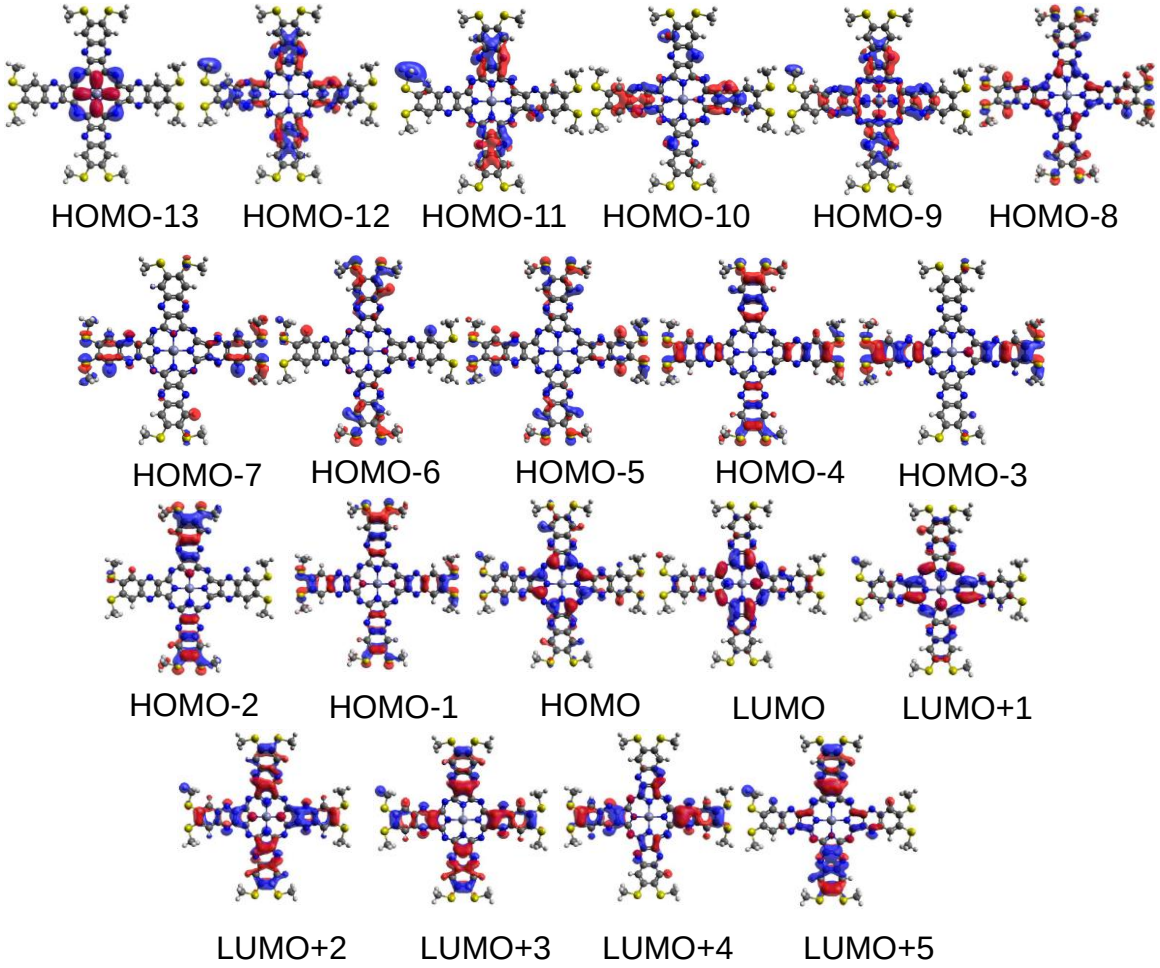
Molecular Orbitals for **Nc**:



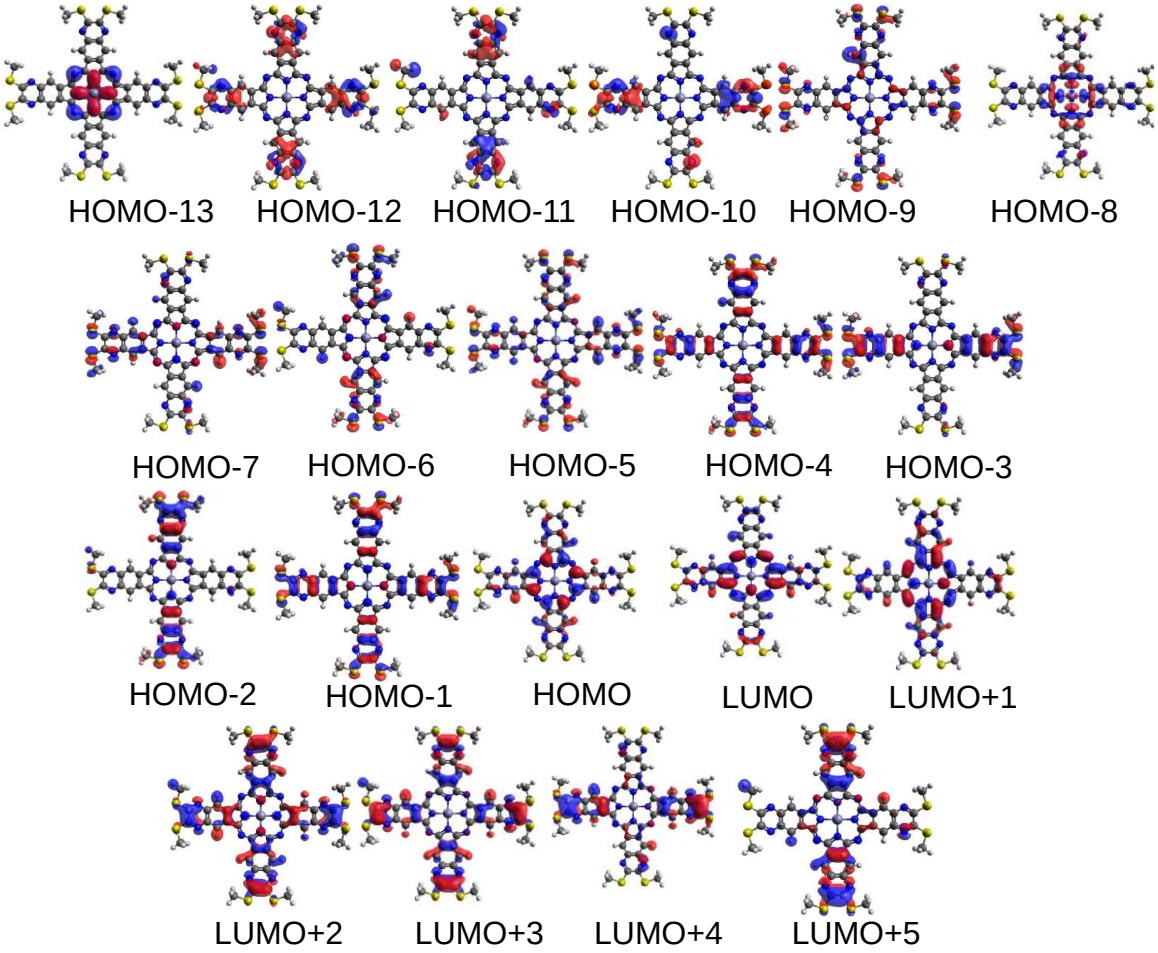
Molecular Orbitals for **TPyzPyzPz**:



Molecular Orbitals for **2,3-TQPz**:



Molecular Orbitals for **6,7-TQPz**:



DFT-PCM predicted compositions for the frontier orbitals

Table S4. DFT-PCM predicted compositions for the frontier orbitals.[a]

			% Composition		
MO	Energy	Symmetry	Zinc	$N_{meso} + N_{pyrr}$[b]	All other atoms
			Pc		
249	-0.692	e_g	0.07	7.71	92.22
248	-0.798	a_{2u}	3.97	5.56	90.47
247	-0.953	b_{2u}	0.00	16.73	83.27
246	-1.225	b_{1u}	0.00	21.26	78.74
245	-2.833	e_g	0.31	30.56	69.13
244	**-2.833**	**e_g**	**0.31**	**30.56**	**69.13**
243	**-4.927**	**a_{1u}**	**0.00**	**0.17**	**99.83**
242	-5.763	b_{2u}	0.00	7.86	92.14
241	-5.781	e_g	0.27	7.01	92.72
240	-5.781	e_g	0.27	7.01	92.72
239	-5.793	a_{2u}	0.14	3.45	96.41
238	-6.366	b_{1u}	0.00	2.26	97.74
237	-6.375	e_g	0.10	7.13	92.77
236	-6.375	e_g	0.10	7.13	92.77
235	-6.602	b_{1u}	27.64	49.61	22.75
234	-6.776	a_{1u}	0.00	0.04	99.96
233	-6.988	a_{2u}	1.63	95.65	2.72
			Nc		
301	-1.412	e_g	0.04	6.72	93.24
300	-1.412	e_g	0.04	6.72	93.24
299	-1.538	a_{2u}	1.80	5.20	93.00
298	-1.644	b_{2u}	0.00	13.47	86.53
297	-2.74	e_g	0.34	29.50	70.16

296	**-2.74**	**e_g**	**0.34**	**29.50**	**70.16**
295	**-4.582**	**a_{1u}**	**0.00**	**0.15**	**99.85**
294	-5.76	b_{1u}	0.00	2.37	97.63
293	-5.794	e_g	0.02	4.89	95.09
292	-5.794	e_g	0.02	4.89	95.09
291	-5.84	b_{2u}	0.00	4.57	95.43
290	-5.854	e_g	0.20	5.75	94.05
289	-5.854	e_g	0.20	5.75	94.05
288	-5.857	a_{2u}	0.07	2.00	97.93
287	-6.239	a_{1u}	0.00	0.05	99.95
286	-6.625	b_{1g}	27.32	50.21	22.47
285	-6.942	a_{2u}	1.51	94.59	3.90
			TPyzPz		
249	-1.748	e_g	0.05	6.07	93.88
248	-1.748	e_g	0.05	6.07	93.88
247	-1.843	a_{2u}	1.40	4.51	94.09
246	-1.934	b_{2u}	0.00	11.63	88.37
245	-3.28	e_g	0.33	32.28	67.39
244	**-3.28**	**e_g**	**0.33**	**32.28**	**67.39**
243	**-5.607**	**a_{1u}**	**0.00**	**0.19**	**99.81**
242	-6.118	b_{2u}	0.00	9.16	90.84
241	-6.14	e_g	0.33	8.57	91.10
240	-6.14	e_g	0.33	8.57	91.10
239	-6.16	a_{2u}	0.15	4.08	95.77
238	-6.759	b_{1g}	17.65	36.68	45.67
237	-6.988	e_g	0.04	2.80	97.16
236	-6.988	e_g	0.04	2.80	97.16
235	-6.993	b_{1u}	0.00	0.77	99.23
234	-7.157	a_{1u}	0.00	0.02	99.98

233	-7.193	e_u	0.10	7.34	92.56
232	-7.193	e_u	0.10	7.34	92.56
231	-7.272	a_{2u}	1.57	96.07	2.36
			TPyzPyzPz		
301	-2.687	e_g	0.01	7.95	92.04
300	-2.687	e_g	0.01	7.95	92.04
299	-2.872	a_{2u}	0.79	4.75	94.46
298	-2.94	b_{2u}	0.00	10.91	89.09
297	-3.523	e_g	0.39	30.48	69.13
296	**-3.523**	**e_g**	**0.39**	**30.48**	**69.13**
295	**-5.705**	**a_{1u}**	**0.00**	**0.20**	**99.80**
294	-6.447	b_{2u}	0.00	6.01	93.99
293	-6.461	e_g	0.21	5.59	94.20
292	-6.461	e_g	0.21	5.59	94.20
291	-6.473	a_{2u}	0.08	2.73	97.19
290	-6.741	b_{1g}	7.27	19.00	73.73
289	-6.929	e_u	0.09	3.23	96.68
288	-6.929	e_u	0.09	3.23	96.68
287	-6.99	b_{1u}	0.00	0.43	99.57
286	-6.991	e_g	0.02	1.48	98.50
285	-6.991	e_g	0.02	1.48	98.50
284	-6.992	a_{1g}	0.08	2.59	97.33
283	-7.086	a_{1u}	0.00	0.01	99.99
282	-7.408	b_{1g}	20.12	33.87	46.01
281	-7.464	a_{2u}	1.44	95.76	2.80
			2,3TQPz		
301	-2.252	e_g	0.02	8.54	91.44
300	-2.252	e_g	0.02	8.54	91.44
299	-2.442	a_{2u}	1.19	5.85	92.96

298	-2.534	b_{2u}	0.00	13.57	86.43
297	-3.274	e_g	0.39	31.06	68.55
296	**-3.274**	**e_g**	**0.39**	**31.06**	**68.55**
295	**-5.327**	**a_{1u}**	**0.00**	**0.17**	**99.83**
294	-6.077	b_{2u}	0.00	4.62	95.38
293	-6.087	e_g	0.14	4.04	95.82
292	-6.087	e_g	0.14	4.04	95.82
291	-6.093	a_{2u}	0.07	2.07	97.86
290	-6.246	b_{1u}	0.00	0.86	99.14
289	-6.26	e_g	0.04	2.87	97.09
288	-6.26	e_g	0.04	2.87	97.09
287	-6.511	a_{1u}	0.00	0.04	99.96
286	-6.712	b_{1g}	11.84	28.36	59.80
285	-7.042	e_u	0.12	7.00	92.88
284	-7.042	e_u	0.12	7.00	92.88
283	-7.174	a_{1g}	0.09	5.28	94.63
282	-7.295	a_{2u}	1.43	95.35	3.22
			6,7-TQPz		
301	-2.028	e_g	0.01	4.91	95.08
300	-2.028	e_g	0.01	4.91	95.08
299	-2.136	a_{2u}	0.83	3.48	95.69
298	-2.198	b_{2u}	0.00	8.74	91.26
297	-2.993	e_g	0.35	29.65	70.00
296	**-2.993**	**e_g**	**0.35**	**29.65**	**70.00**
295	**-4.963**	**a_{1u}**	**0.00**	**0.18**	**99.82**
294	-6.169	b_{2u}	0.00	5.81	94.19
293	-6.182	e_g	0.21	5.12	94.67
292	-6.182	e_g	0.21	5.12	94.67
291	-6.195	a_{2u}	0.07	2.61	97.32

290	-6.498	b_{1u}	0.00	2.35	97.65
289	-6.507	e_g	0.10	7.31	92.59
288	-6.507	e_g	0.10	7.31	92.59
287	-6.797	b_{1g}	26.03	48.06	25.91
286	-6.824	a_{1u}	0.00	0.02	99.98
285	-7.101	e_u	0.01	0.16	99.83
284	-7.101	e_u	0.01	0.16	99.83
283	-7.104	a_{1g}	0.01	0.17	99.82
282	-7.12	a_{2u}	1.52	95.16	3.32

[a]HOMO and LUMO are in bold; [b]N_{meso} are nitrogen atoms in meso-positions and N_{pyrr} are nitrogen atoms directly bonded to the central zinc atom.

Correlations between predicted and experimental data

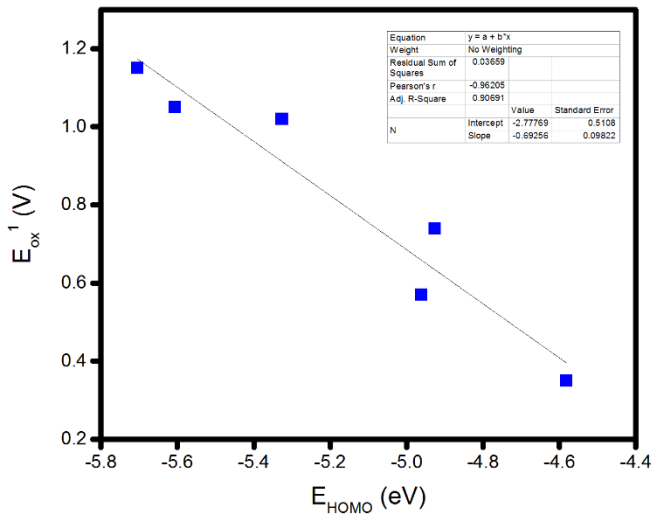


Figure S19. Correlation between DFT-PCM predicted energy of HOMO vs. 1st oxidation state for each of the 6 target compounds.

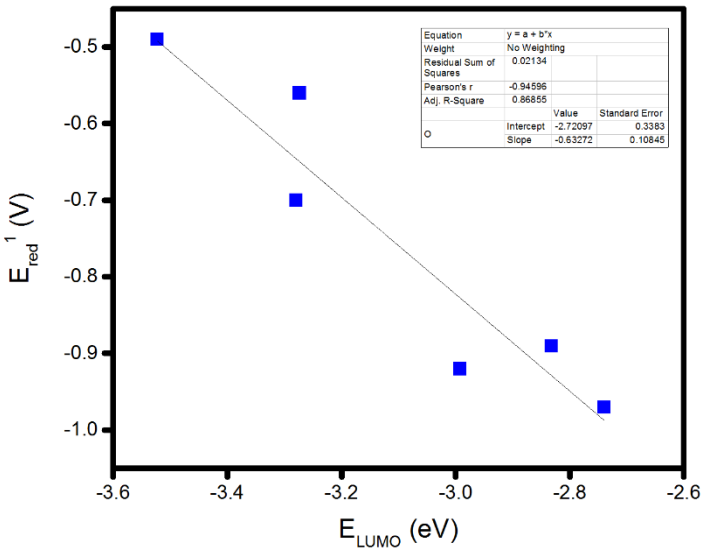


Figure S20. Correlation between DFT-PCM predicted energy of LUMO vs. 1st reduction state for each of the 6 compounds.

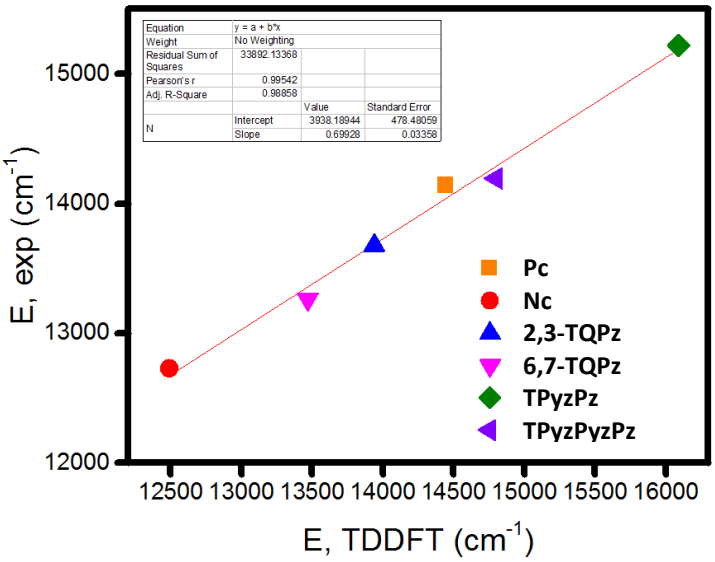


Figure S21. Correlation between TDDFT-PCM predicted and experimentally observed energies of Q-band in target compounds.

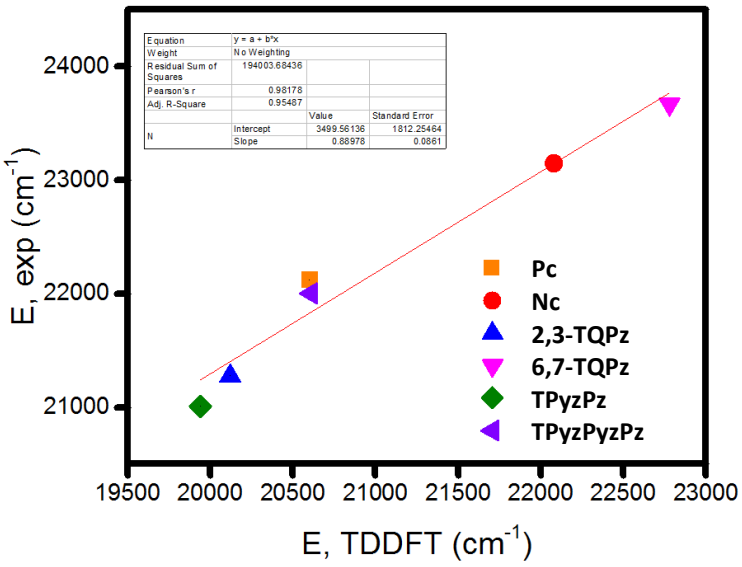


Figure S22. Correlation between TDDFT-PCM predicted and experimentally observed energies of unusual ~450-500 nm in target compounds.

TDDFT-PCM predicted and experimentally observed energies in target compounds.

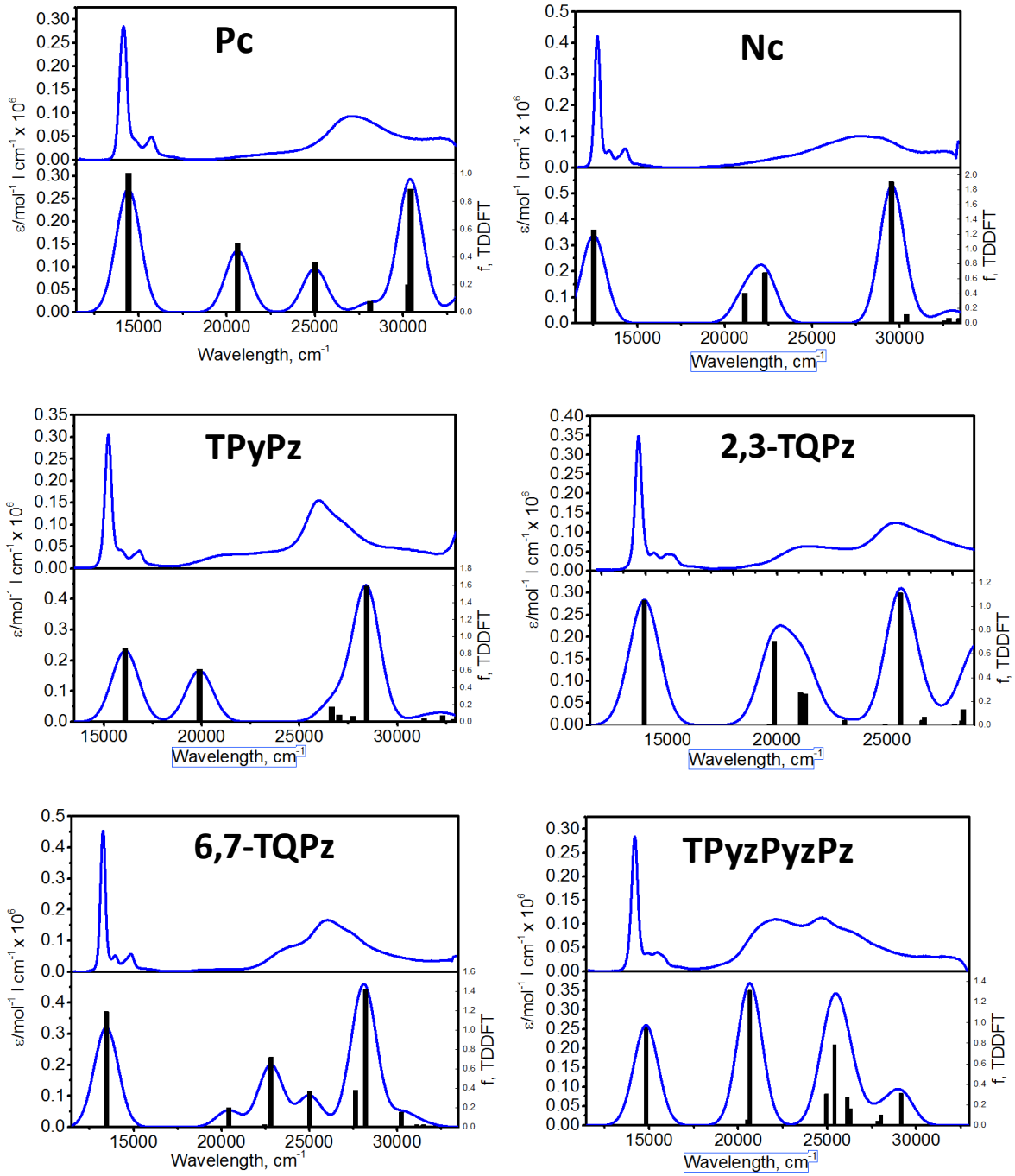


Figure S23. TDDFT-PCM predicted and experimentally observed energies in target compounds.

Optimized geometries for target compounds

Optimized geometries for Pc:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.996184	0.000000
2	7	0	1.996184	0.000000	0.000000
3	7	0	-1.996184	0.000000	0.000000
4	7	0	0.000000	-1.996184	0.000000
5	6	0	1.120211	2.787148	0.000000
6	6	0	-1.120211	2.787148	0.000000
7	6	0	2.787148	1.120211	0.000000
8	6	0	2.787148	-1.120211	0.000000
9	6	0	-2.787148	1.120211	0.000000
10	6	0	-2.787148	-1.120211	0.000000
11	6	0	1.120211	-2.787148	0.000000
12	6	0	-1.120211	-2.787148	0.000000
13	7	0	2.392734	2.392734	0.000000
14	6	0	0.702929	4.186755	0.000000
15	6	0	-0.702929	4.186755	0.000000
16	6	0	4.186755	0.702929	0.000000
17	7	0	2.392734	-2.392734	0.000000
18	6	0	4.186755	-0.702929	0.000000
19	7	0	-2.392734	2.392734	0.000000
20	6	0	-4.186755	0.702929	0.000000
21	6	0	-4.186755	-0.702929	0.000000
22	6	0	0.702929	-4.186755	0.000000
23	7	0	-2.392734	-2.392734	0.000000
24	6	0	-0.702929	-4.186755	0.000000
25	6	0	0.716675	6.590771	0.000000
26	6	0	-0.716675	6.590771	0.000000
27	6	0	-6.590771	0.716675	0.000000
28	6	0	-6.590771	-0.716675	0.000000
29	6	0	-0.716675	-6.590771	0.000000
30	6	0	0.716675	-6.590771	0.000000
31	6	0	6.590771	-0.716675	0.000000
32	6	0	6.590771	0.716675	0.000000
33	30	0	0.000000	0.000000	0.000000
34	6	0	1.418862	5.382357	0.000000
35	1	0	2.501555	5.359451	0.000000
36	6	0	-1.418862	5.382357	0.000000
37	1	0	-2.501555	5.359451	0.000000
38	6	0	-5.382357	1.418862	0.000000
39	1	0	-5.359451	2.501555	0.000000
40	6	0	-5.382357	-1.418862	0.000000
41	1	0	-5.359451	-2.501555	0.000000
42	6	0	-1.418862	-5.382357	0.000000
43	1	0	-2.501555	-5.359451	0.000000
44	6	0	1.418862	-5.382357	0.000000
45	1	0	2.501555	-5.359451	0.000000
46	6	0	5.382357	-1.418862	0.000000
47	1	0	5.359451	-2.501555	0.000000
48	6	0	5.382357	1.418862	0.000000
49	1	0	5.359451	2.501555	0.000000
50	16	0	1.539373	8.175683	0.000000
51	16	0	-1.539373	8.175683	0.000000

52	16	0	-8.175683	1.539373	0.000000
53	16	0	-8.175683	-1.539373	0.000000
54	16	0	-1.539373	-8.175683	0.000000
55	16	0	1.539373	-8.175683	0.000000
56	16	0	8.175683	-1.539373	0.000000
57	16	0	8.175683	1.539373	0.000000
58	6	0	-3.311636	-7.744501	0.000000
59	1	0	-3.587456	-7.186448	0.897735
60	1	0	-3.587456	-7.186448	-0.897735
61	1	0	-3.837024	-8.702318	0.000000
62	6	0	3.311636	-7.744501	0.000000
63	1	0	3.587456	-7.186448	-0.897735
64	1	0	3.587456	-7.186448	0.897735
65	1	0	3.837024	-8.702318	0.000000
66	6	0	7.744501	-3.311636	0.000000
67	1	0	7.186448	-3.587456	0.897735
68	1	0	7.186448	-3.587456	-0.897735
69	1	0	8.702318	-3.837024	0.000000
70	6	0	7.744501	3.311636	0.000000
71	1	0	7.186448	3.587456	-0.897735
72	1	0	7.186448	3.587456	0.897735
73	1	0	8.702318	3.837024	0.000000
74	6	0	3.311636	7.744501	0.000000
75	1	0	3.587456	7.186448	0.897735
76	1	0	3.587456	7.186448	-0.897735
77	1	0	3.837024	8.702318	0.000000
78	6	0	-3.311636	7.744501	0.000000
79	1	0	-3.587456	7.186448	-0.897735
80	1	0	-3.587456	7.186448	0.897735
81	1	0	-3.837024	8.702318	0.000000
82	6	0	-7.744501	3.311636	0.000000
83	1	0	-7.186448	3.587456	0.897735
84	1	0	-7.186448	3.587456	-0.897735
85	1	0	-8.702318	3.837024	0.000000
86	6	0	-7.744501	-3.311636	0.000000
87	1	0	-7.186448	-3.587456	-0.897735
88	1	0	-7.186448	-3.587456	0.897735
89	1	0	-8.702318	-3.837024	0.000000

Optimized geometries for TPyPz:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	2.001853	0.000000
2	7	0	2.001853	0.000000	0.000000
3	7	0	-2.001853	0.000000	0.000000
4	7	0	0.000000	-2.001853	0.000000
5	6	0	1.124911	2.787276	0.000000
6	6	0	-1.124911	2.787276	0.000000
7	6	0	2.787276	1.124911	0.000000
8	6	0	2.787276	-1.124911	0.000000
9	6	0	-2.787276	1.124911	0.000000
10	6	0	-2.787276	-1.124911	0.000000
11	6	0	1.124911	-2.787276	0.000000
12	6	0	-1.124911	-2.787276	0.000000
13	7	0	2.394608	2.394608	0.000000

14	6	0	0.698970	4.186073	0.000000
15	6	0	-0.698970	4.186073	0.000000
16	6	0	4.186073	0.698970	0.000000
17	7	0	2.394608	-2.394608	0.000000
18	6	0	4.186073	-0.698970	0.000000
19	7	0	-2.394608	2.394608	0.000000
20	6	0	-4.186073	0.698970	0.000000
21	6	0	-4.186073	-0.698970	0.000000
22	6	0	0.698970	-4.186073	0.000000
23	7	0	-2.394608	-2.394608	0.000000
24	6	0	-0.698970	-4.186073	0.000000
25	6	0	0.724578	6.439305	0.000000
26	6	0	-0.724578	6.439305	0.000000
27	6	0	-6.439305	0.724578	0.000000
28	6	0	-6.439305	-0.724578	0.000000
29	6	0	-0.724578	-6.439305	0.000000
30	6	0	0.724578	-6.439305	0.000000
31	6	0	6.439305	-0.724578	0.000000
32	6	0	6.439305	0.724578	0.000000
33	30	0	0.000000	0.000000	0.000000
34	16	0	1.576584	7.994266	0.000000
35	16	0	-1.576584	7.994266	0.000000
36	16	0	-7.994266	1.576584	0.000000
37	16	0	-7.994266	-1.576584	0.000000
38	16	0	-1.576584	-7.994266	0.000000
39	16	0	1.576584	-7.994266	0.000000
40	16	0	7.994266	-1.576584	0.000000
41	16	0	7.994266	1.576584	0.000000
42	6	0	-3.319022	-7.448748	0.000000
43	1	0	-3.536671	-6.861949	0.893274
44	1	0	-3.536671	-6.861949	-0.893274
45	1	0	-3.910138	-8.367190	0.000000
46	6	0	3.319022	-7.448748	0.000000
47	1	0	3.536671	-6.861949	-0.893274
48	1	0	3.536671	-6.861949	0.893274
49	1	0	3.910138	-8.367190	0.000000
50	6	0	7.448748	-3.319022	0.000000
51	1	0	6.861949	-3.536671	0.893274
52	1	0	6.861949	-3.536671	-0.893274
53	1	0	8.367190	-3.910138	0.000000
54	6	0	7.448748	3.319022	0.000000
55	1	0	6.861949	3.536671	-0.893274
56	1	0	6.861949	3.536671	0.893274
57	1	0	8.367190	3.910138	0.000000
58	6	0	3.319022	7.448748	0.000000
59	1	0	3.536671	6.861949	0.893274
60	1	0	3.536671	6.861949	-0.893274
61	1	0	3.910138	8.367190	0.000000
62	6	0	-3.319022	7.448748	0.000000
63	1	0	-3.536671	6.861949	-0.893274
64	1	0	-3.536671	6.861949	0.893274
65	1	0	-3.910138	8.367190	0.000000
66	6	0	-7.448748	3.319022	0.000000
67	1	0	-6.861949	3.536671	0.893274
68	1	0	-6.861949	3.536671	-0.893274
69	1	0	-8.367190	3.910138	0.000000
70	6	0	-7.448748	-3.319022	0.000000
71	1	0	-6.861949	-3.536671	-0.893274
72	1	0	-6.861949	-3.536671	0.893274
73	1	0	-8.367190	-3.910138	0.000000

74	7	0	-1.426189	-5.314109	0.000000
75	7	0	1.426189	-5.314109	0.000000
76	7	0	5.314109	-1.426189	0.000000
77	7	0	5.314109	1.426189	0.000000
78	7	0	1.426189	5.314109	0.000000
79	7	0	-1.426189	5.314109	0.000000
80	7	0	-5.314109	1.426189	0.000000
81	7	0	-5.314109	-1.426189	0.000000

Optimized structures for Nc:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	2.003379	0.000000
2	7	0	2.003379	0.000000	0.000000
3	7	0	-2.003379	0.000000	0.000000
4	7	0	0.000000	-2.003379	0.000000
5	6	0	1.122910	2.790646	0.000000
6	6	0	-1.122910	2.790646	0.000000
7	6	0	2.790646	1.122910	0.000000
8	6	0	2.790646	-1.122910	0.000000
9	6	0	-2.790646	1.122910	0.000000
10	6	0	-2.790646	-1.122910	0.000000
11	6	0	1.122910	-2.790646	0.000000
12	6	0	-1.122910	-2.790646	0.000000
13	7	0	2.393838	2.393838	0.000000
14	6	0	0.713759	4.193756	0.000000
15	6	0	-0.713759	4.193756	0.000000
16	6	0	4.193756	0.713759	0.000000
17	7	0	2.393838	-2.393838	0.000000
18	6	0	4.193756	-0.713759	0.000000
19	7	0	-2.393838	2.393838	0.000000
20	6	0	-4.193756	0.713759	0.000000
21	6	0	-4.193756	-0.713759	0.000000
22	6	0	0.713759	-4.193756	0.000000
23	7	0	-2.393838	-2.393838	0.000000
24	6	0	-0.713759	-4.193756	0.000000
25	6	0	0.719652	6.599800	0.000000
26	6	0	-0.719652	6.599800	0.000000
27	6	0	-6.599800	0.719652	0.000000
28	6	0	-6.599800	-0.719652	0.000000
29	6	0	-0.719652	-6.599800	0.000000
30	6	0	0.719652	-6.599800	0.000000
31	6	0	6.599800	-0.719652	0.000000
32	6	0	6.599800	0.719652	0.000000
33	6	0	9.050694	-0.721699	0.000000
34	6	0	9.050694	0.721699	0.000000
35	6	0	-9.050694	-0.721699	0.000000
36	6	0	-9.050694	0.721699	0.000000
37	6	0	0.721699	-9.050694	0.000000
38	6	0	-0.721699	-9.050694	0.000000
39	6	0	0.721699	9.050694	0.000000
40	6	0	-0.721699	9.050694	0.000000
41	30	0	0.000000	0.000000	0.000000
42	16	0	-10.634565	1.544777	0.000000
43	16	0	-10.634565	-1.544777	0.000000
44	16	0	-1.544777	10.634565	0.000000

45	16	0	1.544777	10.634565	0.000000
46	16	0	10.634565	1.544777	0.000000
47	16	0	10.634565	-1.544777	0.000000
48	16	0	-1.544777	-10.634565	0.000000
49	16	0	1.544777	-10.634565	0.000000
50	6	0	10.198073	-3.315115	0.000000
51	1	0	9.637940	-3.587730	0.897548
52	1	0	9.637940	-3.587730	-0.897548
53	1	0	11.153125	-3.845426	0.000000
54	6	0	10.198073	3.315115	0.000000
55	1	0	9.637940	3.587730	-0.897548
56	1	0	9.637940	3.587730	0.897548
57	1	0	11.153125	3.845426	0.000000
58	6	0	3.315115	-10.198073	0.000000
59	1	0	3.587730	-9.637940	-0.897548
60	1	0	3.587730	-9.637940	0.897548
61	1	0	3.845426	-11.153125	0.000000
62	6	0	-3.315115	-10.198073	0.000000
63	1	0	-3.587730	-9.637940	0.897548
64	1	0	-3.587730	-9.637940	-0.897548
65	1	0	-3.845426	-11.153125	0.000000
66	6	0	-10.198073	-3.315115	0.000000
67	1	0	-9.637940	-3.587730	-0.897548
68	1	0	-9.637940	-3.587730	0.897548
69	1	0	-11.153125	-3.845426	0.000000
70	6	0	-10.198073	3.315115	0.000000
71	1	0	-9.637940	3.587730	0.897548
72	1	0	-9.637940	3.587730	-0.897548
73	1	0	-11.153125	3.845426	0.000000
74	6	0	-3.315115	10.198073	0.000000
75	1	0	-3.587730	9.637940	-0.897548
76	1	0	-3.587730	9.637940	0.897548
77	1	0	-3.845426	11.153125	0.000000
78	6	0	3.315115	10.198073	0.000000
79	1	0	3.587730	9.637940	0.897548
80	1	0	3.587730	9.637940	-0.897548
81	1	0	3.845426	11.153125	0.000000
82	6	0	1.429160	5.371913	0.000000
83	1	0	2.515606	5.369868	0.000000
84	6	0	-1.429160	5.371913	0.000000
85	1	0	-2.515606	5.369868	0.000000
86	6	0	-5.371913	1.429160	0.000000
87	1	0	-5.369868	2.515606	0.000000
88	6	0	-5.371913	-1.429160	0.000000
89	1	0	-5.369868	-2.515606	0.000000
90	6	0	-1.429160	-5.371913	0.000000
91	1	0	-2.515606	-5.369868	0.000000
92	6	0	1.429160	-5.371913	0.000000
93	1	0	2.515606	-5.369868	0.000000
94	6	0	5.371913	-1.429160	0.000000
95	1	0	5.369868	-2.515606	0.000000
96	6	0	5.371913	1.429160	0.000000
97	1	0	5.369868	2.515606	0.000000
98	6	0	-1.397882	7.848536	0.000000
99	1	0	-2.481740	7.828415	0.000000
100	6	0	1.397882	7.848536	0.000000
101	1	0	2.481740	7.828415	0.000000
102	6	0	-7.848536	1.397882	0.000000
103	1	0	-7.828415	2.481740	0.000000
104	6	0	-7.848536	-1.397882	0.000000

105	1	0	-7.828415	-2.481740	0.000000
106	6	0	-1.397882	-7.848536	0.000000
107	1	0	-2.481740	-7.828415	0.000000
108	6	0	1.397882	-7.848536	0.000000
109	1	0	2.481740	-7.828415	0.000000
110	6	0	7.848536	-1.397882	0.000000
111	1	0	7.828415	-2.481740	0.000000
112	6	0	7.848536	1.397882	0.000000
113	1	0	7.828415	2.481740	0.000000

Optimized structures for TPyzPyzPz:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	2.010455	0.000000
2	7	0	2.010455	0.000000	0.000000
3	7	0	-2.010455	0.000000	0.000000
4	7	0	0.000000	-2.010455	0.000000
5	6	0	1.127359	2.789280	0.000000
6	6	0	-1.127359	2.789280	0.000000
7	6	0	2.789280	1.127359	0.000000
8	6	0	2.789280	-1.127359	0.000000
9	6	0	-2.789280	1.127359	0.000000
10	6	0	-2.789280	-1.127359	0.000000
11	6	0	1.127359	-2.789280	0.000000
12	6	0	-1.127359	-2.789280	0.000000
13	7	0	2.394168	2.394168	0.000000
14	6	0	0.711571	4.195644	0.000000
15	6	0	-0.711571	4.195644	0.000000
16	6	0	4.195644	0.711571	0.000000
17	7	0	2.394168	-2.394168	0.000000
18	6	0	4.195644	-0.711571	0.000000
19	7	0	-2.394168	2.394168	0.000000
20	6	0	-4.195644	0.711571	0.000000
21	6	0	-4.195644	-0.711571	0.000000
22	6	0	0.711571	-4.195644	0.000000
23	7	0	-2.394168	-2.394168	0.000000
24	6	0	-0.711571	-4.195644	0.000000
25	6	0	0.720462	6.433651	0.000000
26	6	0	-0.720462	6.433651	0.000000
27	6	0	-6.433651	0.720462	0.000000
28	6	0	-6.433651	-0.720462	0.000000
29	6	0	-0.720462	-6.433651	0.000000
30	6	0	0.720462	-6.433651	0.000000
31	6	0	6.433651	-0.720462	0.000000
32	6	0	6.433651	0.720462	0.000000
33	6	0	8.727207	-0.732446	0.000000
34	6	0	8.727207	0.732446	0.000000
35	6	0	-8.727207	-0.732446	0.000000
36	6	0	-8.727207	0.732446	0.000000
37	6	0	0.732446	-8.727207	0.000000
38	6	0	-0.732446	-8.727207	0.000000
39	6	0	0.732446	8.727207	0.000000
40	6	0	-0.732446	8.727207	0.000000
41	30	0	0.000000	0.000000	0.000000
42	16	0	-10.277014	1.579871	0.000000
43	16	0	-10.277014	-1.579871	0.000000

44	16	0	-1.579871	10.277014	0.000000
45	16	0	1.579871	10.277014	0.000000
46	16	0	10.277014	1.579871	0.000000
47	16	0	10.277014	-1.579871	0.000000
48	16	0	-1.579871	-10.277014	0.000000
49	16	0	1.579871	-10.277014	0.000000
50	6	0	9.729076	-3.321062	0.000000
51	1	0	9.141292	-3.534338	0.893658
52	1	0	9.141292	-3.534338	-0.893658
53	1	0	10.645754	-3.914522	0.000000
54	6	0	9.729076	3.321062	0.000000
55	1	0	9.141292	3.534338	-0.893658
56	1	0	9.141292	3.534338	0.893658
57	1	0	10.645754	3.914522	0.000000
58	6	0	3.321062	-9.729076	0.000000
59	1	0	3.534338	-9.141292	-0.893658
60	1	0	3.534338	-9.141292	0.893658
61	1	0	3.914522	-10.645754	0.000000
62	6	0	-3.321062	-9.729076	0.000000
63	1	0	-3.534338	-9.141292	0.893658
64	1	0	-3.534338	-9.141292	-0.893658
65	1	0	-3.914522	-10.645754	0.000000
66	6	0	-9.729076	-3.321062	0.000000
67	1	0	-9.141292	-3.534338	-0.893658
68	1	0	-9.141292	-3.534338	0.893658
69	1	0	-10.645754	-3.914522	0.000000
70	6	0	-9.729076	3.321062	0.000000
71	1	0	-9.141292	3.534338	0.893658
72	1	0	-9.141292	3.534338	-0.893658
73	1	0	-10.645754	3.914522	0.000000
74	6	0	-3.321062	9.729076	0.000000
75	1	0	-3.534338	9.141292	-0.893658
76	1	0	-3.534338	9.141292	0.893658
77	1	0	-3.914522	10.645754	0.000000
78	6	0	3.321062	9.729076	0.000000
79	1	0	3.534338	9.141292	0.893658
80	1	0	3.534338	9.141292	-0.893658
81	1	0	3.914522	10.645754	0.000000
82	7	0	7.610009	-1.410631	0.000000
83	7	0	7.610009	1.410631	0.000000
84	7	0	5.294905	1.447253	0.000000
85	7	0	5.294905	-1.447253	0.000000
86	7	0	1.410631	-7.610009	0.000000
87	7	0	-1.410631	-7.610009	0.000000
88	7	0	1.447253	-5.294905	0.000000
89	7	0	-1.447253	-5.294905	0.000000
90	7	0	-5.294905	-1.447253	0.000000
91	7	0	-5.294905	1.447253	0.000000
92	7	0	-7.610009	1.410631	0.000000
93	7	0	-7.610009	-1.410631	0.000000
94	7	0	-1.447253	5.294905	0.000000
95	7	0	1.447253	5.294905	0.000000
96	7	0	1.410631	7.610009	0.000000
97	7	0	-1.410631	7.610009	0.000000

Optimized structures for 2,3-TQPz

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	2.011162	0.000000
2	7	0	2.011162	0.000000	0.000000
3	7	0	-2.011162	0.000000	0.000000
4	7	0	0.000000	-2.011162	0.000000
5	6	0	1.127927	2.790988	0.000000
6	6	0	-1.127927	2.790988	0.000000
7	6	0	2.790988	1.127927	0.000000
8	6	0	2.790988	-1.127927	0.000000
9	6	0	-2.790988	1.127927	0.000000
10	6	0	-2.790988	-1.127927	0.000000
11	6	0	1.127927	-2.790988	0.000000
12	6	0	-1.127927	-2.790988	0.000000
13	7	0	2.394928	2.394928	0.000000
14	6	0	0.713172	4.197295	0.000000
15	6	0	-0.713172	4.197295	0.000000
16	6	0	4.197295	0.713172	0.000000
17	7	0	2.394928	-2.394928	0.000000
18	6	0	4.197295	-0.713172	0.000000
19	7	0	-2.394928	2.394928	0.000000
20	6	0	-4.197295	0.713172	0.000000
21	6	0	-4.197295	-0.713172	0.000000
22	6	0	0.713172	-4.197295	0.000000
23	7	0	-2.394928	-2.394928	0.000000
24	6	0	-0.713172	-4.197295	0.000000
25	6	0	0.721137	6.445484	0.000000
26	6	0	-0.721137	6.445484	0.000000
27	6	0	-6.445484	0.721137	0.000000
28	6	0	-6.445484	-0.721137	0.000000
29	6	0	-0.721137	-6.445484	0.000000
30	6	0	0.721137	-6.445484	0.000000
31	6	0	6.445484	-0.721137	0.000000
32	6	0	6.445484	0.721137	0.000000
33	6	0	8.886711	-0.724326	0.000000
34	6	0	8.886711	0.724326	0.000000
35	6	0	-8.886711	-0.724326	0.000000
36	6	0	-8.886711	0.724326	0.000000
37	6	0	0.724326	-8.886711	0.000000
38	6	0	-0.724326	-8.886711	0.000000
39	6	0	0.724326	8.886711	0.000000
40	6	0	-0.724326	8.886711	0.000000
41	30	0	0.000000	0.000000	0.000000
42	16	0	-10.465671	1.541938	0.000000
43	16	0	-10.465671	-1.541938	0.000000
44	16	0	-1.541938	10.465671	0.000000
45	16	0	1.541938	10.465671	0.000000
46	16	0	10.465671	1.541938	0.000000
47	16	0	10.465671	-1.541938	0.000000
48	16	0	-1.541938	-10.465671	0.000000
49	16	0	1.541938	-10.465671	0.000000
50	6	0	10.030484	-3.312624	0.000000
51	1	0	9.471106	-3.584212	0.898082
52	1	0	9.471106	-3.584212	-0.898082
53	1	0	10.986660	-3.840690	0.000000
54	6	0	10.030484	3.312624	0.000000
55	1	0	9.471106	3.584212	-0.898082
56	1	0	9.471106	3.584212	0.898082
57	1	0	10.986660	3.840690	0.000000

58	6	0	3.312624	-10.030484	0.000000
59	1	0	3.584212	-9.471106	-0.898082
60	1	0	3.584212	-9.471106	0.898082
61	1	0	3.840690	-10.986660	0.000000
62	6	0	-3.312624	-10.030484	0.000000
63	1	0	-3.584212	-9.471106	0.898082
64	1	0	-3.584212	-9.471106	-0.898082
65	1	0	-3.840690	-10.986660	0.000000
66	6	0	-10.030484	-3.312624	0.000000
67	1	0	-9.471106	-3.584212	-0.898082
68	1	0	-9.471106	-3.584212	0.898082
69	1	0	-10.986660	-3.840690	0.000000
70	6	0	-10.030484	3.312624	0.000000
71	1	0	-9.471106	3.584212	0.898082
72	1	0	-9.471106	3.584212	-0.898082
73	1	0	-10.986660	3.840690	0.000000
74	6	0	-3.312624	10.030484	0.000000
75	1	0	-3.584212	9.471106	-0.898082
76	1	0	-3.584212	9.471106	0.898082
77	1	0	-3.840690	10.986660	0.000000
78	6	0	3.312624	10.030484	0.000000
79	1	0	3.584212	9.471106	0.898082
80	1	0	3.584212	9.471106	-0.898082
81	1	0	3.840690	10.986660	0.000000
82	7	0	5.294336	1.446950	0.000000
83	7	0	5.294336	-1.446950	0.000000
84	7	0	1.446950	-5.294336	0.000000
85	7	0	-1.446950	-5.294336	0.000000
86	7	0	-5.294336	-1.446950	0.000000
87	7	0	-5.294336	1.446950	0.000000
88	7	0	-1.446950	5.294336	0.000000
89	7	0	1.446950	5.294336	0.000000
90	6	0	-1.404798	7.686692	0.000000
91	1	0	-2.486876	7.645098	0.000000
92	6	0	1.404798	7.686692	0.000000
93	1	0	2.486876	7.645098	0.000000
94	6	0	-7.686692	1.404798	0.000000
95	1	0	-7.645098	2.486876	0.000000
96	6	0	-7.686692	-1.404798	0.000000
97	1	0	-7.645098	-2.486876	0.000000
98	6	0	-1.404798	-7.686692	0.000000
99	1	0	-2.486876	-7.645098	0.000000
100	6	0	1.404798	-7.686692	0.000000
101	1	0	2.486876	-7.645098	0.000000
102	6	0	7.686692	-1.404798	0.000000
103	1	0	7.645098	-2.486876	0.000000
104	6	0	7.686692	1.404798	0.000000
105	1	0	7.645098	2.486876	0.000000

Optimized structures for 6,7-TQPz:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	2.003033	0.000000
2	7	0	2.003033	0.000000	0.000000
3	7	0	-2.003033	0.000000	0.000000
4	7	0	0.000000	-2.003033	0.000000
5	6	0	1.122217	2.789099	0.000000

6	6	0	-1.122217	2.789099	0.000000
7	6	0	2.789099	1.122217	0.000000
8	6	0	2.789099	-1.122217	0.000000
9	6	0	-2.789099	1.122217	0.000000
10	6	0	-2.789099	-1.122217	0.000000
11	6	0	1.122217	-2.789099	0.000000
12	6	0	-1.122217	-2.789099	0.000000
13	7	0	2.392739	2.392739	0.000000
14	6	0	0.713019	4.193404	0.000000
15	6	0	-0.713019	4.193404	0.000000
16	6	0	4.193404	0.713019	0.000000
17	7	0	2.392739	-2.392739	0.000000
18	6	0	4.193404	-0.713019	0.000000
19	7	0	-2.392739	2.392739	0.000000
20	6	0	-4.193404	0.713019	0.000000
21	6	0	-4.193404	-0.713019	0.000000
22	6	0	0.713019	-4.193404	0.000000
23	7	0	-2.392739	-2.392739	0.000000
24	6	0	-0.713019	-4.193404	0.000000
25	6	0	0.717730	6.585952	0.000000
26	6	0	-0.717730	6.585952	0.000000
27	6	0	-6.585952	0.717730	0.000000
28	6	0	-6.585952	-0.717730	0.000000
29	6	0	-0.717730	-6.585952	0.000000
30	6	0	0.717730	-6.585952	0.000000
31	6	0	6.585952	-0.717730	0.000000
32	6	0	6.585952	0.717730	0.000000
33	6	0	8.887371	-0.729080	0.000000
34	6	0	8.887371	0.729080	0.000000
35	6	0	-8.887371	-0.729080	0.000000
36	6	0	-8.887371	0.729080	0.000000
37	6	0	0.729080	-8.887371	0.000000
38	6	0	-0.729080	-8.887371	0.000000
39	6	0	0.729080	8.887371	0.000000
40	6	0	-0.729080	8.887371	0.000000
41	30	0	0.000000	0.000000	0.000000
42	16	0	-10.444301	1.582106	0.000000
43	16	0	-10.444301	-1.582106	0.000000
44	16	0	-1.582106	10.444301	0.000000
45	16	0	1.582106	10.444301	0.000000
46	16	0	10.444301	1.582106	0.000000
47	16	0	10.444301	-1.582106	0.000000
48	16	0	-1.582106	-10.444301	0.000000
49	16	0	1.582106	-10.444301	0.000000
50	6	0	9.893666	-3.321944	0.000000
51	1	0	9.305362	-3.537437	0.893106
52	1	0	9.305362	-3.537437	-0.893106
53	1	0	10.808531	-3.918399	0.000000
54	6	0	9.893666	3.321944	0.000000
55	1	0	9.305362	3.537437	-0.893106
56	1	0	9.305362	3.537437	0.893106
57	1	0	10.808531	3.918399	0.000000
58	6	0	3.321944	-9.893666	0.000000
59	1	0	3.537437	-9.305362	-0.893106
60	1	0	3.537437	-9.305362	0.893106
61	1	0	3.918399	-10.808531	0.000000
62	6	0	-3.321944	-9.893666	0.000000
63	1	0	-3.537437	-9.305362	0.893106
64	1	0	-3.537437	-9.305362	-0.893106
65	1	0	-3.918399	-10.808531	0.000000

66	6	0	-9.893666	-3.321944	0.000000
67	1	0	-9.305362	-3.537437	-0.893106
68	1	0	-9.305362	-3.537437	0.893106
69	1	0	-10.808531	-3.918399	0.000000
70	6	0	-9.893666	3.321944	0.000000
71	1	0	-9.305362	3.537437	0.893106
72	1	0	-9.305362	3.537437	-0.893106
73	1	0	-10.808531	3.918399	0.000000
74	6	0	-3.321944	9.893666	0.000000
75	1	0	-3.537437	9.305362	-0.893106
76	1	0	-3.537437	9.305362	0.893106
77	1	0	-3.918399	10.808531	0.000000
78	6	0	3.321944	9.893666	0.000000
79	1	0	3.537437	9.305362	0.893106
80	1	0	3.537437	9.305362	-0.893106
81	1	0	3.918399	10.808531	0.000000
82	7	0	7.770769	-1.406937	0.000000
83	7	0	7.770769	1.406937	0.000000
84	7	0	1.406937	-7.770769	0.000000
85	7	0	-1.406937	-7.770769	0.000000
86	7	0	-7.770769	1.406937	0.000000
87	7	0	-7.770769	-1.406937	0.000000
88	7	0	1.406937	7.770769	0.000000
89	7	0	-1.406937	7.770769	0.000000
90	6	0	1.435443	5.370153	0.000000
91	1	0	2.520332	5.387085	0.000000
92	6	0	-1.435443	5.370153	0.000000
93	1	0	-2.520332	5.387085	0.000000
94	6	0	-5.370153	1.435443	0.000000
95	1	0	-5.387085	2.520332	0.000000
96	6	0	-5.370153	-1.435443	0.000000
97	1	0	-5.387085	-2.520332	0.000000
98	6	0	-1.435443	-5.370153	0.000000
99	1	0	-2.520332	-5.387085	0.000000
100	6	0	1.435443	-5.370153	0.000000
101	1	0	2.520332	-5.387085	0.000000
102	6	0	5.370153	-1.435443	0.000000
103	1	0	5.387085	-2.520332	0.000000
104	6	0	5.370153	1.435443	0.000000
105	1	0	5.387085	2.520332	0.000000

Excitation energies and oscillator strengths: TPyzPz

Excited State 1: Singlet-EU 1.9945 eV 621.63 nm f=0.8599 <S**2>=0.000
231 ->245 0.11185
243 ->244 0.69051
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -7074.62092324
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-EU 1.9945 eV 621.63 nm f=0.8600 <S**2>=0.000
231 ->244 -0.11185
243 ->245 0.69051

Excited state symmetry could not be determined.
Excited State 3: Singlet-?Sym 2.3770 eV 521.60 nm f=0.0000 <S**2>=0.000
240 ->245 0.49735

```
   241 ->244        0.49735

Excited state symmetry could not be determined.
Excited State   4:      Singlet-?Sym    2.3801 eV  520.93 nm  f=0.0000  <S**2>=0.000
   240 ->245       -0.49720
   241 ->244        0.49720

Excited State   5:      Singlet-EU     2.3862 eV  519.59 nm  f=0.0002  <S**2>=0.000
   239 ->244        0.12502
   242 ->244        0.68986

Excited State   6:      Singlet-EU     2.3862 eV  519.59 nm  f=0.0002  <S**2>=0.000
   239 ->245       -0.12502
   242 ->245        0.68986

Excited state symmetry could not be determined.
Excited State   7:      Singlet-?Sym    2.4429 eV  507.53 nm  f=0.0000  <S**2>=0.000
   240 ->244        0.49915
   241 ->245        0.49915

Excited State   8:      Singlet-EU     2.4656 eV  502.85 nm  f=0.6176  <S**2>=0.000
   239 ->245        0.68723
   242 ->245        0.13355

Excited State   9:      Singlet-EU     2.4656 eV  502.85 nm  f=0.6177  <S**2>=0.000
   239 ->244        0.68723
   242 ->244       -0.13355

Excited state symmetry could not be determined.
Excited State  10:      Singlet-?Sym    2.4742 eV  501.11 nm  f=0.0000  <S**2>=0.000
   240 ->244       -0.49888
   241 ->245        0.49888

Excited State  11:      Singlet-EG     2.6776 eV  463.04 nm  f=0.0000  <S**2>=0.000
   238 ->244        0.37966
   238 ->245        0.58372

Excited State  12:      Singlet-EG     2.6776 eV  463.04 nm  f=0.0000  <S**2>=0.000
   238 ->244        0.58372
   238 ->245       -0.37966

Excited State  13:      Singlet-B2G    3.1694 eV  391.19 nm  f=0.0000  <S**2>=0.000
   243 ->246        0.70158

Excited state symmetry could not be determined.
Excited State  14:      Singlet-?Sym    3.2147 eV  385.67 nm  f=0.0000  <S**2>=0.000
   232 ->244        0.49052
   233 ->245        0.49052

Excited state symmetry could not be determined.
Excited State  15:      Singlet-?Sym    3.2214 eV  384.88 nm  f=0.0000  <S**2>=0.000
   232 ->244        0.49328
   233 ->245       -0.49328

Excited State  16:      Singlet-A2G    3.2569 eV  380.68 nm  f=0.0000  <S**2>=0.000
   243 ->247        0.70219

Excited state symmetry could not be determined.
Excited State  17:      Singlet-?Sym    3.2779 eV  378.24 nm  f=0.0000  <S**2>=0.000
   236 ->245       -0.49135
```

237 ->244 0.49135

Excited state symmetry could not be determined.
Excited State 18: Singlet-?Sym 3.2930 eV 376.51 nm f=0.0000 <S**2>=0.000
236 ->245 0.47798
237 ->244 0.47798
242 ->246 -0.12464

Excited State 19: Singlet-EU 3.3041 eV 375.24 nm f=0.1751 <S**2>=0.000
231 ->244 -0.11343
234 ->245 -0.11738
235 ->245 0.67635

Excited State 20: Singlet-EU 3.3041 eV 375.24 nm f=0.1751 <S**2>=0.000
231 ->245 -0.11343
234 ->244 0.11738
235 ->244 0.67635

Excited state symmetry could not be determined.
Excited State 21: Singlet-?Sym 3.3133 eV 374.21 nm f=0.0000 <S**2>=0.000
236 ->244 -0.49670
237 ->245 0.49670

Excited State 22: Singlet-EG 3.3278 eV 372.57 nm f=0.0000 <S**2>=0.000
228 ->244 0.65642
228 ->245 0.24834

Excited State 23: Singlet-EG 3.3278 eV 372.57 nm f=0.0000 <S**2>=0.000
228 ->244 -0.24834
228 ->245 0.65642

Excited state symmetry could not be determined.
Excited State 24: Singlet-?Sym 3.3323 eV 372.07 nm f=0.0000 <S**2>=0.000
232 ->245 0.49089
233 ->244 0.49089

Excited state symmetry could not be determined.
Excited State 25: Singlet-?Sym 3.3335 eV 371.94 nm f=0.0001 <S**2>=0.000
232 ->245 -0.48891
233 ->244 0.48891

Excited state symmetry could not be determined.
Excited State 26: Singlet-?Sym 3.3345 eV 371.82 nm f=0.0000 <S**2>=0.000
236 ->244 0.49744
237 ->245 0.49744

Excited State 27: Singlet-EU 3.3515 eV 369.93 nm f=0.0815 <S**2>=0.000
243 ->249 0.69532

Excited State 28: Singlet-EU 3.3515 eV 369.93 nm f=0.0815 <S**2>=0.000
243 ->248 0.69532

Excited State 29: Singlet-EG 3.3828 eV 366.51 nm f=0.0000 <S**2>=0.000
229 ->244 -0.41134
229 ->245 -0.16532
230 ->244 0.49688
230 ->245 -0.19970

Excited State 30: Singlet-EG 3.3828 eV 366.51 nm f=0.0000 <S**2>=0.000
229 ->244 -0.16532

229 ->245 0.41134
230 ->244 0.19970
230 ->245 0.49688

Excited State 31: Singlet-EU 3.4397 eV 360.45 nm f=0.0669 <S**2>=0.000
231 ->244 0.32936
234 ->245 0.59633
235 ->245 0.16356

Excited State 32: Singlet-EU 3.4397 eV 360.45 nm f=0.0669 <S**2>=0.000
231 ->245 -0.32936
234 ->244 0.59633
235 ->244 -0.16356

Excited State 33: Singlet-B1G 3.4631 eV 358.01 nm f=0.0000 <S**2>=0.000
239 ->246 -0.10065
242 ->247 -0.10062
243 ->250 0.67700

Excited State 34: Singlet-EG 3.4944 eV 354.81 nm f=0.0000 <S**2>=0.000
229 ->245 0.52846
230 ->245 -0.43970

Excited State 35: Singlet-EG 3.4944 eV 354.81 nm f=0.0000 <S**2>=0.000
229 ->244 0.52846
230 ->244 0.43970

Excited State 36: Singlet-EU 3.5248 eV 351.75 nm f=1.5941 <S**2>=0.000
231 ->244 0.46891
234 ->245 -0.23877
239 ->248 -0.19294
240 ->246 -0.29719
240 ->247 0.21456
242 ->248 0.19520

Excited State 37: Singlet-EU 3.5248 eV 351.75 nm f=1.5941 <S**2>=0.000
231 ->245 0.46891
234 ->244 0.23876
239 ->249 0.19294
241 ->246 -0.29719
241 ->247 -0.21456
242 ->249 0.19520

Excited State 38: Singlet-B1G 3.6844 eV 336.51 nm f=0.0000 <S**2>=0.000
239 ->246 0.43323
240 ->248 0.25415
241 ->249 -0.25415
242 ->247 0.35790
243 ->250 0.17295

Excited State 39: Singlet-A1G 3.7865 eV 327.44 nm f=0.0000 <S**2>=0.000
236 ->245 0.13417
237 ->244 0.13417
239 ->247 0.20332
240 ->248 -0.19889
241 ->249 -0.19889
242 ->246 0.57734

Excited State 40: Singlet-EU 3.8541 eV 321.70 nm f=0.0166 <S**2>=0.000
231 ->244 0.33458

234 ->245 -0.25329
240 ->246 0.44516
240 ->247 -0.20824
242 ->248 -0.18619

Excited State 41: Singlet-EU 3.8541 eV 321.70 nm f=0.0166 <S**2>=0.000
231 ->245 0.33458
234 ->244 0.25328
241 ->246 0.44516
241 ->247 0.20824
242 ->249 -0.18619

Excited State 42: Singlet-B1G 3.8878 eV 318.90 nm f=0.0000 <S**2>=0.000
239 ->246 0.49711
242 ->247 -0.49207

Excited State 43: Singlet-EU 3.8903 eV 318.70 nm f=0.0347 <S**2>=0.000
240 ->246 0.41997
240 ->247 0.52932
242 ->248 0.16355

Excited State 44: Singlet-EU 3.8903 eV 318.70 nm f=0.0347 <S**2>=0.000
241 ->246 -0.41997
241 ->247 0.52932
242 ->249 -0.16355

Excited state symmetry could not be determined.
Excited State 45: Singlet-?Sym 3.8990 eV 317.99 nm f=0.0100 <S**2>=0.000
226 ->245 0.47581
227 ->244 0.47581
228 ->250 -0.14620

Excited state symmetry could not be determined.
Excited State 46: Singlet-?Sym 3.9011 eV 317.82 nm f=0.0000 <S**2>=0.000
226 ->244 -0.49025
227 ->245 0.49025

Excited state symmetry could not be determined.
Excited State 47: Singlet-?Sym 3.9033 eV 317.64 nm f=0.0000 <S**2>=0.000
226 ->244 0.49407
227 ->245 0.49407

Excited State 48: Singlet-A1G 3.9036 eV 317.61 nm f=0.0000 <S**2>=0.000
239 ->247 0.54222
240 ->248 -0.19243
241 ->249 -0.19243
242 ->246 -0.35272

Excited state symmetry could not be determined.
Excited State 49: Singlet-?Sym 3.9226 eV 316.08 nm f=0.0000 <S**2>=0.000
226 ->245 -0.48726
227 ->244 0.48726

Excited State 50: Singlet-A2G 3.9943 eV 310.40 nm f=0.0000 <S**2>=0.000
240 ->249 -0.35582
241 ->248 0.35582
242 ->250 0.49121

Excited State 51: Singlet-EU 4.0080 eV 309.34 nm f=0.0694 <S**2>=0.000
239 ->248 0.29995

240 ->247 -0.16567
241 ->250 0.37170
242 ->248 0.48064

Excited State 52: Singlet-EU 4.0080 eV 309.34 nm f=0.0694 <S**2>=0.000
239 ->249 -0.29995
240 ->250 -0.37169
241 ->247 0.16567
242 ->249 0.48064

Excited state symmetry could not be determined.
Excited State 53: Singlet-?Sym 4.0176 eV 308.61 nm f=0.0000 <S**2>=0.000
239 ->250 0.25413
240 ->249 0.46366
241 ->248 0.46366

Excited State 54: Singlet-A2U 4.0562 eV 305.67 nm f=0.0072 <S**2>=0.000
229 ->246 -0.11005
230 ->247 0.21911
232 ->249 0.23295
233 ->248 0.23295
238 ->246 0.54846

Excited State 55: Singlet-A2G 4.0706 eV 304.59 nm f=0.0000 <S**2>=0.000
240 ->249 0.35045
241 ->248 -0.35045
242 ->250 0.50169

Excited state symmetry could not be determined.
Excited State 56: Singlet-?Sym 4.0715 eV 304.52 nm f=0.0000 <S**2>=0.000
239 ->246 0.22076
240 ->248 -0.40840
241 ->249 0.40840
242 ->247 0.33814

Excited State 57: Singlet-EU 4.0768 eV 304.12 nm f=0.0267 <S**2>=0.000
239 ->248 0.10046
240 ->247 0.20096
241 ->250 0.52247
242 ->248 -0.39907

Excited State 58: Singlet-EU 4.0768 eV 304.12 nm f=0.0267 <S**2>=0.000
239 ->249 0.10047
240 ->250 0.52247
241 ->247 0.20096
242 ->249 0.39907

Excited state symmetry could not be determined.
Excited State 59: Singlet-?Sym 4.0789 eV 303.96 nm f=0.0000 <S**2>=0.000
239 ->247 0.38924
240 ->248 0.40203
241 ->249 0.40203
242 ->246 0.15137

Excited State 60: Singlet-B2U 4.0931 eV 302.91 nm f=0.0000 <S**2>=0.000
229 ->247 -0.15624
230 ->246 0.26636
232 ->249 0.27149
233 ->248 -0.27149
238 ->247 0.48010

Excited State 61: Singlet-EU 4.0938 eV 302.86 nm f=0.0013 <S**2>=0.000
239 ->248 0.58508
240 ->246 -0.12371
240 ->247 0.23600
241 ->250 -0.27732

Excited State 62: Singlet-EU 4.0938 eV 302.86 nm f=0.0013 <S**2>=0.000
239 ->249 0.58508
240 ->250 -0.27732
241 ->246 0.12371
241 ->247 0.23600

Excited State 63: Singlet-EG 4.1137 eV 301.39 nm f=0.0000 <S**2>=0.000
229 ->248 -0.16483
230 ->248 -0.25105
233 ->246 0.34028
233 ->247 -0.32345
238 ->248 0.40230

Excited State 64: Singlet-EG 4.1137 eV 301.39 nm f=0.0000 <S**2>=0.000
229 ->249 -0.16483
230 ->249 0.25105
232 ->246 0.34028
232 ->247 0.32345
238 ->249 0.40230

Excited State 65: Singlet-B2G 4.1179 eV 301.09 nm f=0.0000 <S**2>=0.000
239 ->250 0.65084
240 ->249 -0.18465
241 ->248 -0.18465

Excited state symmetry could not be determined.
Excited State 66: Singlet-?Sym 4.2815 eV 289.58 nm f=0.0000 <S**2>=0.000
224 ->245 -0.48225
225 ->244 0.48225

Excited State 67: Singlet-A1U 4.4029 eV 281.60 nm f=0.0000 <S**2>=0.000
238 ->250 0.68683

Excited state symmetry could not be determined.
Excited State 68: Singlet-?Sym 4.4129 eV 280.96 nm f=0.0000 <S**2>=0.000
224 ->245 0.46407
225 ->244 0.46407
234 ->246 -0.11222
235 ->247 -0.12169
236 ->248 -0.10196
237 ->249 0.10196

Excited State 69: Singlet-A2U 4.4251 eV 280.19 nm f=0.0103 <S**2>=0.000
229 ->246 0.33203
230 ->247 -0.27909
232 ->249 -0.25171
233 ->248 -0.25171
238 ->246 0.41236

Excited State 70: Singlet-EU 4.4645 eV 277.71 nm f=0.0366 <S**2>=0.000
223 ->244 -0.19508
234 ->249 -0.22998
235 ->249 -0.28903

```
   237 ->246        0.44100
   237 ->247        0.34151
SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 LETran=    1270.
Leave Link  914 at Sun Jul 20 18:16:02 2014, MaxMem= 2359296000 cpu:  382628.6
(Enter /usr/local/g09/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.


 Excitation energies and oscillator strengths: Pc

 Excited State   1:      Singlet-EU     1.7876 eV  693.60 nm  f=1.0068  <S**2>=0.000
   243 ->244        0.57476
   243 ->245       -0.40016
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -6946.33055278
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-EU     1.7876 eV  693.60 nm  f=1.0068  <S**2>=0.000
   243 ->244        0.40016
   243 ->245        0.57476

 Excited state symmetry could not be determined.
 Excited State   3:      Singlet-?Sym    2.4779 eV  500.35 nm  f=0.0000  <S**2>=0.000
   240 ->244        0.49712
   241 ->245        0.49712

 Excited state symmetry could not be determined.
 Excited State   4:      Singlet-?Sym    2.4812 eV  499.69 nm  f=0.0000  <S**2>=0.000
   240 ->244       -0.49638
   241 ->245        0.49638

 Excited State   5:      Singlet-EU     2.4859 eV  498.75 nm  f=0.0043  <S**2>=0.000
   239 ->244        0.12995
   239 ->245       -0.13357
   242 ->244        0.47222
   242 ->245        0.48538

 Excited State   6:      Singlet-EU     2.4859 eV  498.75 nm  f=0.0043  <S**2>=0.000
   239 ->244        0.13357
   239 ->245        0.12995
   242 ->244        0.48538
   242 ->245       -0.47222

 Excited state symmetry could not be determined.
 Excited State   7:      Singlet-?Sym    2.5430 eV  487.55 nm  f=0.0000  <S**2>=0.000
   240 ->245        0.49893
   241 ->244        0.49893

 Excited State   8:      Singlet-EU     2.5565 eV  484.98 nm  f=0.4999  <S**2>=0.000
   239 ->244        0.67669
   242 ->244       -0.19075

 Excited State   9:      Singlet-EU     2.5565 eV  484.98 nm  f=0.4999  <S**2>=0.000
   239 ->245        0.67669
   242 ->245        0.19075

 Excited state symmetry could not be determined.
 Excited State  10:      Singlet-?Sym    2.5595 eV  484.42 nm  f=0.0000  <S**2>=0.000
   240 ->245       -0.49774
   241 ->244        0.49774
```

Excited State 11: Singlet-EG 2.9169 eV 425.06 nm f=0.0000 <S**2>=0.000
235 ->244 0.68971
235 ->245 -0.14937

Excited State 12: Singlet-EG 2.9169 eV 425.06 nm f=0.0000 <S**2>=0.000
235 ->244 0.14937
235 ->245 0.68971

Excited state symmetry could not be determined.
Excited State 13: Singlet-?Sym 3.0745 eV 403.27 nm f=0.0000 <S**2>=0.000
236 ->244 -0.49287
237 ->245 0.49287

Excited state symmetry could not be determined.
Excited State 14: Singlet-?Sym 3.0889 eV 401.39 nm f=0.0000 <S**2>=0.000
236 ->245 -0.49746
237 ->244 0.49746

Excited State 15: Singlet-EU 3.0985 eV 400.14 nm f=0.3582 <S**2>=0.000
238 ->245 0.69501

Excited State 16: Singlet-EU 3.0985 eV 400.14 nm f=0.3582 <S**2>=0.000
238 ->244 0.69501

Excited state symmetry could not be determined.
Excited State 17: Singlet-?Sym 3.1332 eV 395.71 nm f=0.0000 <S**2>=0.000
236 ->245 0.49727
237 ->244 0.49727

Excited state symmetry could not be determined.
Excited State 18: Singlet-?Sym 3.1577 eV 392.64 nm f=0.0000 <S**2>=0.000
236 ->244 0.49188
237 ->245 0.49188

Excited State 19: Singlet-B1G 3.2503 eV 381.46 nm f=0.0000 <S**2>=0.000
243 ->246 0.69804

Excited State 20: Singlet-EU 3.4859 eV 355.68 nm f=0.0785 <S**2>=0.000
233 ->244 0.33676
234 ->245 0.61178

Excited State 21: Singlet-EU 3.4859 eV 355.68 nm f=0.0785 <S**2>=0.000
233 ->245 -0.33676
234 ->244 0.61178

Excited State 22: Singlet-B2G 3.5080 eV 353.43 nm f=0.0000 <S**2>=0.000
243 ->247 0.69984

Excited State 23: Singlet-EG 3.5278 eV 351.45 nm f=0.0000 <S**2>=0.000
232 ->244 0.58107
232 ->245 0.39461

Excited State 24: Singlet-EG 3.5278 eV 351.45 nm f=0.0000 <S**2>=0.000
232 ->244 -0.39461
232 ->245 0.58107

Excited State 25: Singlet-A2G 3.6491 eV 339.77 nm f=0.0000 <S**2>=0.000
243 ->248 0.70278

Excited State 26: Singlet-EU 3.7567 eV 330.03 nm f=0.1997 <S**2>=0.000
233 ->244 0.33993
233 ->245 0.18334
234 ->245 -0.17341
243 ->249 0.25146
243 ->250 0.46622

Excited State 27: Singlet-EU 3.7567 eV 330.03 nm f=0.1996 <S**2>=0.000
233 ->244 -0.18334
233 ->245 0.33993
234 ->244 0.17341
243 ->249 0.46622
243 ->250 -0.25146

Excited State 28: Singlet-EU 3.7717 eV 328.72 nm f=0.8907 <S**2>=0.000
233 ->245 -0.43949
234 ->244 -0.26238
243 ->249 0.45902

Excited State 29: Singlet-EU 3.7717 eV 328.72 nm f=0.8907 <S**2>=0.000
233 ->244 -0.43949
234 ->245 0.26238
243 ->250 0.45902

Excited state symmetry could not be determined.
Excited State 30: Singlet-?Sym 4.0114 eV 309.08 nm f=0.0000 <S**2>=0.000
230 ->244 0.49313
231 ->245 -0.49313

Excited state symmetry could not be determined.
Excited State 31: Singlet-?Sym 4.0149 eV 308.81 nm f=0.0057 <S**2>=0.000
230 ->245 0.48813
231 ->244 0.48813
232 ->246 -0.13915

Excited state symmetry could not be determined.
Excited State 32: Singlet-?Sym 4.0197 eV 308.44 nm f=0.0000 <S**2>=0.000
230 ->245 -0.49745
231 ->244 0.49745

Excited state symmetry could not be determined.
Excited State 33: Singlet-?Sym 4.0244 eV 308.08 nm f=0.0000 <S**2>=0.000
230 ->244 0.49625
231 ->245 0.49625

Excited State 34: Singlet-A2G 4.1309 eV 300.14 nm f=0.0000 <S**2>=0.000
242 ->246 0.68745

Excited State 35: Singlet-EU 4.1560 eV 298.33 nm f=0.1327 <S**2>=0.000
241 ->246 0.69333

Excited State 36: Singlet-EU 4.1560 eV 298.33 nm f=0.1327 <S**2>=0.000
240 ->246 0.69333

Excited State 37: Singlet-B2G 4.1907 eV 295.85 nm f=0.0000 <S**2>=0.000
228 ->245 0.10441
229 ->244 0.10441
239 ->246 0.68273

Excited state symmetry could not be determined.

Excited State 38: Singlet-?Sym 4.2581 eV 291.17 nm f=0.0000 <S**2>=0.000
224 ->245 0.13641
225 ->244 0.13641
228 ->245 -0.46485
229 ->244 0.46485
242 ->246 -0.13335

Excited State 39: Singlet-B1G 4.2637 eV 290.79 nm f=0.0000 <S**2>=0.000
239 ->247 0.48662
240 ->250 0.25519
241 ->249 -0.25519
242 ->248 0.32518

Excited State 40: Singlet-EU 4.2921 eV 288.86 nm f=0.3564 <S**2>=0.000
236 ->246 -0.10668
237 ->246 0.12916
239 ->249 -0.17112
239 ->250 -0.14133
240 ->247 -0.29224
240 ->248 -0.18489
241 ->247 0.35383
241 ->248 -0.22385
242 ->249 0.18317
242 ->250 -0.15129

Excited State 41: Singlet-EU 4.2921 eV 288.86 nm f=0.3564 <S**2>=0.000
236 ->246 0.12916
237 ->246 0.10668
239 ->249 -0.14133
239 ->250 0.17112
240 ->247 0.35383
240 ->248 0.22385
241 ->247 0.29224
241 ->248 -0.18489
242 ->249 0.15129
242 ->250 0.18317

Excited State 42: Singlet-A1G 4.3013 eV 288.25 nm f=0.0000 <S**2>=0.000
228 ->244 0.14833
229 ->245 0.14833
238 ->246 0.17336
239 ->248 0.24904
240 ->250 0.20943
241 ->249 0.20943
242 ->247 0.48024
243 ->255 0.13842

Excited state symmetry could not be determined.
Excited State 43: Singlet-?Sym 4.3595 eV 284.40 nm f=0.0000 <S**2>=0.000
224 ->245 -0.19193
225 ->244 0.19193
228 ->245 0.44337
229 ->244 0.44337
239 ->246 -0.14882

Excited state symmetry could not be determined.
Excited State 44: Singlet-?Sym 4.4035 eV 281.56 nm f=0.0000 <S**2>=0.000
228 ->244 -0.49304
229 ->245 0.49304

Excited state symmetry could not be determined.
Excited State 45: Singlet-?Sym 4.4419 eV 279.12 nm f=0.0000 <S**2>=0.000
228 ->244 0.47220
229 ->245 0.47220
242 ->247 -0.12463

Excited State 46: Singlet-EU 4.4773 eV 276.92 nm f=0.0063 <S**2>=0.000
222 ->245 0.13810
227 ->244 0.14444
227 ->245 0.66060

Excited State 47: Singlet-EU 4.4773 eV 276.92 nm f=0.0063 <S**2>=0.000
222 ->244 -0.13810
227 ->244 0.66060
227 ->245 -0.14444

Excited State 48: Singlet-B1G 4.5345 eV 273.42 nm f=0.0000 <S**2>=0.000
239 ->247 -0.47125
240 ->250 0.11868
241 ->249 -0.11868
242 ->248 0.48823

Excited State 49: Singlet-EU 4.5383 eV 273.20 nm f=0.0216 <S**2>=0.000
239 ->249 0.11929
241 ->247 0.48256
241 ->248 0.45733
242 ->249 -0.14906

Excited State 50: Singlet-EU 4.5383 eV 273.20 nm f=0.0216 <S**2>=0.000
239 ->250 -0.11929
240 ->247 0.48256
240 ->248 -0.45733
242 ->250 -0.14906

Excited State 51: Singlet-A1G 4.5384 eV 273.19 nm f=0.0000 <S**2>=0.000
238 ->246 -0.12303
239 ->248 -0.44745
240 ->250 -0.15920
241 ->249 -0.15920
242 ->247 0.46737

Excited State 52: Singlet-EU 4.6057 eV 269.20 nm f=0.0351 <S**2>=0.000
226 ->244 0.68639
240 ->248 -0.10235

Excited State 53: Singlet-EU 4.6057 eV 269.20 nm f=0.0351 <S**2>=0.000
226 ->245 0.68639
241 ->248 0.10235

Excited state symmetry could not be determined.
Excited State 54: Singlet-?Sym 4.6239 eV 268.14 nm f=0.0000 <S**2>=0.000
224 ->245 0.47507
225 ->244 0.47507
228 ->245 0.14428
229 ->244 -0.14428

Excited state symmetry could not be determined.
Excited State 55: Singlet-?Sym 4.6392 eV 267.25 nm f=0.0000 <S**2>=0.000
224 ->245 -0.45532
225 ->244 0.45532

228 ->245 -0.19360
229 ->244 -0.19360

Excited State 56: Singlet-A1U 4.6560 eV 266.29 nm f=0.0000 <S**2>=0.000
235 ->246 0.69221

Excited state symmetry could not be determined.
Excited State 57: Singlet-?Sym 4.6628 eV 265.90 nm f=0.0000 <S**2>=0.000
224 ->244 0.48591
225 ->245 -0.48591

Excited State 58: Singlet-A1U 4.6633 eV 265.87 nm f=0.0000 <S**2>=0.000
243 ->251 0.69430

Excited state symmetry could not be determined.
Excited State 59: Singlet-?Sym 4.6785 eV 265.01 nm f=0.0000 <S**2>=0.000
224 ->244 0.48639
225 ->245 0.48639
242 ->248 -0.13670

Excited State 60: Singlet-EG 4.6786 eV 265.00 nm f=0.0000 <S**2>=0.000
243 ->252 -0.46496
243 ->253 0.51541

Excited State 61: Singlet-EG 4.6786 eV 265.00 nm f=0.0000 <S**2>=0.000
243 ->252 0.51541
243 ->253 0.46496

Excited State 62: Singlet-B1U 4.6865 eV 264.56 nm f=0.0000 <S**2>=0.000
243 ->254 0.69401

Excited State 63: Singlet-EU 4.7265 eV 262.32 nm f=0.0007 <S**2>=0.000
236 ->246 0.12248
239 ->250 -0.22519
240 ->248 -0.25313
242 ->250 0.59107

Excited State 64: Singlet-EU 4.7265 eV 262.32 nm f=0.0007 <S**2>=0.000
237 ->246 0.12248
239 ->249 0.22519
241 ->248 0.25313
242 ->249 0.59107

Excited state symmetry could not be determined.
Excited State 65: Singlet-?Sym 4.7323 eV 261.99 nm f=0.0000 <S**2>=0.000
240 ->249 0.49699
241 ->250 0.49699

Excited state symmetry could not be determined.
Excited State 66: Singlet-?Sym 4.7340 eV 261.90 nm f=0.0000 <S**2>=0.000
240 ->249 -0.49604
241 ->250 0.49604

Excited State 67: Singlet-EU 4.7421 eV 261.46 nm f=0.1498 <S**2>=0.000
236 ->246 -0.17169
237 ->246 -0.38968
239 ->249 0.40676
239 ->250 -0.17921
240 ->248 0.11979
241 ->247 0.11871

```
   241 ->248        -0.27190

 Excited State  68:      Singlet-EU     4.7421 eV  261.46 nm  f=0.1498  <S**2>=0.000
   236 ->246         0.38968
   237 ->246        -0.17169
   239 ->249         0.17921
   239 ->250         0.40676
   240 ->247        -0.11871
   240 ->248        -0.27190
   241 ->248        -0.11979

 Excited State  69:      Singlet-A1G    4.7474 eV  261.16 nm  f=0.0000  <S**2>=0.000
   238 ->246        -0.37185
   239 ->248         0.44073
   240 ->250        -0.26726
   241 ->249        -0.26726
   242 ->247         0.13894

 Excited state symmetry could not be determined.
 Excited State  70:      Singlet-?Sym    4.7554 eV  260.72 nm  f=0.0000  <S**2>=0.000
   239 ->247         0.18284
   240 ->250        -0.40205
   241 ->249         0.40205
   242 ->248         0.36099
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 LETran=    1270.
 Leave Link  914 at Sun Jul 20 19:51:47 2014, MaxMem= 2359296000 cpu:  789314.6
 (Enter /usr/local/g09/l601.exe)
 Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.


 TPyzPyzPz
 Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-EU     1.8381 eV  674.53 nm  f=0.9650  <S**2>=0.000
   295 -> 296         0.49906
   295 -> 297         0.48447
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -7817.51602671
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-EU     1.8381 eV  674.53 nm  f=0.9650  <S**2>=0.000
   295 -> 296        -0.48447
   295 -> 297         0.49906

 Excited State   3:      Singlet-B2G    2.3063 eV  537.60 nm  f=0.0000  <S**2>=0.000
   295 -> 298         0.69987

 Excited State   4:      Singlet-A2G    2.3724 eV  522.62 nm  f=0.0000  <S**2>=0.000
   295 -> 299         0.69210

 Excited State   5:      Singlet-EG     2.5374 eV  488.62 nm  f=0.0000  <S**2>=0.000
   282 -> 296         0.11895
   290 -> 296         0.56699
   290 -> 297        -0.36352

 Excited State   6:      Singlet-EG     2.5374 eV  488.62 nm  f=0.0000  <S**2>=0.000
   282 -> 297         0.11895
   290 -> 296         0.36352
   290 -> 297         0.56699
```

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 2.5417 eV 487.80 nm f=0.0000 <S**2>=0.000
292 -> 296 -0.49309
293 -> 297 0.49309

Excited State 8: Singlet-EU 2.5428 eV 487.58 nm f=0.0526 <S**2>=0.000
294 -> 296 0.68927

Excited State 9: Singlet-EU 2.5428 eV 487.58 nm f=0.0526 <S**2>=0.000
294 -> 297 0.68927

Excited state symmetry could not be determined.
Excited State 10: Singlet-?Sym 2.5434 eV 487.47 nm f=0.0000 <S**2>=0.000
292 -> 296 0.48792
293 -> 297 0.48792
295 -> 299 0.13549

Excited State 11: Singlet-EU 2.5607 eV 484.19 nm f=1.3128 <S**2>=0.000
291 -> 297 0.49741
294 -> 297 -0.10826
295 -> 301 0.45721

Excited State 12: Singlet-EU 2.5607 eV 484.19 nm f=1.3128 <S**2>=0.000
291 -> 296 0.49741
294 -> 296 0.10826
295 -> 300 0.45721

Excited state symmetry could not be determined.
Excited State 13: Singlet-?Sym 2.5686 eV 482.70 nm f=0.0000 <S**2>=0.000
292 -> 297 0.49419
293 -> 296 0.49419

Excited State 14: Singlet-EU 2.5921 eV 478.31 nm f=0.0052 <S**2>=0.000
291 -> 296 -0.47488
295 -> 300 0.50577

Excited State 15: Singlet-EU 2.5921 eV 478.31 nm f=0.0052 <S**2>=0.000
291 -> 297 -0.47488
295 -> 301 0.50577

Excited state symmetry could not be determined.
Excited State 16: Singlet-?Sym 2.6148 eV 474.15 nm f=0.0000 <S**2>=0.000
292 -> 297 -0.49676
293 -> 296 0.49676

Excited state symmetry could not be determined.
Excited State 17: Singlet-?Sym 2.7412 eV 452.29 nm f=0.0001 <S**2>=0.000
284 -> 299 -0.20237
288 -> 297 -0.39918
288 -> 300 0.14943
289 -> 296 0.39918
289 -> 301 0.14943
290 -> 298 0.29663

Excited state symmetry could not be determined.
Excited State 18: Singlet-?Sym 2.7515 eV 450.61 nm f=0.0000 <S**2>=0.000
284 -> 298 -0.23525
288 -> 297 0.40678
288 -> 300 -0.15088
289 -> 296 0.40678

289 -> 301 0.15088
290 -> 299 0.24550

Excited State 19: Singlet-EG 2.8389 eV 436.74 nm f=0.0000 <S**2>=0.000
284 -> 296 0.35465
284 -> 297 -0.42156
288 -> 298 0.18805
288 -> 299 -0.16757
289 -> 298 -0.15820
289 -> 299 -0.14097
290 -> 300 0.16686
290 -> 301 -0.14038

Excited State 20: Singlet-EG 2.8389 eV 436.74 nm f=0.0000 <S**2>=0.000
284 -> 296 0.42156
284 -> 297 0.35465
288 -> 298 -0.15820
288 -> 299 0.14097
289 -> 298 -0.18805
289 -> 299 -0.16757
290 -> 300 -0.14038
290 -> 301 -0.16686

Excited state symmetry could not be determined.
Excited State 21: Singlet-?Sym 2.8420 eV 436.25 nm f=0.0000 <S**2>=0.000
288 -> 296 0.48836
289 -> 297 0.48835

Excited state symmetry could not be determined.
Excited State 22: Singlet-?Sym 2.8447 eV 435.84 nm f=0.0000 <S**2>=0.000
288 -> 296 -0.48975
289 -> 297 0.48976

Excited state symmetry could not be determined.
Excited State 23: Singlet-?Sym 3.0825 eV 402.22 nm f=0.0000 <S**2>=0.000
285 -> 296 -0.36781
286 -> 297 0.36781
291 -> 299 -0.21405
292 -> 300 0.14507
293 -> 301 0.14507
294 -> 298 -0.36255

Excited State 24: Singlet-B1G 3.0826 eV 402.21 nm f=0.0000 <S**2>=0.000
285 -> 296 -0.25220
286 -> 297 -0.25220
291 -> 298 0.39200
292 -> 300 0.19324
293 -> 301 -0.19324
294 -> 299 0.34496
295 -> 302 -0.10342

Excited State 25: Singlet-EU 3.0939 eV 400.74 nm f=0.3062 <S**2>=0.000
283 -> 296 0.14454
283 -> 297 -0.12736
287 -> 296 -0.28460
287 -> 297 -0.25077
291 -> 300 0.12181
291 -> 301 -0.10733
292 -> 298 0.29539
292 -> 299 -0.21471

293 -> 298 0.26028
293 -> 299 0.18918
294 -> 300 -0.13284
294 -> 301 -0.11705

Excited State 26: Singlet-EU 3.0939 eV 400.74 nm f=0.3062 <S**2>=0.000
283 -> 296 -0.12736
283 -> 297 -0.14454
287 -> 296 0.25077
287 -> 297 -0.28460
291 -> 300 -0.10733
291 -> 301 -0.12181
292 -> 298 -0.26028
292 -> 299 0.18918
293 -> 298 0.29539
293 -> 299 0.21471
294 -> 300 0.11705
294 -> 301 -0.13284

Excited State 27: Singlet-EG 3.0945 eV 400.66 nm f=0.0000 <S**2>=0.000
282 -> 296 0.35424
282 -> 297 0.26354
284 -> 296 -0.29885
284 -> 297 0.22234
284 -> 300 0.11341
284 -> 301 0.15244
288 -> 298 0.12550
288 -> 299 -0.12594
289 -> 298 -0.16869
289 -> 299 -0.16929
290 -> 300 0.10428
290 -> 301 -0.14017

Excited State 28: Singlet-EG 3.0945 eV 400.66 nm f=0.0000 <S**2>=0.000
282 -> 296 -0.26354
282 -> 297 0.35424
284 -> 296 0.22234
284 -> 297 0.29885
284 -> 300 0.15244
284 -> 301 -0.11341
288 -> 298 0.16869
288 -> 299 -0.16929
289 -> 298 0.12550
289 -> 299 0.12594
290 -> 300 0.14017
290 -> 301 0.10428

Excited state symmetry could not be determined.
Excited State 29: Singlet-?Sym 3.1262 eV 396.59 nm f=0.0000 <S**2>=0.000
285 -> 297 0.49262
286 -> 296 0.49262

Excited state symmetry could not be determined.
Excited State 30: Singlet-?Sym 3.1362 eV 395.33 nm f=0.0000 <S**2>=0.000
285 -> 297 -0.49248
286 -> 296 0.49248

Excited state symmetry could not be determined.
Excited State 31: Singlet-?Sym 3.1475 eV 393.92 nm f=0.0000 <S**2>=0.000
285 -> 296 0.42675

286 -> 297 0.42675
291 -> 298 0.23506
294 -> 299 0.19939
295 -> 302 -0.13366

Excited State 32: Singlet-EU 3.1496 eV 393.64 nm f=0.7871 <S**2>=0.000
283 -> 297 -0.19979
287 -> 296 -0.18980
287 -> 297 0.54832
293 -> 298 0.22595
293 -> 299 0.14803

Excited State 33: Singlet-EU 3.1496 eV 393.64 nm f=0.7871 <S**2>=0.000
283 -> 296 0.19979
287 -> 296 0.54832
287 -> 297 0.18980
292 -> 298 0.22595
292 -> 299 -0.14803

Excited State 34: Singlet-B2U 3.1672 eV 391.47 nm f=0.0000 <S**2>=0.000
284 -> 298 -0.23047
288 -> 297 -0.28003
288 -> 300 -0.22954
289 -> 296 -0.28003
289 -> 301 0.22954
290 -> 299 0.41751

Excited State 35: Singlet-A2U 3.1723 eV 390.83 nm f=0.0002 <S**2>=0.000
284 -> 299 -0.23081
288 -> 297 0.29517
288 -> 300 0.21442
289 -> 296 -0.29517
289 -> 301 0.21442
290 -> 298 0.41750

Excited State 36: Singlet-A1G 3.2368 eV 383.04 nm f=0.0000 <S**2>=0.000
285 -> 296 -0.27407
286 -> 297 0.27407
294 -> 298 0.58109

Excited State 37: Singlet-EU 3.2379 eV 382.92 nm f=0.2793 <S**2>=0.000
281 -> 297 0.22226
283 -> 296 0.58464
292 -> 298 -0.30379

Excited State 38: Singlet-EU 3.2379 eV 382.92 nm f=0.2793 <S**2>=0.000
281 -> 296 -0.22226
283 -> 297 0.58464
293 -> 298 0.30379

Excited State 39: Singlet-B1G 3.2566 eV 380.72 nm f=0.0000 <S**2>=0.000
291 -> 298 0.49605
294 -> 299 -0.49417

Excited State 40: Singlet-EU 3.2624 eV 380.04 nm f=0.1624 <S**2>=0.000
283 -> 296 0.17207
292 -> 298 0.36589
292 -> 299 0.53207
293 -> 299 -0.13253

Excited State 41: Singlet-EU 3.2624 eV 380.04 nm f=0.1624 <S**2>=0.000
283 -> 297 0.17207
292 -> 299 0.13253
293 -> 298 -0.36589
293 -> 299 0.53207

Excited State 42: Singlet-EG 3.2728 eV 378.83 nm f=0.0000 <S**2>=0.000
280 -> 296 0.69630

Excited State 43: Singlet-EG 3.2728 eV 378.83 nm f=0.0000 <S**2>=0.000
280 -> 297 0.69630

Excited State 44: Singlet-A1G 3.2866 eV 377.24 nm f=0.0000 <S**2>=0.000
285 -> 296 -0.18807
286 -> 297 0.18807
291 -> 299 0.61284
292 -> 300 -0.14086
293 -> 301 -0.14086
294 -> 298 -0.10101

Excited State 45: Singlet-EG 3.2882 eV 377.06 nm f=0.0000 <S**2>=0.000
282 -> 297 0.50104
284 -> 297 -0.21232
284 -> 300 -0.13137
288 -> 298 -0.19562
288 -> 299 0.21586
290 -> 297 -0.17096
290 -> 300 -0.22576

Excited State 46: Singlet-EG 3.2882 eV 377.06 nm f=0.0000 <S**2>=0.000
282 -> 296 0.50104
284 -> 296 0.21232
284 -> 301 -0.13137
289 -> 298 0.19562
289 -> 299 0.21586
290 -> 296 -0.17096
290 -> 301 0.22576

Excited State 47: Singlet-B1G 3.3985 eV 364.82 nm f=0.0000 <S**2>=0.000
291 -> 298 0.12944
292 -> 300 -0.11333
293 -> 301 0.11333
294 -> 299 0.21444
295 -> 302 0.63269

Excited State 48: Singlet-EU 3.4522 eV 359.15 nm f=0.0444 <S**2>=0.000
291 -> 300 0.13550
291 -> 301 -0.20553
293 -> 299 0.11008
294 -> 300 0.35224
294 -> 301 0.53428

Excited State 49: Singlet-EU 3.4522 eV 359.15 nm f=0.0444 <S**2>=0.000
291 -> 300 0.20553
291 -> 301 0.13550
292 -> 299 -0.11008
294 -> 300 0.53428
294 -> 301 -0.35224

Excited state symmetry could not be determined.

Excited State 50: Singlet-?Sym 3.4576 eV 358.58 nm f=0.0000 <S**2>=0.000
292 -> 301 -0.49622
293 -> 300 0.49622

Excited state symmetry could not be determined.
Excited State 51: Singlet-?Sym 3.4579 eV 358.55 nm f=0.0000 <S**2>=0.000
292 -> 301 0.49674
293 -> 300 0.49674

Excited State 52: Singlet-EU 3.4719 eV 357.11 nm f=0.1016 <S**2>=0.000
281 -> 297 -0.26120
291 -> 300 0.54585
292 -> 298 -0.17941
292 -> 299 0.25719
294 -> 300 -0.15470

Excited State 53: Singlet-EU 3.4719 eV 357.11 nm f=0.1016 <S**2>=0.000
281 -> 296 0.26120
291 -> 301 0.54585
293 -> 298 0.17941
293 -> 299 0.25719
294 -> 301 0.15470

Excited state symmetry could not be determined.
Excited State 54: Singlet-?Sym 3.4781 eV 356.48 nm f=0.0000 <S**2>=0.000
291 -> 299 0.25865
292 -> 300 0.45202
293 -> 301 0.45202
294 -> 298 0.13036

Excited state symmetry could not be determined.
Excited State 55: Singlet-?Sym 3.4850 eV 355.76 nm f=0.0000 <S**2>=0.000
291 -> 298 0.13808
292 -> 300 -0.42901
293 -> 301 0.42901
294 -> 299 0.21483
295 -> 302 -0.24618

Excited State 56: Singlet-A2U 3.4946 eV 354.79 nm f=0.0000 <S**2>=0.000
282 -> 298 0.23448
284 -> 299 0.35540
288 -> 300 -0.20611
289 -> 301 -0.20611
290 -> 298 0.45608

Excited State 57: Singlet-B2U 3.5603 eV 348.24 nm f=0.0000 <S**2>=0.000
282 -> 299 0.18037
284 -> 298 0.40946
288 -> 300 0.14745
289 -> 301 -0.14745
290 -> 299 0.48036

Excited State 58: Singlet-EU 3.6137 eV 343.10 nm f=0.3128 <S**2>=0.000
281 -> 296 0.10463
281 -> 297 0.54300
283 -> 296 -0.14297
286 -> 298 0.12234
291 -> 300 0.28778
295 -> 296 -0.10337

Excited State 59: Singlet-EU 3.6137 eV 343.10 nm f=0.3128 <S**2>=0.000
281 -> 296 -0.54300
281 -> 297 0.10463
283 -> 297 -0.14297
285 -> 298 -0.12234
291 -> 301 0.28778
295 -> 297 -0.10337

Excited State 60: Singlet-EG 3.6438 eV 340.26 nm f=0.0000 <S**2>=0.000
284 -> 300 -0.10663
288 -> 298 -0.30284
289 -> 298 -0.26578
290 -> 300 0.40438
290 -> 301 0.35490

Excited State 61: Singlet-EG 3.6438 eV 340.26 nm f=0.0000 <S**2>=0.000
284 -> 301 -0.10663
288 -> 298 -0.26578
289 -> 298 0.30284
290 -> 300 0.35490
290 -> 301 -0.40438

Excited State 62: Singlet-EU 3.6456 eV 340.10 nm f=0.0001 <S**2>=0.000
283 -> 296 -0.11456
283 -> 301 0.14664
285 -> 298 0.25877
285 -> 299 -0.19562
286 -> 298 -0.41032
286 -> 299 -0.31018
287 -> 300 0.12359
287 -> 301 0.19598

Excited State 63: Singlet-EU 3.6456 eV 340.10 nm f=0.0001 <S**2>=0.000
283 -> 297 -0.11456
283 -> 300 -0.14664
285 -> 298 0.41032
285 -> 299 -0.31019
286 -> 298 0.25877
286 -> 299 0.19562
287 -> 300 0.19598
287 -> 301 -0.12359

Excited State 64: Singlet-A2G 3.6495 eV 339.73 nm f=0.0000 <S**2>=0.000
283 -> 299 0.29370
285 -> 300 0.22906
286 -> 301 -0.22906
287 -> 298 0.53760

Excited State 65: Singlet-B2G 3.6669 eV 338.11 nm f=0.0000 <S**2>=0.000
283 -> 298 0.39265
285 -> 300 -0.24782
286 -> 301 -0.24782
287 -> 299 0.45438

Excited State 66: Singlet-EG 3.6856 eV 336.40 nm f=0.0000 <S**2>=0.000
284 -> 300 -0.13403
288 -> 298 0.34977
288 -> 299 0.46181
289 -> 298 -0.15709
289 -> 299 0.20741

```
   290 -> 300        0.22556
   290 -> 301       -0.10130

Excited State  67:      Singlet-EG     3.6856 eV  336.40 nm  f=0.0000  <S**2>=0.000
   284 -> 301        0.13403
   288 -> 298        0.15709
   288 -> 299        0.20741
   289 -> 298        0.34977
   289 -> 299       -0.46181
   290 -> 300        0.10130
   290 -> 301        0.22556

Excited state symmetry could not be determined.
Excited State  68:      Singlet-?Sym    3.6942 eV  335.62 nm  f=0.0000  <S**2>=0.000
   271 -> 297       -0.15082
   272 -> 296       -0.15082
   278 -> 297       -0.44074
   279 -> 296        0.44074
   280 -> 298        0.23097

Excited state symmetry could not be determined.
Excited State  69:      Singlet-?Sym    3.7255 eV  332.80 nm  f=0.0000  <S**2>=0.000
   271 -> 296       -0.12180
   272 -> 297       -0.12180
   278 -> 296       -0.44987
   279 -> 297        0.44987
   284 -> 298        0.18752

Excited state symmetry could not be determined.
Excited State  70:      Singlet-?Sym    3.7646 eV  329.34 nm  f=0.0002  <S**2>=0.000
   271 -> 296        0.10999
   272 -> 297       -0.11000
   278 -> 296        0.44502
   279 -> 297        0.44502
   282 -> 298        0.10629
   284 -> 299       -0.17975
SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 LETran=    1270.
Leave Link  914 at Tue Jul 22 12:24:58 2014, MaxMem= 2359296000 cpu: 1756552.9
(Enter /usr/local/g09/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

 NC Excitation energies and oscillator strengths:

Excited State   1:      Singlet-EU     1.5510 eV  799.38 nm  f=1.2592  <S**2>=0.000
   295 -> 296        0.60192
   295 -> 297       -0.36597
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) =  -7560.91906521
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State   2:      Singlet-EU     1.5510 eV  799.38 nm  f=1.2592  <S**2>=0.000
   295 -> 296        0.36597
   295 -> 297        0.60192

Excited State   3:      Singlet-B2G    2.5329 eV  489.50 nm  f=0.0000  <S**2>=0.000
   295 -> 298        0.69393

Excited State   4:      Singlet-EU     2.6235 eV  472.60 nm  f=0.4055  <S**2>=0.000
   291 -> 297        0.12620
   294 -> 296        0.66962
```

294 -> 297 0.16392

Excited State 5: Singlet-EU 2.6235 eV 472.60 nm f=0.4055 <S**2>=0.000
291 -> 296 -0.12620
294 -> 296 -0.16392
294 -> 297 0.66962

Excited State 6: Singlet-A2G 2.6251 eV 472.30 nm f=0.0000 <S**2>=0.000
289 -> 296 -0.16818
290 -> 297 -0.16818
292 -> 297 -0.19676
293 -> 296 -0.19676
295 -> 299 0.60138

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 2.6362 eV 470.31 nm f=0.0000 <S**2>=0.000
289 -> 297 0.15109
290 -> 296 0.15109
292 -> 296 0.47310
293 -> 297 0.47310

Excited state symmetry could not be determined.
Excited State 8: Singlet-?Sym 2.6450 eV 468.76 nm f=0.0000 <S**2>=0.000
292 -> 297 0.45661
293 -> 296 0.45661
295 -> 299 0.26920

Excited state symmetry could not be determined.
Excited State 9: Singlet-?Sym 2.6713 eV 464.14 nm f=0.0000 <S**2>=0.000
289 -> 296 0.29271
290 -> 297 -0.29271
292 -> 297 -0.40249
293 -> 296 0.40249

Excited state symmetry could not be determined.
Excited State 10: Singlet-?Sym 2.6795 eV 462.71 nm f=0.0000 <S**2>=0.000
289 -> 297 0.15330
290 -> 296 -0.15330
292 -> 296 0.47048
293 -> 297 -0.47048

Excited State 11: Singlet-EU 2.7146 eV 456.73 nm f=0.0106 <S**2>=0.000
288 -> 296 -0.14389
288 -> 297 -0.21248
291 -> 296 -0.31067
291 -> 297 0.45875
295 -> 300 0.18148
295 -> 301 0.26798

Excited State 12: Singlet-EU 2.7146 eV 456.73 nm f=0.0106 <S**2>=0.000
288 -> 296 0.21248
288 -> 297 -0.14389
291 -> 296 0.45875
291 -> 297 0.31067
295 -> 300 -0.26798
295 -> 301 0.18148

Excited state symmetry could not be determined.
Excited State 13: Singlet-?Sym 2.7326 eV 453.72 nm f=0.0000 <S**2>=0.000
289 -> 296 0.39425

290 -> 297 -0.39425
292 -> 297 0.28999
293 -> 296 -0.28999
295 -> 298 -0.12409

Excited state symmetry could not be determined.
Excited State 14: Singlet-?Sym 2.7327 eV 453.71 nm f=0.0000 <S**2>=0.000
289 -> 296 0.46356
290 -> 297 0.46356
295 -> 299 0.25102

Excited State 15: Singlet-EU 2.7650 eV 448.41 nm f=0.6819 <S**2>=0.000
288 -> 296 0.13073
288 -> 297 0.55160
291 -> 297 0.35800
295 -> 301 -0.18884

Excited State 16: Singlet-EU 2.7650 eV 448.41 nm f=0.6819 <S**2>=0.000
288 -> 296 0.55160
288 -> 297 -0.13073
291 -> 296 -0.35800
295 -> 300 -0.18884

Excited state symmetry could not be determined.
Excited State 17: Singlet-?Sym 2.7660 eV 448.25 nm f=0.0000 <S**2>=0.000
289 -> 297 0.47365
290 -> 296 0.47365
292 -> 296 -0.15372
293 -> 297 -0.15372

Excited State 18: Singlet-EU 2.7848 eV 445.22 nm f=0.0132 <S**2>=0.000
288 -> 297 0.32396
291 -> 297 -0.18239
295 -> 301 0.59320

Excited State 19: Singlet-EU 2.7848 eV 445.22 nm f=0.0132 <S**2>=0.000
288 -> 296 0.32396
291 -> 296 0.18239
295 -> 300 0.59320

Excited state symmetry could not be determined.
Excited State 20: Singlet-?Sym 2.8331 eV 437.63 nm f=0.0000 <S**2>=0.000
289 -> 297 -0.47439
290 -> 296 0.47439
292 -> 296 0.15061
293 -> 297 -0.15061

Excited State 21: Singlet-B1G 3.0028 eV 412.89 nm f=0.0000 <S**2>=0.000
295 -> 302 0.70234

Excited State 22: Singlet-EG 3.0477 eV 406.82 nm f=0.0000 <S**2>=0.000
286 -> 296 0.61414
286 -> 297 -0.34647

Excited State 23: Singlet-EG 3.0477 eV 406.82 nm f=0.0000 <S**2>=0.000
286 -> 296 0.34647
286 -> 297 0.61414

Excited State 24: Singlet-EU 3.1298 eV 396.14 nm f=0.0004 <S**2>=0.000
285 -> 297 -0.13710

287 -> 296 0.65785
287 -> 297 -0.18237

Excited State 25: Singlet-EU 3.1298 eV 396.14 nm f=0.0004 <S**2>=0.000
285 -> 296 0.13710
287 -> 296 0.18237
287 -> 297 0.65785

Excited State 26: Singlet-EG 3.5634 eV 347.94 nm f=0.0000 <S**2>=0.000
284 -> 296 0.57958
284 -> 297 -0.39503

Excited State 27: Singlet-EG 3.5634 eV 347.94 nm f=0.0000 <S**2>=0.000
284 -> 296 0.39503
284 -> 297 0.57958

Excited State 28: Singlet-EU 3.6605 eV 338.71 nm f=1.9099 <S**2>=0.000
285 -> 297 0.43461
288 -> 300 -0.20471
289 -> 298 0.33666
289 -> 299 -0.24351
291 -> 300 -0.20656
293 -> 298 -0.15406

Excited State 29: Singlet-EU 3.6605 eV 338.71 nm f=1.9099 <S**2>=0.000
285 -> 296 0.43461
288 -> 301 0.20471
290 -> 298 0.33666
290 -> 299 0.24351
291 -> 301 -0.20656
292 -> 298 -0.15406

Excited State 30: Singlet-B1G 3.7017 eV 334.94 nm f=0.0000 <S**2>=0.000
288 -> 298 0.45846
289 -> 300 -0.22930
290 -> 301 0.22930
291 -> 299 -0.35020
292 -> 301 -0.13325
293 -> 300 0.13325

Excited State 31: Singlet-A1G 3.7344 eV 332.00 nm f=0.0000 <S**2>=0.000
288 -> 299 -0.30022
289 -> 300 -0.24063
290 -> 301 -0.24063
291 -> 298 0.46033
294 -> 302 0.16870
295 -> 303 -0.17910

Excited State 32: Singlet-A2G 3.7520 eV 330.45 nm f=0.0000 <S**2>=0.000
292 -> 300 -0.14315
293 -> 301 0.14315
294 -> 298 0.65714

Excited State 33: Singlet-EU 3.7676 eV 329.08 nm f=0.1208 <S**2>=0.000
285 -> 296 0.27523
287 -> 297 -0.10739
290 -> 299 -0.12427
292 -> 298 0.52148
292 -> 299 -0.16834
294 -> 300 -0.22725

Excited State 34: Singlet-EU 3.7676 eV 329.08 nm f=0.1208 <S**2>=0.000
285 -> 297 0.27523
287 -> 296 0.10739
289 -> 299 0.12427
293 -> 298 0.52148
293 -> 299 0.16834
294 -> 301 0.22725

Excited State 35: Singlet-EU 3.7999 eV 326.28 nm f=0.0106 <S**2>=0.000
285 -> 296 0.17278
285 -> 297 0.34200
287 -> 296 0.10328
288 -> 300 0.10544
289 -> 298 -0.27434
289 -> 299 0.13514
290 -> 298 -0.13860
291 -> 300 0.10431
292 -> 298 -0.12544
292 -> 302 -0.12224
293 -> 298 -0.24829
293 -> 299 -0.14836
295 -> 304 -0.16462

Excited State 36: Singlet-EU 3.7999 eV 326.28 nm f=0.0106 <S**2>=0.000
285 -> 296 0.34200
285 -> 297 -0.17278
287 -> 297 -0.10328
288 -> 301 -0.10544
289 -> 298 0.13860
290 -> 298 -0.27434
290 -> 299 -0.13514
291 -> 301 0.10431
292 -> 298 -0.24829
292 -> 299 0.14836
293 -> 298 0.12544
293 -> 302 0.12224
295 -> 305 -0.16462

Excited State 37: Singlet-B2G 3.8339 eV 323.39 nm f=0.0000 <S**2>=0.000
287 -> 298 -0.13007
292 -> 300 0.23959
293 -> 301 0.23959
294 -> 299 0.59173

Excited State 38: Singlet-EU 3.9047 eV 317.53 nm f=0.0091 <S**2>=0.000
289 -> 299 0.10130
290 -> 299 0.11527
292 -> 298 0.22057
292 -> 299 0.42999
293 -> 298 -0.19383
293 -> 299 0.37786
294 -> 300 0.15228
294 -> 301 0.13382

Excited State 39: Singlet-EU 3.9047 eV 317.53 nm f=0.0091 <S**2>=0.000
289 -> 299 0.11527
290 -> 299 -0.10130
292 -> 298 -0.19383
292 -> 299 -0.37786

293 -> 298 -0.22057
293 -> 299 0.42999
294 -> 300 -0.13382
294 -> 301 0.15228

Excited state symmetry could not be determined.
Excited State 40: Singlet-?Sym 3.9373 eV 314.89 nm f=0.0000 <S**2>=0.000
277 -> 296 0.13314
278 -> 297 -0.13314
282 -> 297 0.45673
283 -> 296 0.45673
294 -> 298 -0.10961

Excited State 41: Singlet-B1G 3.9666 eV 312.57 nm f=0.0000 <S**2>=0.000
288 -> 298 0.49243
291 -> 299 0.47383

Excited State 42: Singlet-EU 3.9678 eV 312.48 nm f=0.0151 <S**2>=0.000
289 -> 298 0.47427
289 -> 299 0.42475
291 -> 300 0.11519
293 -> 298 -0.12422
293 -> 299 -0.15165

Excited State 43: Singlet-EU 3.9678 eV 312.48 nm f=0.0151 <S**2>=0.000
290 -> 298 0.47427
290 -> 299 -0.42475
291 -> 301 0.11520
292 -> 298 -0.12422
292 -> 299 0.15165

Excited State 44: Singlet-A1G 3.9683 eV 312.44 nm f=0.0000 <S**2>=0.000
288 -> 299 0.45517
289 -> 300 0.13815
290 -> 301 0.13815
291 -> 298 0.49007

Excited state symmetry could not be determined.
Excited State 45: Singlet-?Sym 3.9802 eV 311.51 nm f=0.0000 <S**2>=0.000
282 -> 296 0.47360
283 -> 297 0.47360
292 -> 301 0.11489
293 -> 300 -0.11489

Excited state symmetry could not be determined.
Excited State 46: Singlet-?Sym 4.0005 eV 309.92 nm f=0.0000 <S**2>=0.000
277 -> 296 0.13929
278 -> 297 0.13929
282 -> 297 -0.46591
283 -> 296 0.46591

Excited state symmetry could not be determined.
Excited State 47: Singlet-?Sym 4.0138 eV 308.89 nm f=0.0000 <S**2>=0.000
282 -> 296 0.48818
283 -> 297 -0.48818

Excited state symmetry could not be determined.
Excited State 48: Singlet-?Sym 4.0156 eV 308.76 nm f=0.0000 <S**2>=0.000
275 -> 296 0.48834
276 -> 297 -0.48834

284 -> 298 0.12440

Excited state symmetry could not be determined.
Excited State 49: Singlet-?Sym 4.0328 eV 307.44 nm f=0.0000 <S**2>=0.000
275 -> 297 0.49639
276 -> 296 -0.49638

Excited state symmetry could not be determined.
Excited State 50: Singlet-?Sym 4.0351 eV 307.26 nm f=0.0000 <S**2>=0.000
282 -> 297 0.10661
283 -> 296 0.10661
287 -> 299 0.18055
289 -> 301 -0.12535
290 -> 300 0.12535
292 -> 300 0.41668
293 -> 301 -0.41668
294 -> 298 0.22229

Excited State 51: Singlet-EU 4.0429 eV 306.67 nm f=0.0354 <S**2>=0.000
281 -> 296 0.15117
281 -> 297 0.58427
290 -> 299 0.11048
292 -> 299 0.14593
294 -> 300 -0.26345

Excited State 52: Singlet-EU 4.0429 eV 306.67 nm f=0.0354 <S**2>=0.000
281 -> 296 0.58427
281 -> 297 -0.15117
289 -> 299 -0.11048
293 -> 299 -0.14593
294 -> 301 0.26345

Excited state symmetry could not be determined.
Excited State 53: Singlet-?Sym 4.0547 eV 305.78 nm f=0.0000 <S**2>=0.000
287 -> 298 -0.21013
292 -> 300 0.39352
293 -> 301 0.39352
294 -> 299 -0.37177

Excited State 54: Singlet-EU 4.0670 eV 304.85 nm f=0.0699 <S**2>=0.000
281 -> 296 -0.31600
289 -> 299 -0.16907
293 -> 299 -0.17397
294 -> 300 -0.16445
294 -> 301 0.52539

Excited State 55: Singlet-EU 4.0670 eV 304.85 nm f=0.0699 <S**2>=0.000
281 -> 297 0.31600
290 -> 299 -0.16907
292 -> 299 -0.17397
294 -> 300 0.52539
294 -> 301 0.16445

Excited state symmetry could not be determined.
Excited State 56: Singlet-?Sym 4.0707 eV 304.58 nm f=0.0046 <S**2>=0.000
275 -> 297 0.48563
276 -> 296 0.48563
284 -> 302 -0.11966

Excited state symmetry could not be determined.

Excited State 57: Singlet-?Sym 4.0719 eV 304.48 nm f=0.0000 <S**2>=0.000
282 -> 296 0.12025
283 -> 297 0.12025
291 -> 299 0.18201
292 -> 301 -0.45552
293 -> 300 0.45552

Excited state symmetry could not be determined.
Excited State 58: Singlet-?Sym 4.0781 eV 304.02 nm f=0.0000 <S**2>=0.000
275 -> 296 0.49586
276 -> 297 0.49586

Excited state symmetry could not be determined.
Excited State 59: Singlet-?Sym 4.0793 eV 303.94 nm f=0.0000 <S**2>=0.000
288 -> 299 -0.13497
292 -> 301 0.47093
293 -> 300 0.47093
295 -> 303 -0.11003

Excited state symmetry could not be determined.
Excited State 60: Singlet-?Sym 4.1383 eV 299.60 nm f=0.0000 <S**2>=0.000
277 -> 296 -0.16671
278 -> 297 0.16671
289 -> 301 -0.43468
290 -> 300 0.43468
291 -> 302 0.13081
292 -> 300 -0.13232
293 -> 301 0.13232

Excited State 61: Singlet-EU 4.1407 eV 299.43 nm f=0.0665 <S**2>=0.000
279 -> 297 -0.12637
288 -> 300 -0.26325
289 -> 299 -0.16511
291 -> 300 0.59523

Excited State 62: Singlet-EU 4.1407 eV 299.43 nm f=0.0665 <S**2>=0.000
279 -> 296 0.12636
288 -> 301 0.26325
290 -> 299 0.16511
291 -> 301 0.59523

Excited state symmetry could not be determined.
Excited State 63: Singlet-?Sym 4.1508 eV 298.70 nm f=0.0000 <S**2>=0.000
289 -> 301 0.48213
290 -> 300 0.48213

Excited State 64: Singlet-A1G 4.1563 eV 298.30 nm f=0.0000 <S**2>=0.000
288 -> 299 0.40922
289 -> 300 -0.35171
290 -> 301 -0.35171
291 -> 298 -0.17498
292 -> 301 0.13163
293 -> 300 0.13163

Excited State 65: Singlet-EU 4.1565 eV 298.29 nm f=0.0300 <S**2>=0.000
279 -> 297 0.13308
288 -> 300 0.51202
289 -> 298 0.17301
289 -> 299 -0.32451
291 -> 300 0.15366

```
   293 -> 299        0.11677
   295 -> 304       -0.12583

 Excited State  66:      Singlet-EU     4.1565 eV  298.29 nm  f=0.0300  <S**2>=0.000
   279 -> 296        0.13307
   288 -> 301        0.51203
   290 -> 298       -0.17301
   290 -> 299       -0.32451
   291 -> 301       -0.15366
   292 -> 299        0.11677
   295 -> 305        0.12583

 Excited state symmetry could not be determined.
 Excited State  67:      Singlet-?Sym    4.1609 eV  297.98 nm  f=0.0000  <S**2>=0.000
   288 -> 298        0.17462
   289 -> 300        0.41676
   290 -> 301       -0.41676
   291 -> 299       -0.33594

 Excited state symmetry could not be determined.
 Excited State  68:      Singlet-?Sym    4.1898 eV  295.92 nm  f=0.0000  <S**2>=0.000
   277 -> 296        0.43360
   278 -> 297       -0.43360
   282 -> 297       -0.13813
   283 -> 296       -0.13813
   289 -> 301       -0.17327
   290 -> 300        0.17327

 Excited state symmetry could not be determined.
 Excited State  69:      Singlet-?Sym    4.1949 eV  295.56 nm  f=0.0000  <S**2>=0.000
   277 -> 296        0.46795
   278 -> 297        0.46795
   282 -> 297        0.13351
   283 -> 296       -0.13351

 Excited State  70:      Singlet-EU     4.1980 eV  295.34 nm  f=0.0004  <S**2>=0.000
   274 -> 297       -0.16549
   279 -> 296       -0.10621
   279 -> 297        0.61482
   288 -> 300       -0.21152
   295 -> 304       -0.11313
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 LETran=    1270.
 Leave Link  914 at Sun Jul 20 00:20:20 2014, MaxMem= 2359296000 cpu: 1348588.9
 (Enter /usr/local/g09/l601.exe)
 Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

2,3-TQPz
Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-EU     1.7292 eV  716.98 nm  f=1.0524  <S**2>=0.000
   295 -> 296        0.33959
   295 -> 297        0.61196
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -7689.18336470
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-EU     1.7292 eV  716.98 nm  f=1.0524  <S**2>=0.000
   295 -> 296        0.61196
   295 -> 297       -0.33959
```

Excited State 3: Singlet-B2G 2.3405 eV 529.74 nm f=0.0000 <S**2>=0.000
292 -> 296 -0.14326
293 -> 297 0.14326
295 -> 298 0.67360

Excited State 4: Singlet-A2G 2.4038 eV 515.77 nm f=0.0000 <S**2>=0.000
292 -> 296 -0.37136
293 -> 297 -0.37136
295 -> 299 0.46812

Excited State 5: Singlet-EU 2.4374 eV 508.68 nm f=0.0075 <S**2>=0.000
291 -> 296 0.13719
294 -> 296 0.66474
294 -> 297 -0.14512

Excited State 6: Singlet-EU 2.4374 eV 508.68 nm f=0.0075 <S**2>=0.000
291 -> 297 -0.13719
294 -> 296 0.14512
294 -> 297 0.66474

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 2.4438 eV 507.35 nm f=0.0000 <S**2>=0.000
292 -> 296 0.47181
293 -> 297 -0.47181
295 -> 298 0.20486

Excited State 8: Singlet-EU 2.4644 eV 503.10 nm f=0.7062 <S**2>=0.000
291 -> 296 0.67048
291 -> 297 0.14454
294 -> 296 -0.13812

Excited State 9: Singlet-EU 2.4644 eV 503.10 nm f=0.7062 <S**2>=0.000
291 -> 296 -0.14454
291 -> 297 0.67048
294 -> 297 0.13812

Excited state symmetry could not be determined.
Excited State 10: Singlet-?Sym 2.4649 eV 502.99 nm f=0.0000 <S**2>=0.000
292 -> 297 0.49147
293 -> 296 0.49147

Excited State 11: Singlet-A2G 2.4692 eV 502.13 nm f=0.0000 <S**2>=0.000
292 -> 296 0.33102
293 -> 297 0.33102
295 -> 299 0.52621

Excited state symmetry could not be determined.
Excited State 12: Singlet-?Sym 2.4779 eV 500.35 nm f=0.0000 <S**2>=0.000
288 -> 296 -0.15024
289 -> 297 0.15024
292 -> 297 -0.47414
293 -> 296 0.47414

Excited state symmetry could not be determined.
Excited State 13: Singlet-?Sym 2.6115 eV 474.76 nm f=0.0000 <S**2>=0.000
288 -> 297 0.49546
289 -> 296 0.49546

Excited State 14: Singlet-EU 2.6126 eV 474.57 nm f=0.2721 <S**2>=0.000
290 -> 296 0.13364

290 -> 297 0.68209

Excited State 15: Singlet-EU 2.6126 eV 474.57 nm f=0.2721 <S**2>=0.000
290 -> 296 0.68209
290 -> 297 -0.13364

Excited state symmetry could not be determined.
Excited State 16: Singlet-?Sym 2.6163 eV 473.89 nm f=0.0000 <S**2>=0.000
288 -> 296 0.49085
289 -> 297 0.49085

Excited state symmetry could not be determined.
Excited State 17: Singlet-?Sym 2.6260 eV 472.14 nm f=0.0000 <S**2>=0.000
288 -> 297 -0.49182
289 -> 296 0.49182

Excited State 18: Singlet-EU 2.6378 eV 470.03 nm f=0.2637 <S**2>=0.000
295 -> 301 0.69345

Excited State 19: Singlet-EU 2.6378 eV 470.03 nm f=0.2637 <S**2>=0.000
295 -> 300 0.69345

Excited state symmetry could not be determined.
Excited State 20: Singlet-?Sym 2.6710 eV 464.19 nm f=0.0000 <S**2>=0.000
288 -> 296 -0.46488
289 -> 297 0.46488
292 -> 297 0.15497
293 -> 296 -0.15497

Excited State 21: Singlet-EG 2.6922 eV 460.53 nm f=0.0000 <S**2>=0.000
286 -> 296 -0.27838
286 -> 297 0.63338

Excited State 22: Singlet-EG 2.6922 eV 460.53 nm f=0.0000 <S**2>=0.000
286 -> 296 0.63338
286 -> 297 0.27838

Excited State 23: Singlet-EU 2.8605 eV 433.44 nm f=0.0439 <S**2>=0.000
287 -> 296 0.60003
287 -> 297 -0.28736
292 -> 298 -0.10710

Excited State 24: Singlet-EU 2.8605 eV 433.44 nm f=0.0439 <S**2>=0.000
287 -> 296 0.28736
287 -> 297 0.60003
293 -> 298 0.10710

Excited state symmetry could not be determined.
Excited State 25: Singlet-?Sym 3.0896 eV 401.29 nm f=0.0029 <S**2>=0.000
283 -> 299 -0.13831
284 -> 297 -0.43648
284 -> 300 -0.10757
285 -> 296 0.43648
285 -> 301 -0.10757
286 -> 298 -0.26106

Excited state symmetry could not be determined.
Excited State 26: Singlet-?Sym 3.1043 eV 399.40 nm f=0.0000 <S**2>=0.000
283 -> 298 0.17583
284 -> 297 0.45142

284 -> 300 0.10485
285 -> 296 0.45142
285 -> 301 -0.10485
286 -> 299 0.17837

Excited state symmetry could not be determined.
Excited State 27: Singlet-?Sym 3.1127 eV 398.31 nm f=0.0000 <S**2>=0.000
284 -> 296 0.49107
285 -> 297 0.49107

Excited state symmetry could not be determined.
Excited State 28: Singlet-?Sym 3.1181 eV 397.63 nm f=0.0000 <S**2>=0.000
284 -> 296 -0.49314
285 -> 297 0.49314

Excited State 29: Singlet-B1G 3.1491 eV 393.71 nm f=0.0000 <S**2>=0.000
291 -> 298 0.51907
292 -> 300 -0.20046
293 -> 301 0.20046
294 -> 299 0.35161
295 -> 302 -0.10423

Excited State 30: Singlet-EU 3.1760 eV 390.38 nm f=1.1140 <S**2>=0.000
282 -> 296 -0.16727
287 -> 297 -0.12534
291 -> 301 0.14181
292 -> 298 0.25724
292 -> 299 0.14379
293 -> 298 0.46234
293 -> 299 -0.25843
294 -> 301 -0.15677

Excited State 31: Singlet-EU 3.1760 eV 390.38 nm f=1.1140 <S**2>=0.000
282 -> 297 -0.16727
287 -> 296 0.12534
291 -> 300 -0.14181
292 -> 298 0.46234
292 -> 299 0.25843
293 -> 298 -0.25724
293 -> 299 0.14379
294 -> 300 -0.15677

Excited State 32: Singlet-A1G 3.2168 eV 385.43 nm f=0.0000 <S**2>=0.000
291 -> 299 0.20641
292 -> 300 -0.14019
293 -> 301 -0.14019
294 -> 298 0.62018

Excited State 33: Singlet-EG 3.2281 eV 384.08 nm f=0.0000 <S**2>=0.000
283 -> 296 0.20384
283 -> 297 0.57265
284 -> 298 0.20020
284 -> 299 0.16088
286 -> 300 0.17159

Excited State 34: Singlet-EG 3.2281 eV 384.08 nm f=0.0000 <S**2>=0.000
283 -> 296 0.57265
283 -> 297 -0.20384
285 -> 298 0.20020
285 -> 299 -0.16088

286 -> 301 0.17159

Excited State 35: Singlet-EU 3.2997 eV 375.75 nm f=0.0415 <S**2>=0.000
287 -> 301 -0.12575
288 -> 298 -0.25375
288 -> 299 -0.15796
289 -> 298 0.43373
289 -> 299 -0.27000
290 -> 300 0.10272
290 -> 301 0.17558
292 -> 298 -0.13374
292 -> 299 0.18305
293 -> 299 0.10709

Excited State 36: Singlet-EU 3.2997 eV 375.75 nm f=0.0415 <S**2>=0.000
287 -> 300 -0.12575
288 -> 298 0.43373
288 -> 299 0.27000
289 -> 298 0.25375
289 -> 299 -0.15796
290 -> 300 -0.17558
290 -> 301 0.10272
292 -> 299 0.10709
293 -> 298 -0.13374
293 -> 299 -0.18304

Excited State 37: Singlet-B1G 3.3021 eV 375.47 nm f=0.0000 <S**2>=0.000
291 -> 298 -0.44201
294 -> 299 0.49585
295 -> 302 -0.20725

Excited State 38: Singlet-A2G 3.3056 eV 375.07 nm f=0.0000 <S**2>=0.000
287 -> 299 0.18621
288 -> 300 -0.20557
289 -> 301 0.20557
290 -> 298 0.60697

Excited State 39: Singlet-EU 3.3114 eV 374.42 nm f=0.0703 <S**2>=0.000
288 -> 298 0.15523
288 -> 299 0.10583
289 -> 298 0.12650
292 -> 298 0.23606
292 -> 299 -0.32539
293 -> 298 0.28968
293 -> 299 0.39931

Excited State 40: Singlet-EU 3.3114 eV 374.42 nm f=0.0703 <S**2>=0.000
288 -> 298 0.12650
289 -> 298 -0.15523
289 -> 299 0.10583
292 -> 298 -0.28968
292 -> 299 0.39931
293 -> 298 0.23606
293 -> 299 0.32539

Excited State 41: Singlet-A1G 3.3208 eV 373.35 nm f=0.0000 <S**2>=0.000
291 -> 299 0.60831
292 -> 300 -0.13237
293 -> 301 -0.13237
294 -> 298 -0.28992

Excited State 42: Singlet-B1G 3.3274 eV 372.61 nm f=0.0000 <S**2>=0.000
294 -> 299 0.22006
295 -> 302 0.65707

Excited State 43: Singlet-EG 3.3349 eV 371.78 nm f=0.0000 <S**2>=0.000
281 -> 296 0.14420
281 -> 297 0.68358

Excited State 44: Singlet-EG 3.3349 eV 371.78 nm f=0.0000 <S**2>=0.000
281 -> 296 0.68358
281 -> 297 -0.14420

Excited State 45: Singlet-B2G 3.3518 eV 369.91 nm f=0.0000 <S**2>=0.000
287 -> 298 0.27648
288 -> 300 -0.25184
289 -> 301 -0.25184
290 -> 299 0.53143

Excited State 46: Singlet-EG 3.3921 eV 365.50 nm f=0.0000 <S**2>=0.000
280 -> 296 0.60699
283 -> 296 -0.21235
283 -> 301 -0.12975
285 -> 298 0.15551
285 -> 299 -0.13903
286 -> 301 0.11039

Excited State 47: Singlet-EG 3.3921 eV 365.50 nm f=0.0000 <S**2>=0.000
280 -> 297 0.60699
283 -> 297 0.21235
283 -> 300 -0.12975
284 -> 298 -0.15551
284 -> 299 -0.13903
286 -> 300 -0.11039

Excited State 48: Singlet-EU 3.4823 eV 356.04 nm f=0.0046 <S**2>=0.000
289 -> 298 0.41466
289 -> 299 0.55421
290 -> 301 -0.12156

Excited State 49: Singlet-EU 3.4823 eV 356.04 nm f=0.0046 <S**2>=0.000
288 -> 298 -0.41466
288 -> 299 0.55421
290 -> 300 -0.12156

Excited State 50: Singlet-A2U 3.5192 eV 352.31 nm f=0.0047 <S**2>=0.000
283 -> 299 0.18508
284 -> 297 -0.23510
284 -> 300 0.18965
285 -> 296 0.23510
285 -> 301 0.18965
286 -> 298 0.52503

Excited State 51: Singlet-EU 3.5218 eV 352.04 nm f=0.0355 <S**2>=0.000
291 -> 301 0.20536
293 -> 299 -0.14124
294 -> 300 0.18067
294 -> 301 0.62060

Excited State 52: Singlet-EU 3.5218 eV 352.04 nm f=0.0355 <S**2>=0.000

291 -> 300 -0.20536
292 -> 299 0.14124
294 -> 300 0.62060
294 -> 301 -0.18067

Excited state symmetry could not be determined.
Excited State 53: Singlet-?Sym 3.5264 eV 351.58 nm f=0.0000 <S**2>=0.000
292 -> 301 0.49452
293 -> 300 0.49452

Excited state symmetry could not be determined.
Excited State 54: Singlet-?Sym 3.5282 eV 351.41 nm f=0.0000 <S**2>=0.000
292 -> 301 -0.49569
293 -> 300 0.49569

Excited State 55: Singlet-B2U 3.5297 eV 351.26 nm f=0.0000 <S**2>=0.000
283 -> 298 0.21546
284 -> 297 -0.19751
284 -> 300 0.22837
285 -> 296 -0.19751
285 -> 301 -0.22837
286 -> 299 0.50146

Excited State 56: Singlet-EU 3.5316 eV 351.07 nm f=0.1332 <S**2>=0.000
282 -> 297 0.26021
291 -> 300 0.56153
292 -> 298 0.15834
292 -> 299 0.25328
294 -> 300 0.12789

Excited State 57: Singlet-EU 3.5316 eV 351.07 nm f=0.1332 <S**2>=0.000
282 -> 296 -0.26021
291 -> 301 0.56153
293 -> 298 -0.15834
293 -> 299 0.25328
294 -> 301 -0.12789

Excited state symmetry could not be determined.
Excited State 58: Singlet-?Sym 3.5354 eV 350.69 nm f=0.0000 <S**2>=0.000
291 -> 298 -0.15741
292 -> 300 -0.44268
293 -> 301 0.44268
294 -> 299 -0.27739

Excited state symmetry could not be determined.
Excited State 59: Singlet-?Sym 3.5385 eV 350.39 nm f=0.0000 <S**2>=0.000
291 -> 299 0.27529
292 -> 300 0.44197
293 -> 301 0.44197
294 -> 298 0.13452

Excited State 60: Singlet-A2G 3.5877 eV 345.58 nm f=0.0000 <S**2>=0.000
287 -> 299 0.40329
288 -> 300 -0.32479
289 -> 301 0.32479
290 -> 298 -0.35002

Excited State 61: Singlet-B2G 3.5974 eV 344.65 nm f=0.0000 <S**2>=0.000
287 -> 298 0.52893
288 -> 300 -0.14646

289 -> 301 -0.14646
290 -> 299 -0.41661

Excited State 62: Singlet-EU 3.6304 eV 341.51 nm f=0.5945 <S**2>=0.000
282 -> 296 0.53453
287 -> 297 -0.12393
287 -> 300 -0.14021
290 -> 300 0.24424
291 -> 301 0.26792

Excited State 63: Singlet-EU 3.6304 eV 341.51 nm f=0.5945 <S**2>=0.000
282 -> 297 0.53453
287 -> 296 0.12393
287 -> 301 -0.14021
290 -> 301 -0.24424
291 -> 300 -0.26792

Excited State 64: Singlet-EG 3.6311 eV 341.45 nm f=0.0000 <S**2>=0.000
280 -> 297 0.32098
283 -> 297 -0.27376
283 -> 300 0.18113
284 -> 298 0.26552
284 -> 299 0.28400
286 -> 300 0.34086

Excited State 65: Singlet-EG 3.6311 eV 341.45 nm f=0.0000 <S**2>=0.000
280 -> 296 -0.32098
283 -> 296 -0.27376
283 -> 301 -0.18113
285 -> 298 0.26552
285 -> 299 -0.28400
286 -> 301 0.34086

Excited state symmetry could not be determined.
Excited State 66: Singlet-?Sym 3.7036 eV 334.77 nm f=0.0000 <S**2>=0.000
288 -> 301 -0.49256
289 -> 300 0.49256

Excited State 67: Singlet-EU 3.7073 eV 334.43 nm f=0.0023 <S**2>=0.000
282 -> 296 -0.19570
288 -> 298 0.12784
288 -> 299 0.22645
290 -> 300 0.59400

Excited State 68: Singlet-EU 3.7073 eV 334.43 nm f=0.0023 <S**2>=0.000
282 -> 297 0.19571
289 -> 298 -0.12784
289 -> 299 0.22645
290 -> 301 0.59400

Excited state symmetry could not be determined.
Excited State 69: Singlet-?Sym 3.7139 eV 333.84 nm f=0.0000 <S**2>=0.000
288 -> 301 0.48674
289 -> 300 0.48674
292 -> 300 -0.10049
293 -> 301 -0.10049

Excited state symmetry could not be determined.
Excited State 70: Singlet-?Sym 3.7354 eV 331.92 nm f=0.0000 <S**2>=0.000
287 -> 298 0.36863

288 -> 300 0.40348
289 -> 301 0.40348
290 -> 299 0.18933
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 1270.
Leave Link 914 at Sat Jul 19 02:43:00 2014, MaxMem= 2359296000 cpu: 1383131.9
(Enter /usr/local/g09/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

6,7-TQPz

Excitation energies and oscillator strengths:

Excited State 1: Singlet-EU 1.6670 eV 743.76 nm f=1.1882 <S**2>=0.000
295 -> 296 0.39106
295 -> 297 0.58354
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -7689.25620417
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-EU 1.6670 eV 743.76 nm f=1.1882 <S**2>=0.000
295 -> 296 0.58354
295 -> 297 -0.39106

Excited State 3: Singlet-B2G 2.3563 eV 526.19 nm f=0.0000 <S**2>=0.000
295 -> 298 0.70377

Excited State 4: Singlet-A2G 2.4173 eV 512.90 nm f=0.0000 <S**2>=0.000
295 -> 299 0.70306

Excited State 5: Singlet-EU 2.5303 eV 490.01 nm f=0.2012 <S**2>=0.000
295 -> 300 0.69618

Excited State 6: Singlet-EU 2.5303 eV 490.01 nm f=0.2012 <S**2>=0.000
295 -> 301 0.69618

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 2.7780 eV 446.31 nm f=0.0000 <S**2>=0.000
292 -> 296 -0.49145
293 -> 297 0.49145

Excited state symmetry could not be determined.
Excited State 8: Singlet-?Sym 2.7789 eV 446.16 nm f=0.0000 <S**2>=0.000
292 -> 296 0.49431
293 -> 297 0.49431

Excited State 9: Singlet-EU 2.7840 eV 445.34 nm f=0.0273 <S**2>=0.000
291 -> 297 -0.13770
294 -> 296 -0.14336
294 -> 297 0.66749

Excited State 10: Singlet-EU 2.7840 eV 445.34 nm f=0.0273 <S**2>=0.000
291 -> 296 0.13770
294 -> 296 0.66749
294 -> 297 0.14336

Excited state symmetry could not be determined.
Excited State 11: Singlet-?Sym 2.8224 eV 439.29 nm f=0.0000 <S**2>=0.000
292 -> 297 0.49522
293 -> 296 0.49522

Excited State 12: Singlet-EU 2.8289 eV 438.27 nm f=0.7186 <S**2>=0.000
291 -> 296 0.68469
294 -> 296 -0.14245

Excited State 13: Singlet-EU 2.8289 eV 438.27 nm f=0.7186 <S**2>=0.000
291 -> 297 0.68469
294 -> 297 0.14245

Excited state symmetry could not be determined.
Excited State 14: Singlet-?Sym 2.8408 eV 436.44 nm f=0.0000 <S**2>=0.000
292 -> 297 -0.48977
293 -> 296 0.48977

Excited State 15: Singlet-EG 2.9783 eV 416.29 nm f=0.0000 <S**2>=0.000
287 -> 296 0.68339
287 -> 297 -0.13978

Excited State 16: Singlet-EG 2.9783 eV 416.29 nm f=0.0000 <S**2>=0.000
287 -> 296 0.13978
287 -> 297 0.68339

Excited State 17: Singlet-B1G 3.0676 eV 404.18 nm f=0.0000 <S**2>=0.000
288 -> 296 -0.34825
289 -> 297 -0.34825
295 -> 302 0.49850

Excited state symmetry could not be determined.
Excited State 18: Singlet-?Sym 3.0885 eV 401.44 nm f=0.0000 <S**2>=0.000
288 -> 297 0.49349
289 -> 296 0.49349

Excited State 19: Singlet-B1G 3.0977 eV 400.25 nm f=0.0000 <S**2>=0.000
288 -> 296 0.35042
289 -> 297 0.35042
295 -> 302 0.49145

Excited State 20: Singlet-EU 3.1014 eV 399.77 nm f=0.3759 <S**2>=0.000
290 -> 296 0.69195

Excited State 21: Singlet-EU 3.1014 eV 399.77 nm f=0.3759 <S**2>=0.000
290 -> 297 0.69195

Excited state symmetry could not be determined.
Excited State 22: Singlet-?Sym 3.1382 eV 395.08 nm f=0.0000 <S**2>=0.000
288 -> 297 -0.49318
289 -> 296 0.49318

Excited state symmetry could not be determined.
Excited State 23: Singlet-?Sym 3.1500 eV 393.60 nm f=0.0000 <S**2>=0.000
288 -> 296 -0.47165
289 -> 297 0.47165
294 -> 298 -0.10965

Excited State 24: Singlet-EU 3.4246 eV 362.04 nm f=0.3796 <S**2>=0.000
286 -> 297 0.52192
291 -> 301 -0.17267
293 -> 298 -0.27502
293 -> 299 0.23361
294 -> 301 0.19352

Excited State 25: Singlet-EU 3.4246 eV 362.04 nm f=0.3796 <S**2>=0.000
286 -> 296 0.52192
291 -> 300 -0.17267
292 -> 298 0.27502
292 -> 299 0.23361
294 -> 300 -0.19352

Excited State 26: Singlet-B1G 3.4769 eV 356.59 nm f=0.0000 <S**2>=0.000
291 -> 298 0.41869
292 -> 300 -0.27421
293 -> 301 0.27421
294 -> 299 0.38351

Excited State 27: Singlet-EU 3.4963 eV 354.62 nm f=1.4196 <S**2>=0.000
282 -> 296 0.36260
282 -> 297 0.15187
286 -> 296 -0.13515
286 -> 297 0.32268
291 -> 301 0.16227
292 -> 298 0.11511
293 -> 298 0.27483
293 -> 299 -0.22106
294 -> 301 -0.16591

Excited State 28: Singlet-EU 3.4963 eV 354.62 nm f=1.4196 <S**2>=0.000
282 -> 296 -0.15187
282 -> 297 0.36260
286 -> 296 -0.32268
286 -> 297 -0.13515
291 -> 300 -0.16227
292 -> 298 0.27483
292 -> 299 0.22106
293 -> 298 -0.11511
294 -> 300 -0.16591

Excited State 29: Singlet-EG 3.4993 eV 354.31 nm f=0.0000 <S**2>=0.000
280 -> 297 0.69829

Excited State 30: Singlet-EG 3.4993 eV 354.31 nm f=0.0000 <S**2>=0.000
280 -> 296 0.69829

Excited State 31: Singlet-A1G 3.5553 eV 348.73 nm f=0.0000 <S**2>=0.000
288 -> 296 -0.12798
289 -> 297 0.12798
291 -> 299 0.32071
292 -> 300 -0.25067
293 -> 301 -0.25067
294 -> 298 0.46470
295 -> 306 -0.10476

Excited state symmetry could not be determined.
Excited State 32: Singlet-?Sym 3.6169 eV 342.79 nm f=0.0053 <S**2>=0.000
281 -> 298 -0.20467
283 -> 299 -0.19757
284 -> 297 0.41916
284 -> 300 -0.16641
285 -> 296 0.41916
285 -> 301 0.16641
287 -> 298 0.10070

Excited state symmetry could not be determined.
Excited State 33: Singlet-?Sym 3.6178 eV 342.71 nm f=0.0000 <S**2>=0.000
281 -> 299 0.18655
283 -> 298 0.21940
284 -> 297 -0.42022
284 -> 300 0.16651
285 -> 296 0.42022
285 -> 301 0.16651

Excited State 34: Singlet-EG 3.6233 eV 342.18 nm f=0.0000 <S**2>=0.000
281 -> 296 -0.33938
281 -> 301 -0.15678
283 -> 296 0.46357
283 -> 297 0.11293
283 -> 301 0.15792
285 -> 298 0.21482
285 -> 299 -0.19389

Excited State 35: Singlet-EG 3.6233 eV 342.18 nm f=0.0000 <S**2>=0.000
281 -> 297 0.33938
281 -> 300 -0.15678
283 -> 296 -0.11293
283 -> 297 0.46357
283 -> 300 -0.15792
284 -> 298 -0.21482
284 -> 299 -0.19389

Excited state symmetry could not be determined.
Excited State 36: Singlet-?Sym 3.6387 eV 340.74 nm f=0.0000 <S**2>=0.000
284 -> 296 -0.49377
285 -> 297 0.49377

Excited state symmetry could not be determined.
Excited State 37: Singlet-?Sym 3.6389 eV 340.72 nm f=0.0000 <S**2>=0.000
284 -> 296 0.49394
285 -> 297 0.49394

Excited State 38: Singlet-EG 3.6477 eV 339.90 nm f=0.0000 <S**2>=0.000
281 -> 297 0.53724
283 -> 297 -0.43805

Excited State 39: Singlet-EG 3.6477 eV 339.90 nm f=0.0000 <S**2>=0.000
281 -> 296 0.53724
283 -> 296 0.43805

Excited State 40: Singlet-B1G 3.7321 eV 332.21 nm f=0.0000 <S**2>=0.000
291 -> 298 0.51240
294 -> 299 -0.47926

Excited State 41: Singlet-EU 3.7322 eV 332.20 nm f=0.0104 <S**2>=0.000
292 -> 298 0.18474
292 -> 299 -0.18467
293 -> 298 0.45441
293 -> 299 0.45424

Excited State 42: Singlet-EU 3.7322 eV 332.20 nm f=0.0104 <S**2>=0.000
292 -> 298 0.45441
292 -> 299 -0.45424
293 -> 298 -0.18474

293 -> 299 -0.18467

Excited State 43: Singlet-A1G 3.7352 eV 331.93 nm f=0.0000 <S**2>=0.000
291 -> 299 0.48715
292 -> 300 -0.12081
293 -> 301 -0.12081
294 -> 298 -0.48079

Excited State 44: Singlet-EU 3.7489 eV 330.72 nm f=0.1540 <S**2>=0.000
282 -> 296 -0.14825
282 -> 297 0.50322
286 -> 296 0.28541
292 -> 298 -0.20288
292 -> 299 -0.12599
294 -> 300 0.10354
295 -> 304 -0.14353

Excited State 45: Singlet-EU 3.7489 eV 330.72 nm f=0.1540 <S**2>=0.000
282 -> 296 0.50322
282 -> 297 0.14825
286 -> 297 -0.28541
293 -> 298 -0.20288
293 -> 299 0.12599
294 -> 301 0.10354
295 -> 305 -0.14353

Excited state symmetry could not be determined.
Excited State 46: Singlet-?Sym 3.8545 eV 321.66 nm f=0.0000 <S**2>=0.000
288 -> 300 0.13538
289 -> 301 -0.13538
290 -> 298 -0.26747
292 -> 301 -0.42640
293 -> 300 0.42640

Excited State 47: Singlet-EU 3.8567 eV 321.48 nm f=0.0274 <S**2>=0.000
288 -> 298 0.10247
289 -> 298 0.16093
291 -> 300 -0.24359
291 -> 301 0.15510
292 -> 299 0.13732
294 -> 300 0.46856
294 -> 301 0.29835

Excited State 48: Singlet-EU 3.8567 eV 321.48 nm f=0.0274 <S**2>=0.000
288 -> 298 0.16093
289 -> 298 -0.10247
291 -> 300 0.15510
291 -> 301 0.24359
293 -> 299 -0.13732
294 -> 300 -0.29835
294 -> 301 0.46856

Excited state symmetry could not be determined.
Excited State 49: Singlet-?Sym 3.8613 eV 321.09 nm f=0.0000 <S**2>=0.000
292 -> 301 0.48874
293 -> 300 0.48874

Excited state symmetry could not be determined.
Excited State 50: Singlet-?Sym 3.8866 eV 319.00 nm f=0.0000 <S**2>=0.000
291 -> 298 0.23028

292 -> 300 0.40006
293 -> 301 -0.40006
294 -> 299 0.34062

Excited state symmetry could not be determined.
Excited State 51: Singlet-?Sym 3.8914 eV 318.61 nm f=0.0000 <S**2>=0.000
291 -> 299 0.38028
292 -> 300 0.39869
293 -> 301 0.39869
294 -> 298 0.18037

Excited State 52: Singlet-A2G 3.8933 eV 318.45 nm f=0.0000 <S**2>=0.000
278 -> 297 0.19895
279 -> 296 0.19895
286 -> 299 0.14001
288 -> 300 -0.20433
289 -> 301 0.20433
290 -> 298 0.42130
292 -> 301 -0.25216
293 -> 300 0.25216

Excited State 53: Singlet-EU 3.8944 eV 318.37 nm f=0.0022 <S**2>=0.000
286 -> 300 -0.11708
288 -> 298 0.36888
288 -> 299 0.27012
290 -> 300 -0.20935
291 -> 301 0.24866
293 -> 298 -0.12523
293 -> 299 0.21564
294 -> 301 -0.29503

Excited State 54: Singlet-EU 3.8944 eV 318.37 nm f=0.0022 <S**2>=0.000
286 -> 301 -0.11708
289 -> 298 0.36888
289 -> 299 -0.27012
290 -> 301 0.20935
291 -> 300 -0.24866
292 -> 298 -0.12523
292 -> 299 -0.21564
294 -> 300 -0.29503

Excited State 55: Singlet-EU 3.9041 eV 317.57 nm f=0.0234 <S**2>=0.000
288 -> 298 -0.26353
288 -> 299 -0.17791
290 -> 300 0.16572
291 -> 300 0.11568
291 -> 301 0.50974
293 -> 298 -0.11897
293 -> 299 0.21487

Excited State 56: Singlet-EU 3.9041 eV 317.57 nm f=0.0234 <S**2>=0.000
289 -> 298 0.26353
289 -> 299 -0.17791
290 -> 301 0.16572
291 -> 300 0.50974
291 -> 301 -0.11568
292 -> 298 0.11897
292 -> 299 0.21487

Excited State 57: Singlet-B2G 3.9175 eV 316.48 nm f=0.0000 <S**2>=0.000

278 -> 297 0.16133
279 -> 296 -0.16133
286 -> 298 0.18139
288 -> 300 -0.28111
289 -> 301 -0.28111
290 -> 299 0.47754
295 -> 303 -0.10695

Excited state symmetry could not be determined.
Excited State 58: Singlet-?Sym 3.9562 eV 313.39 nm f=0.0000 <S**2>=0.000
274 -> 297 -0.48482
275 -> 296 0.48482
280 -> 298 0.14295

Excited state symmetry could not be determined.
Excited State 59: Singlet-?Sym 3.9562 eV 313.39 nm f=0.0000 <S**2>=0.000
278 -> 297 0.42545
279 -> 296 0.42545
290 -> 298 -0.29689
295 -> 307 0.11591

Excited State 60: Singlet-A2U 3.9690 eV 312.38 nm f=0.0081 <S**2>=0.000
281 -> 298 -0.23474
283 -> 299 -0.27504
284 -> 297 -0.26130
284 -> 300 -0.24681
285 -> 296 -0.26130
285 -> 301 0.24681
287 -> 298 0.30132

Excited State 61: Singlet-B2U 3.9731 eV 312.06 nm f=0.0000 <S**2>=0.000
274 -> 296 0.21394
275 -> 297 -0.21394
281 -> 299 0.25500
283 -> 298 0.27477
284 -> 297 0.24107
284 -> 300 0.24532
285 -> 296 -0.24107
285 -> 301 0.24532
287 -> 299 -0.15614

Excited state symmetry could not be determined.
Excited State 62: Singlet-?Sym 3.9768 eV 311.77 nm f=0.0000 <S**2>=0.000
274 -> 296 -0.44651
275 -> 297 0.44651
281 -> 299 0.10676
283 -> 298 0.12222
284 -> 297 0.11851
284 -> 300 0.11071
285 -> 296 -0.11851
285 -> 301 0.11071
287 -> 299 -0.12258

Excited State 63: Singlet-EG 3.9790 eV 311.60 nm f=0.0000 <S**2>=0.000
281 -> 297 0.27122
281 -> 300 0.25245
283 -> 297 0.27192
283 -> 300 0.27009
284 -> 298 0.30705
284 -> 299 0.30763

287 -> 300 -0.13431

Excited State 64: Singlet-EG 3.9790 eV 311.60 nm f=0.0000 <S**2>=0.000
281 -> 296 -0.27122
281 -> 301 0.25245
283 -> 296 0.27192
283 -> 301 -0.27009
285 -> 298 -0.30705
285 -> 299 0.30763
287 -> 301 -0.13431

Excited state symmetry could not be determined.
Excited State 65: Singlet-?Sym 3.9856 eV 311.08 nm f=0.0000 <S**2>=0.000
278 -> 296 0.48337
279 -> 297 0.48337

Excited state symmetry could not be determined.
Excited State 66: Singlet-?Sym 3.9965 eV 310.24 nm f=0.0000 <S**2>=0.000
278 -> 297 -0.41697
279 -> 296 0.41697
290 -> 299 0.13078
295 -> 303 -0.33027

Excited state symmetry could not be determined.
Excited State 67: Singlet-?Sym 4.0004 eV 309.93 nm f=0.0015 <S**2>=0.000
274 -> 296 0.45049
275 -> 297 0.45049
280 -> 302 -0.11330
281 -> 298 -0.11983
287 -> 298 -0.16863

Excited state symmetry could not be determined.
Excited State 68: Singlet-?Sym 4.0027 eV 309.75 nm f=0.0000 <S**2>=0.000
278 -> 296 -0.48956
279 -> 297 0.48956

Excited state symmetry could not be determined.
Excited State 69: Singlet-?Sym 4.0151 eV 308.80 nm f=0.0000 <S**2>=0.000
274 -> 297 0.49441
275 -> 296 0.49441

Excited State 70: Singlet-EU 4.0271 eV 307.87 nm f=0.0004 <S**2>=0.000
277 -> 297 0.51192
288 -> 298 -0.35341
288 -> 299 0.29140
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 1270.
Leave Link 914 at Sat Jul 19 07:03:43 2014, MaxMem= 2359296000 cpu: 1246107.6
(Enter /usr/local/g09/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

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