Supporting Information

Design of D-π-A type photoacid generators for high efficiency excitation at 405 nm and 800 nm

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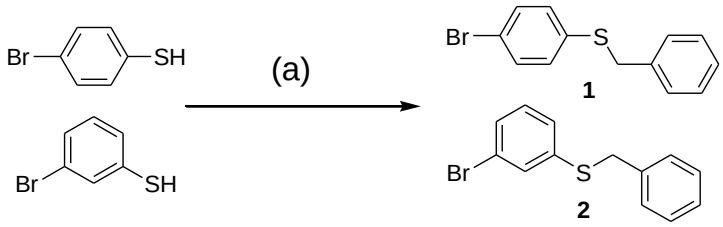
Contents:

I. General materials, characterizations and synthesis procedures (Schemes, Procedures, NMR spectra, MS spectra).

All reagents were purchased from commercial available sources such as Aldrich or Fisher and used without further purification. Solvents were dried prior to use as required: dichloromethane (DCM) were distilled under an atmosphere of anhydrous nitrogen from CaH_2; DMF was distilled under reduced pressure from $CaSO_4$, and THF was dried by distilling under an atmosphere of nitrogen from sodium and benzophenone.

Proton and carbon nuclear magnetic resonance spectra (^1H, ^{13}C NMR) were recorded on a Bruker Avance 500 (400 MHz) spectrometer. Chemical shifts were reported in parts per million (ppm) downfield from the Me_4Si resonance which was used as the internal standard when recording NMR spectra. Mass spectra were recorded on a Micromass GCTTM and a Micromass LCTTM.

Scheme S1:



(a) Benzyl bromide, K_2CO_3, Acetone, Refluxing, 24 h.

4-(benzylthio)-4'-bromobenzene (1):

To a solution of benzyl bromide 8.55 g (50 mmol, 1 equiv) and 4-bromobenzenethiol 9.45 g (50 mmol, 1 equiv) in 250 mL of acetone, K_2CO_3 8.28 g (60 mmol, 1.2 equiv) was added. After addition the resulting mixture was allowed to stir at refluxing for 24 h. TLC showed that the rare materials disappeared and then the inorganic salts were filtered off and solvent was removed by rotary evaporation. The crude product was purified via recrystallization from ethanol as white powder (13.0 g, 93% yield).

^1H NMR (400 MHz, $CDCl_3$, δ_{ppm}): 7.35 (d, *J = 8.5 Hz*, 2H); 7.27 (m, 5H, Benzyl); 7.14 (d, *J = 8.5 Hz*, 2H); 4.08 (s, 2H, CH_2).

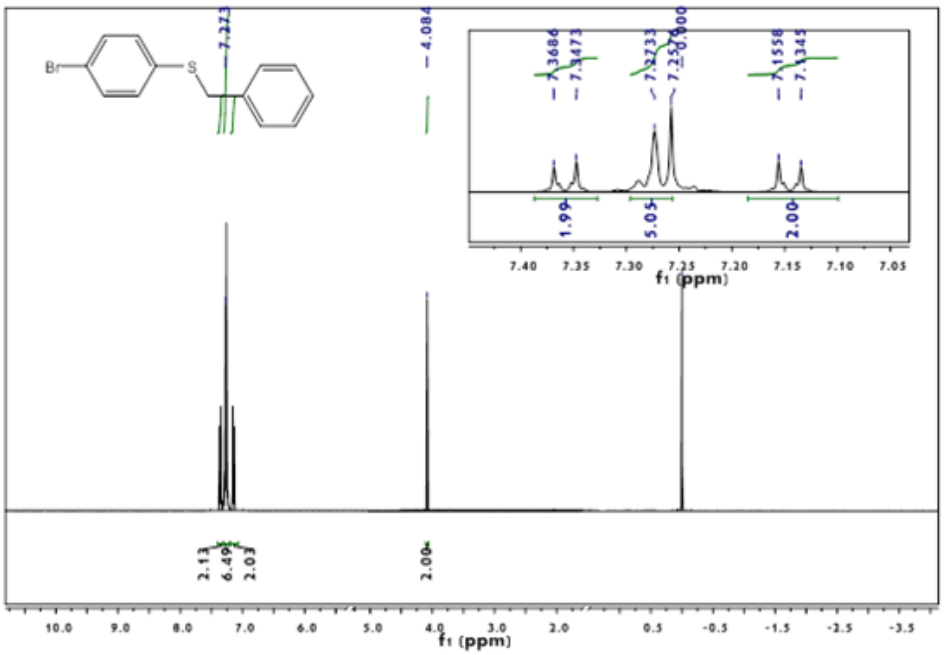


Fig. S1. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1**.

3-(benzylthio)-4'-bromobenzene (2):

To a solution of benzyl bromide 8.55 g (50 mmol, 1 equiv) and 3-bromobenzenethiol 9.45 g (50 mmol, 1 equiv) in 250 mL of acetone, K_2CO_3 8.28 g (60 mmol, 1.2 equiv) was added. After addition the resulting mixture was allowed to stir at refluxing for 24 h. TLC showed that the rare materials disappeared and then the inorganic salts were filtered off and solvent was removed by rotary evaporation. The crude product was purified via recrystallization from ethanol as white powder (12.4 g, 89% yield).

^{1}H NMR (400 MHz, $CDCl_3$, δ_{ppm}): 7.43 (st, *J = 1.8 Hz*, 1H); 7.27 (m, 5H, Benzyl); 7.25 (d, 1H); 7.19 (dt, *J = 7.8 Hz* and *1.2 Hz*, 1H); 7.09 (t, *J = 7.8 Hz*, 1H); 4.11 (s, 2H, CH_2).

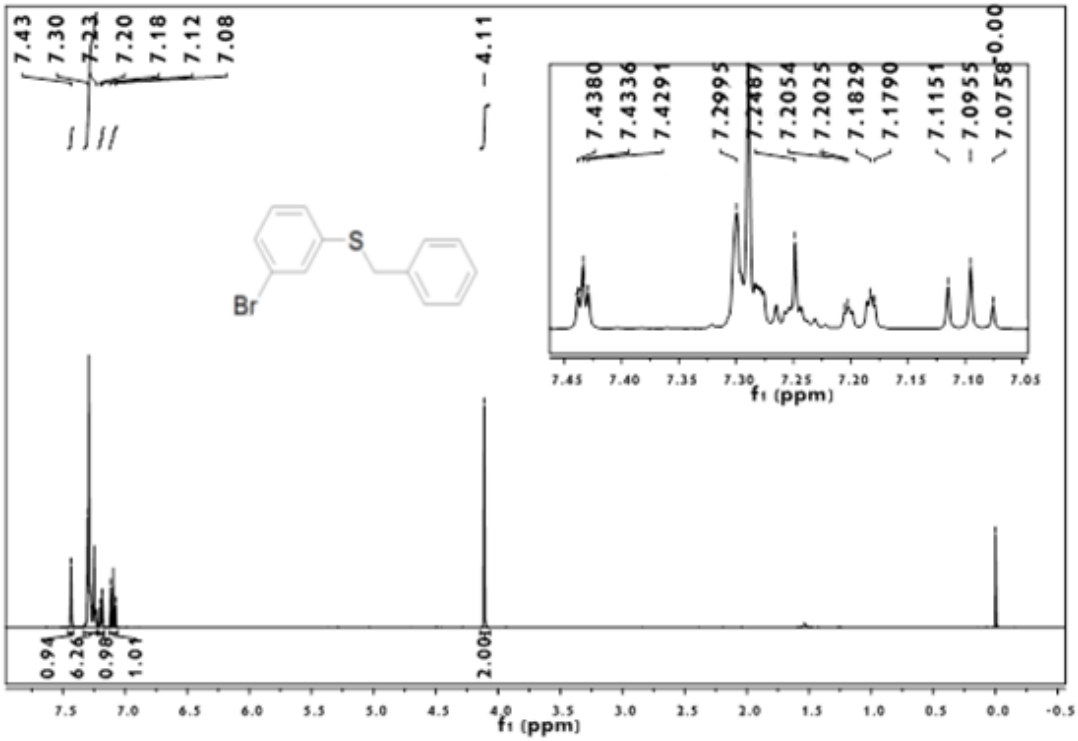
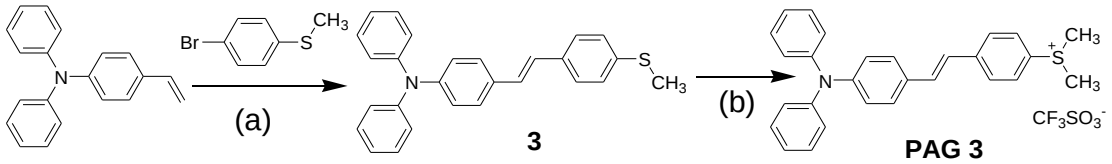


Fig. S2. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **2**.

Scheme S2:



(a) $Pd(OAc)_2$, Triethanolamine, 120 ^oC, 24 h; (b) Methyl trifluoromethanesulfonate, CH_2Cl_2, -78 ^oC, 2 h, r.t. 24 h.

(*E*)-4-(N,N-diphenyl)amine-4'-methylthiostilbene (3):

To a solution of 4-(N,N-diphenyl)amine-styrene[1] 2.71g (10 mmol, 1 equiv) in 10 mL of triethanolamine, 4-bromothioanisole 2.22g (11 mmol, 1.1 equiv) and $Pd(OAc)_2$ 22.4mg (0.1 mmol, 0.01 equiv) were added and the mixture was stirred for 24 hours in 120 ^oC oil bath under the atmosphere of nitrogen and then was poured into 200 mL of water after being cooled to room temperature. Extraction was applied with dichloromethane (100 mL × 3 times) and the organic layer was washed by brine for 3 times, dried over anhydrous magnesium sulfate and filtered over a short pad of silica gel to get off the Pd catalyst. Solvent was then removed to get green-yellow powder as crude product. The product can be purified by recrystallization from chloroform and ethanol at 80 ^oC (2.76g, 70.3 % yield).

^{1}H NMR (400 MHz, $CDCl_3$, δ_{ppm}): 7.42 (d, *J = 8.2 Hz*, 2H, PhH); 7.38 (d, *J = 8.4 Hz*, 2H, PhH); 7.23-7.29 (m, 8H, PhH, $CDCl_3$); 7.12 (d, *J = 7.8 Hz*, 4H, PhH); 7.05~6.99

(m, 5H, PhH, CH=CH); 6.96 (d, *J* = *16.3 Hz*, 1H, CH=CH); 2.48 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ_{ppm}): 147.46; 147.23; 137.29; 134.54; 131.41; 129.23; 127.50; 127.22; 126.69; 126.64; 126.29; 124.41; 123.54; 122.97; 15.84. EI-MS (m/z): calcd for $C_{27}H_{23}NS$, 393.2; found, 393.2 $[M]^+$; Anal. calcd for $C_{27}H_{23}NS$: C, 82.40; H, 5.89; N, 3.56; Found: C, 82.41; H, 6.01; N, 3.49.

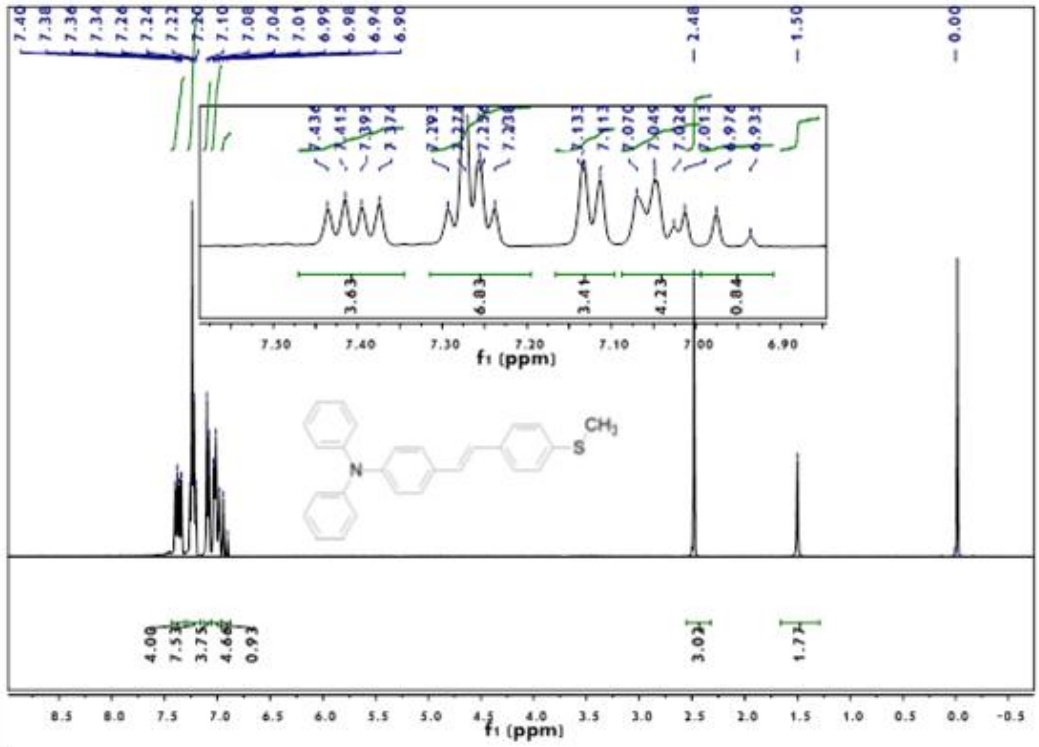


Fig. S3. ^1H NMR (400 MHz, $CDCl_3$) of compound **3**.

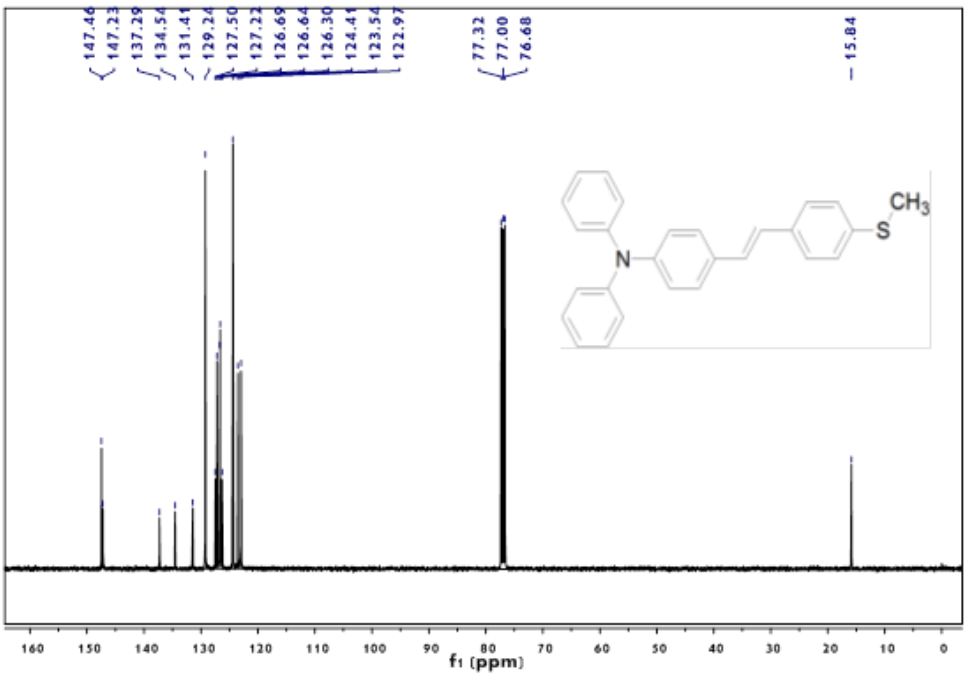


Fig. S3-2. ^{13}C NMR (100 MHz, $CDCl_3$) of compound **3**.

(*E*)-4-(((N,N-diphenyl)amino)-styryl)-phenyl-dimethylsulfonium trifluoromethanesulfonate (PAG 3)[2]:

Due to the high sensitivity to ambient light, all the preparation was carried out in dark. Firstly, to a solution of precursor compound **3** 393mg (1.0 mmol, 1 equiv) in 5 mL of dried dichloromethane at -78 ^{o}C, methyl trifluoromethanesulfonate 180mg (1.1 mmol, 1.1 equiv) was syringed into the solution. After stirring at this temperature for 2h, the mixture was warmed to room temperature and stirred for another 24 hours. Subsequently, dichloromethane was removed and residue was dissolved in acetonitrile. 10 times volume ethyl ether was added to the solution dropwise, slowly forming the crystal. Solid was collected by filtration and washed with ethyl ether. Then it was dissolved in acetonitrile again for another crystal formation by dropping 10 times volume ethyl ether. Yellow product was gained (423 mg, 76.0% yield).

^{1}H NMR (400 MHz, CD_3CN, δ_{ppm}): 7.86~7.80 (m, 4H, PhH); 7.51 (d, *J = 8.6 Hz*, 2H, PhH); 7.38 (d, *J = 16.4 Hz*, 1H, CH=CH); 7.32 (m, 4H, PhH); 7.14 (d, *J = 15.9 Hz*, 1H, CH=CH); 7.09 (m, 6H, PhH); 7.00 (d, *J = 8.7 Hz*, 2H, PhH); 3.12 (s, 6H, CH_3). ^{13}C NMR (100 MHz, CD_3CN, δ_{ppm}): 149.27; 148.09; 144.88; 133.57; 131.17; 130.92; 130.42; 128.99; 128.88; 125.71; 124.87; 124.59; 123.27; 122.94; 29.43. EI-MS (m/z): calcd for $C_{29}H_{26}F_3NO_3S_2$, 557.1306, found: 408.1754, $[M\text{-}CF_3SO_3^-]^+$; Anal. calcd for $C_{29}H_{26}F_3NO_3S_2$: C, 62.46; H, 4.70; N, 2.51; Found: C, 62.35; H, 4.85; N, 2.47.

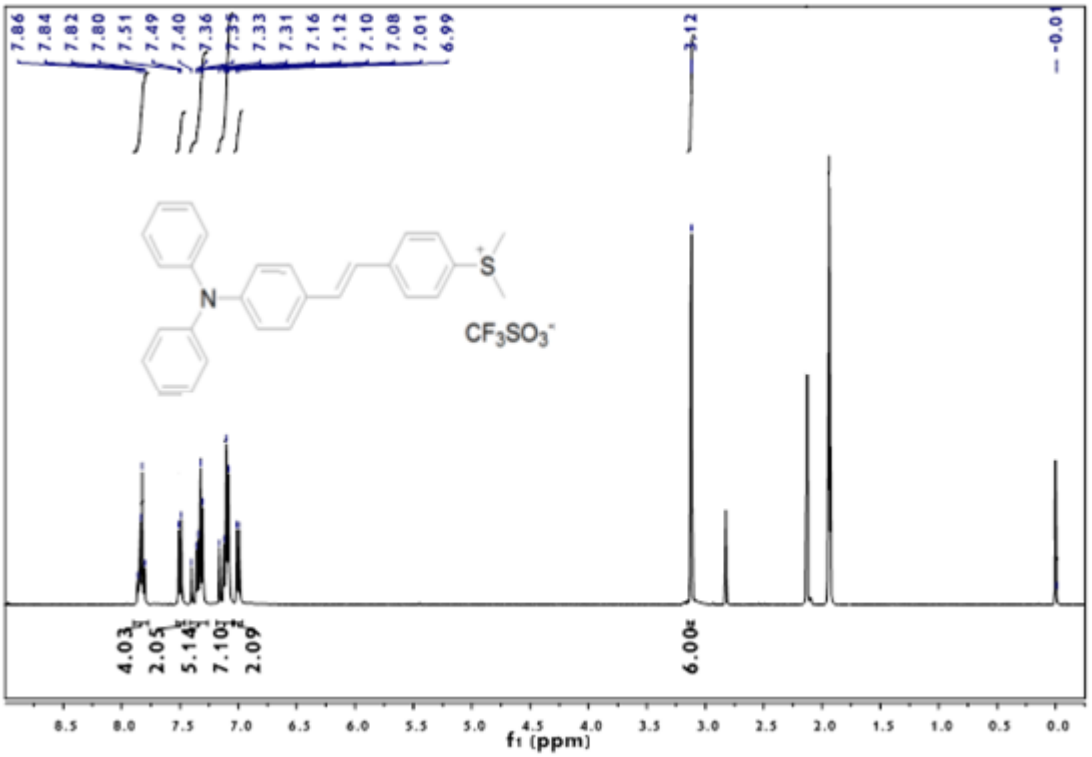


Fig. S4. ^{1}H NMR (400 MHz, CD_3CN) of PAG **3**.

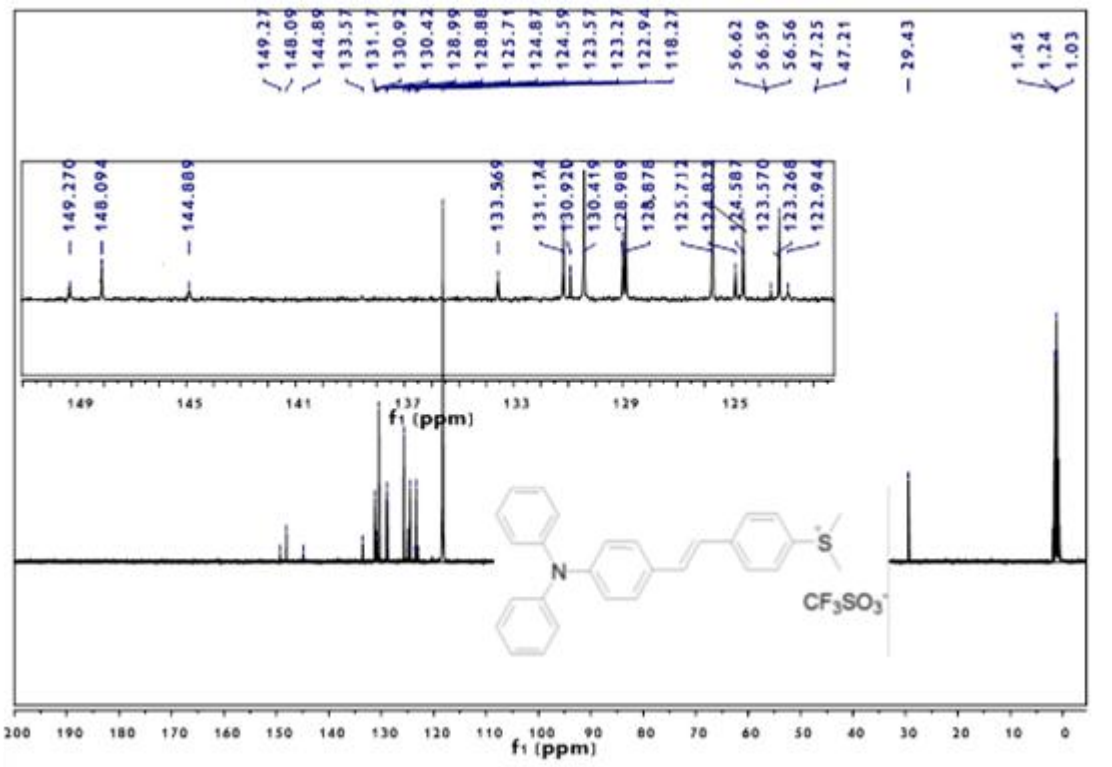


Fig. S4-2. ^{13}C NMR (100 MHz, CD_3CN) of PAG **3**.

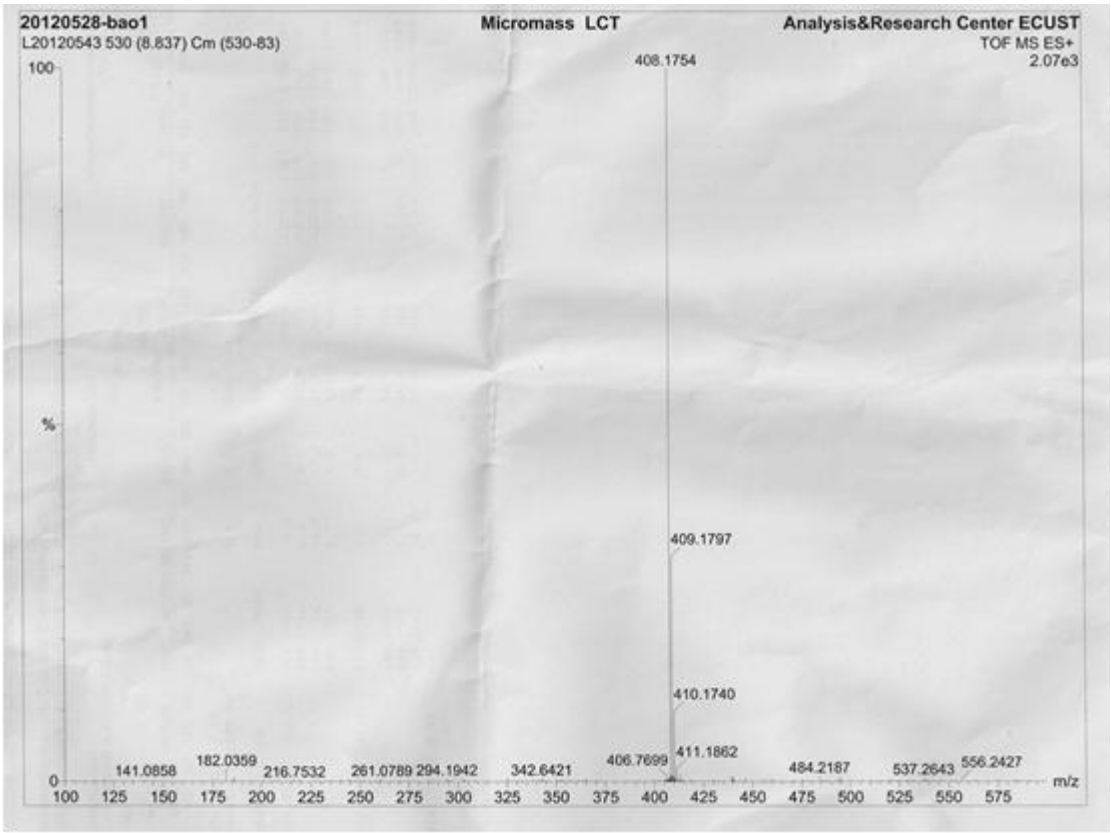
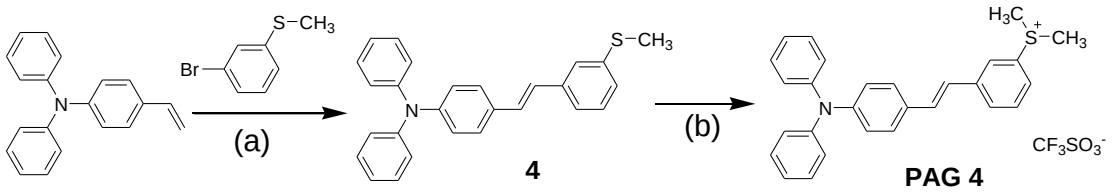


Fig. S4-3. TOF-MS of PAG **3**.

Scheme S3:



(a) $Pd(OAc)_2$, Triethanolamine, 120 ^oC, 24 h; (b) Methyl trifluoromethanesulfonate, CH_2Cl_2, -78 ^oC, 2 h, r.t. 24 h.

(*E*)-4-(N,N-diphenyl)amine-3'-methylthiostilbene (4):

Compound **4** was prepared with the same method as **3** by 4-(N, N-diphenyl)amine-styrene 1.35g (50 mmol, 1 equiv) and 3-bromothioanisole 1.11g (55 mmol, 1.1 equiv). Recrystallization was applied with chloroform and ethanol mixture in 80 ^oC and pale yellowish powder was obtained as pure **4** (1.20g, 61.2% yield).

^1H NMR (400 MHz, $CDCl_3$, δ_{ppm}): 7.38 (d, *J = 8.5 Hz*, 2H, PhH); 7.37 (s, 1H, PhH); 7.28~7.24 (m, 5H, PhH and $CDCl_3$); 7.12 (d, *J = 8.6 Hz*, 4H, PhH); 7.01-7.07 (m, 5H, PhH and CH=CH); 6.94 (d, *J = 16.4 Hz*, 1H, CH=CH); 2.52 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ_{ppm}): 147.42; 138.17; 131.11; 129.24; 128.99; 128.71; 127.36; 126.29; 125.26; 124.47; 124.32; 123.39; 123.06; 123.03; 15.82. EI-MS (m/z): calcd for $C_{27}H_{23}NS$, 393.2; found, 393.2 $[M]^+$; Anal. calcd for $C_{27}H_{23}NS$: C, 82.40; H, 5.89; N, 3.56; Found: C, 82.31; H, 6.05; N, 3.47.

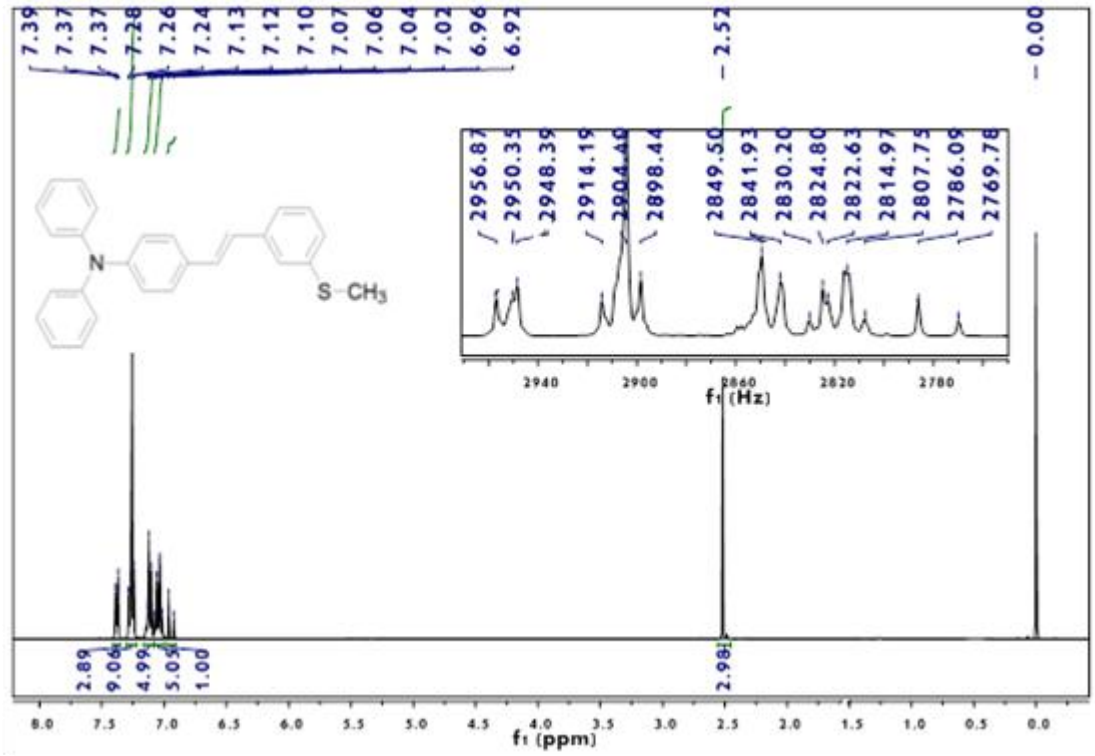


Fig. S5. ^1H NMR (400 MHz, $CDCl_3$) of compound **4**.

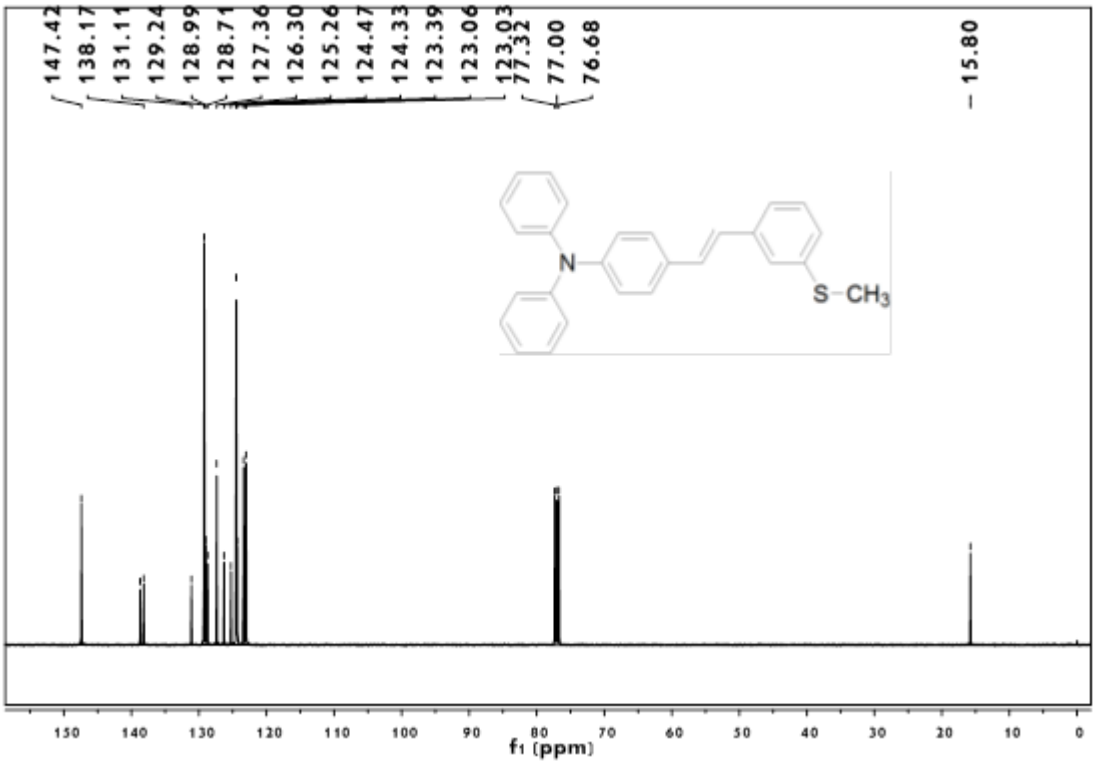


Fig. S5-2. ^{13}C NMR (100 MHz, $CDCl_3$) of compound **4**.

(*E*)-3-(((N,N-diphenyl)amino)-styryl)-phenyl-dimethylsulfonium trifluoromethanesulfonate (PAG 4):

PAG 4 was prepared by the same method as **PAG 3** with the equivalent mole rare materials. Finally, shallow yellow product was gained (340 mg, 61.0 % yield).

^{1}H NMR (400 MHz, CD_3CN, δ_{ppm}): 8.03 (s, 1H, PhH); 7.89 (d, *J = 7.6 Hz*, 1H, PhH); 7.73 (d, *J = 7.7 Hz*, 1H, PhH); 7.67 (t, *J = 7.8 Hz, 7.9 Hz*, 1H, PhH); 7.63 (d, *J = 22.9 Hz*, 1H, CH=CH); 7.48 (d, *J = 8.6 Hz*, 2H, PhH); 7.36~7.29 (m, 5H; PhH and CH=CH); 7.14~7.07 (m, 6H, PhH); 7.01 (d, *J = 8.6 Hz*, 2H, PhH); 3.15 (s, 6H, CH_3). ^{13}C NMR (100 MHz, CD_3CN, δ_{ppm}): 149.14; 148.23; 141.79; 132.73; 132.49; 132.03; 131.20; 130.48; 128.88; 128.69; 127.70; 126.80; 125.71; 125.79; 124.80; 124.58; 124.53; 29.26. EI-MS (m/z): calcd for $C_{29}H_{26}F_3NO_3S_2$, 557.1306, found: 408.1783, $[M\text{-}CF_3SO_3^-]^+$; Anal. calcd for $C_{29}H_{26}F_3NO_3S_2$: C, 62.46; H, 4.70; N, 2.51; Found: C, 62.38; H, 4.75; N, 2.49.

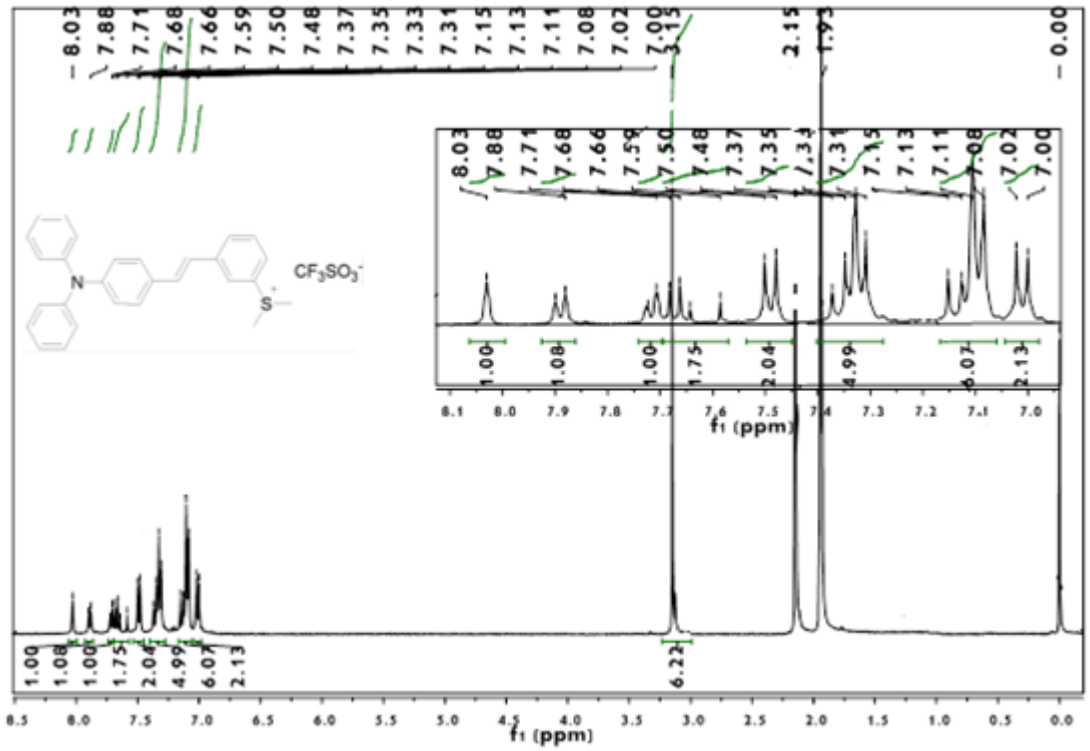


Fig. S6. ^{1}H NMR (400 MHz, CD_3CN) of PAG **4**.

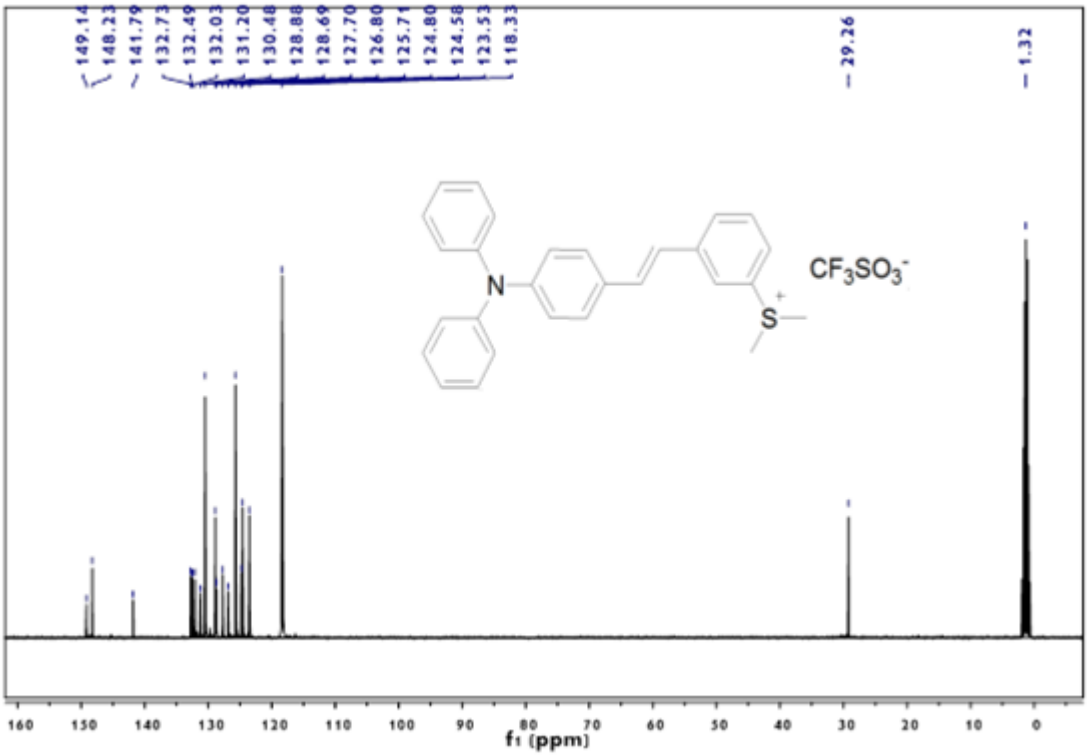


Fig. S6-2. ^{13}C NMR (100 MHz, CD_3CN) of PAG **3**.

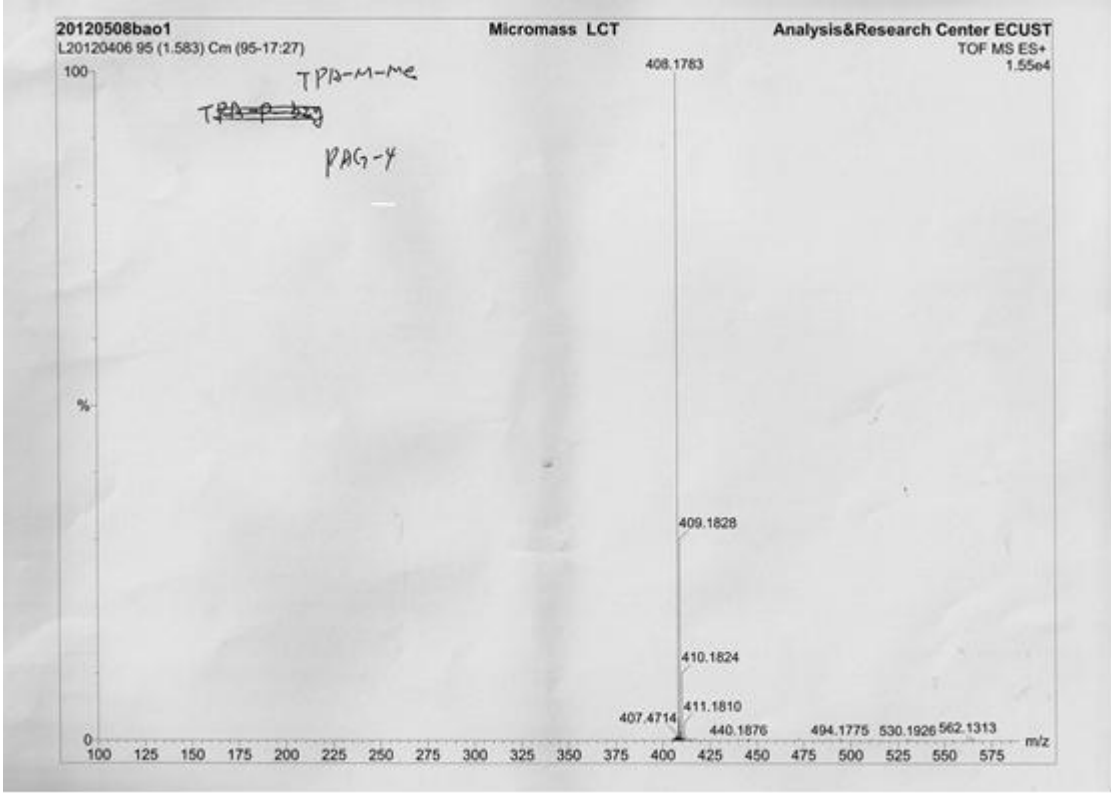
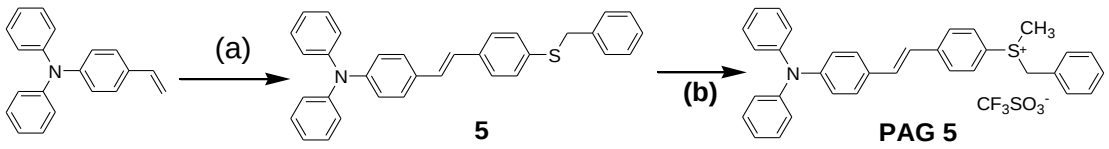


Fig. S6-3. TOF-MS of PAG **4.**

Scheme S4:



(a) Compound **1**, $Pd(OAc)_2$, Triethanolamine, 120 ^oC, 24 h; (b) Methyl trifluoromethanesulfonate, CH_2Cl_2, -78 ^oC, 2 h, r.t. 24 h.

(*E*)-4-(N,N-diphenyl)amine-4'-benzylthiostilbene (5):

Compound **5** was prepared with the similar method as **3** by 4-(N,N-diphenyl)amine-styrene 1.35 g (5 mmol, 1 equiv) and compound **1** 1.53 g (5.5mmol, 1.1 equiv) catalyst by $Pd(OAc)_2$ 11.2 mg(0.05mmol, 0.01equiv). The product can be purified by column chromatography with DCM/petroleum ether (1/5; v/v) as eluent to give a yellow product (1.66 g, 63.5% yield).

^1H NMR (400 MHz, $CDCl_3$, δ_{ppm}): 7.37 (d, *J = 8.3 Hz*, 2H, PhH); 7.36 (d, *J = 8.6 Hz*, 2H, PhH); 7.23-7.30 (m, 11H, PhH, $CDCl_3$); 7.11 (d, *J = 7.6 Hz*, 4H, PhH); 7.04~6.99 (m, 5H, PhH, CH=CH); 6.94 (d, *J = 16.3 Hz*, 1H, CH=CH); 4.12 (s, 2H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$, δ_{ppm}): 147.46; 147.35; 137.36; 135.76; 135.16; 131.27; 129.91; 129.28; 128.81; 128.49; 128.06; 127.32; 127.18; 126.64; 126.19; 124.48;

123.46; 123.04; 39.00. EI-MS (m/z): calcd for $C_{27}H_{23}NS$, 469.2; found, 469.2 $[M]^+$; Anal. calcd for $C_{33}H_{27}NS$: C, 84.40; H, 5.79; N, 2.98; Found: C, 84.41; H, 5.90; N, 3.04.

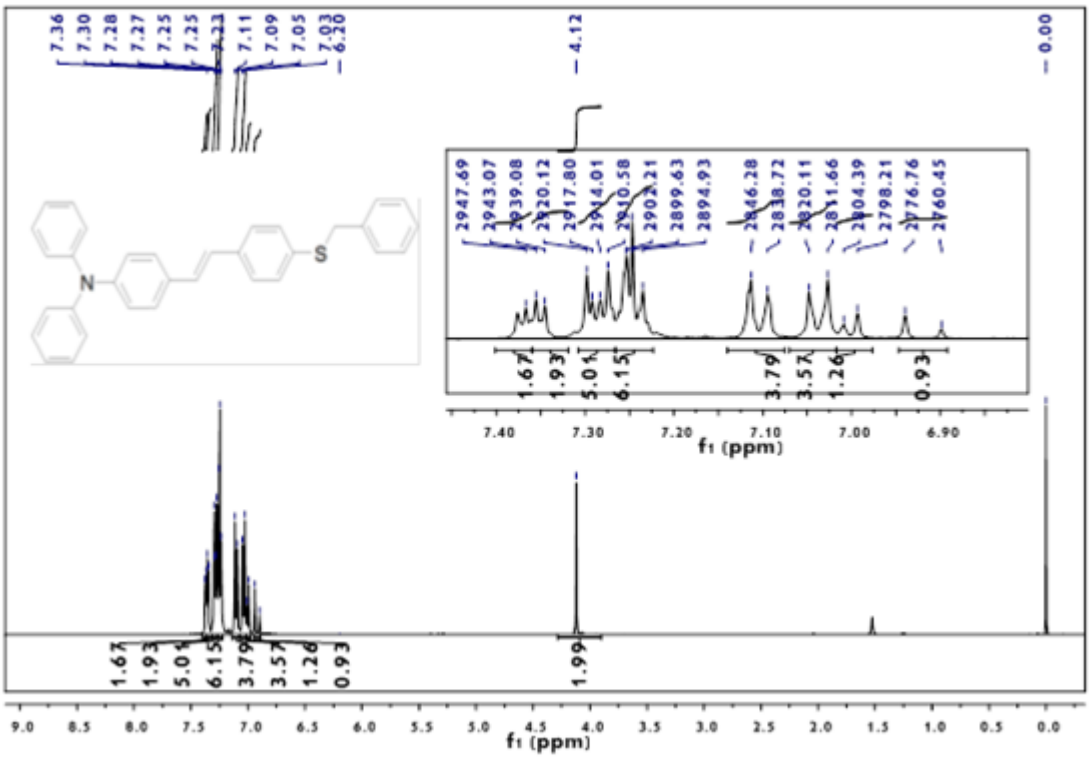


Fig. S7. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **5**.

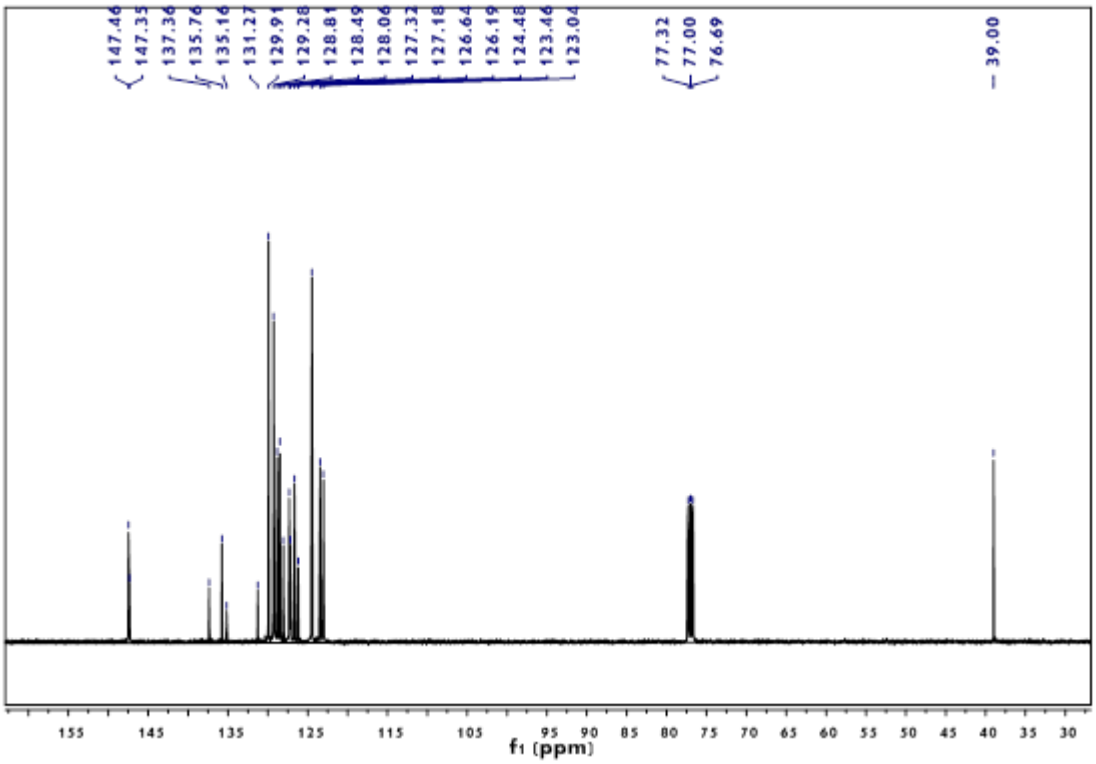


Fig. S7-2. ^{13}C NMR (400 MHz, $CDCl_3$) of compound **5**.

(*E*)-4-(((N,N-diphenyl)amino)-styryl)-phenyl-methyl-benzyl-sulfonium trifluoromethanesulfonate (PAG 5):

Due to the high sensitivity to ambient light, all the preparation was carried out in dark. Firstly, to a solution of precursor compound **5** 469 mg (1.0 mmol, 1 equiv) in 5 mL of dried dichloromethane at -78 ^oC, methyl trifluoromethanesulfonate 180mg (1.1 mmol, 1.1 equiv) was syringed into the solution. After stirring at this temperature for 2h, the mixture was warmed to room temperature and stirred for another 24 hours. Subsequently, dichloromethane was removed and residue was dissolved in acetonitrile. 10 times volume ethyl ether was added to the solution dropwise, slowly forming the crystal. Solid was collected by filtration and washed with ethyl ether. Then it was dissolved in acetonitrile again for another crystal formation by dropping 10 times volume ethyl ether. Yellow product was gained (399 mg, 63.0% yield).

^1H NMR (400 MHz, CD_3CN, δ_{ppm}): 7.75 (d, *J = 8.6 Hz*, 2 H, PhH); 7.64 (d, *J = 8.6 Hz*, 2H, PhH); 7.49 (d, *J = 8.6 Hz*, 2H, PhH); 7.43 (d, *J = 7.3 Hz*, 1H, PhH); 7.38 (d, *J = 7.6 Hz*, 2H, PhH); 7.33 (m, 5H, PhH); 7.22 (d, *J = 7.2 Hz*, 2H, PhH); 7.09 (m, 7H, PhH); 7.00 (d, *J = 8.6 Hz*, 2H, PhH); 4.83 (d, *J = 12.8 Hz*, 1H, CH_2); 4.67 (d, *J = 12.8 Hz*, 1 H, CH_2); 3.14 (s, 3H, CH_3). ^{13}C NMR (100 MHz, CD_3CN, δppm): 148.27; 133.48; 132.29; 131.64; 131.12; 130.56; 130.39; 130.34; 129.16; 128.93; 125.92; 124.94; 124.88; 124.78; 123.37; 29.62; 25.87. EI-MS (m/z): calcd for c, 633.1619, found: 484.2090 $[M\text{-}CF_3SO_3^-]^+$; Anal. calcd for 633.1619: C, 66.33; H, 4.77; N, 2.21; Found: C, 66.35; H, 4.86; N, 2.17.

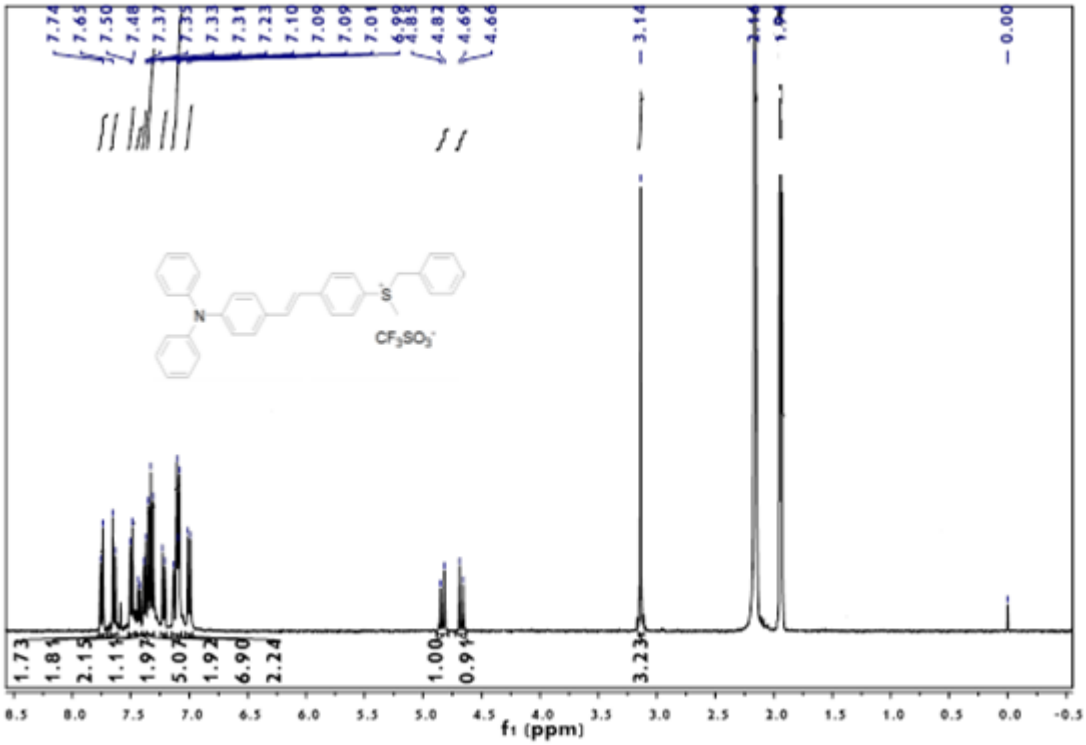


Fig. S8. ^1H NMR (400 MHz, CD_3CN) of PAG **5**.

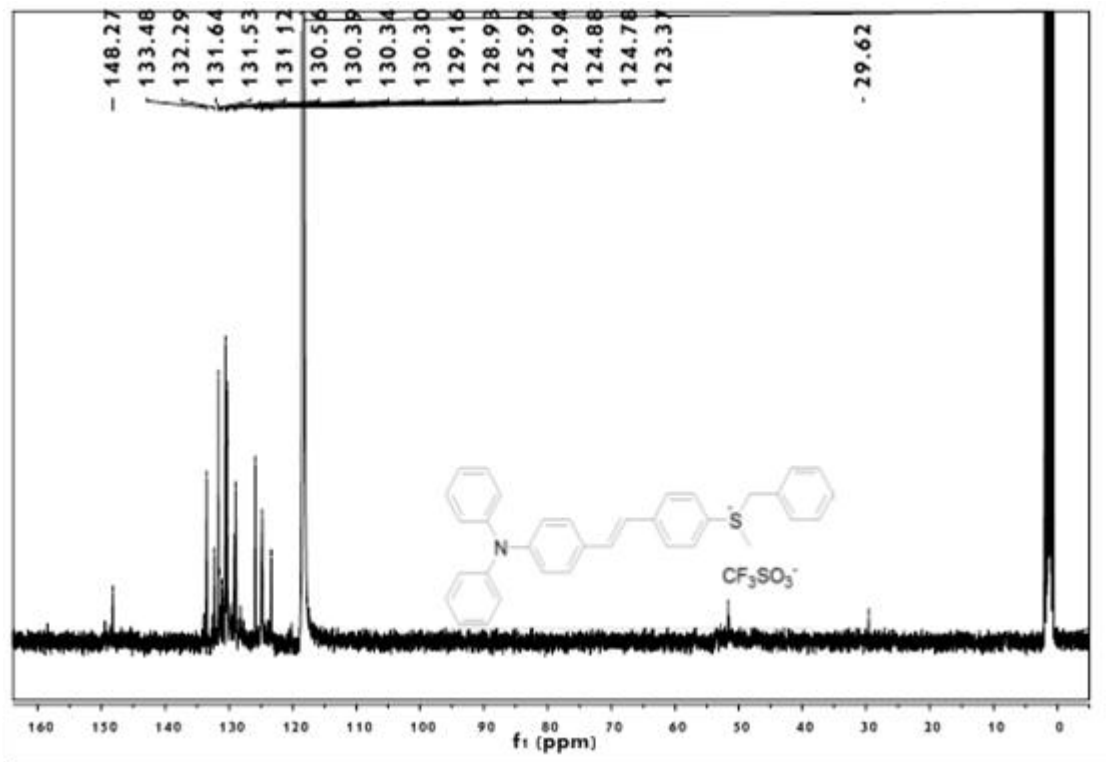


Fig. S8-2. ^{13}C NMR (100 MHz, CD_3CN) of PAG **5**.

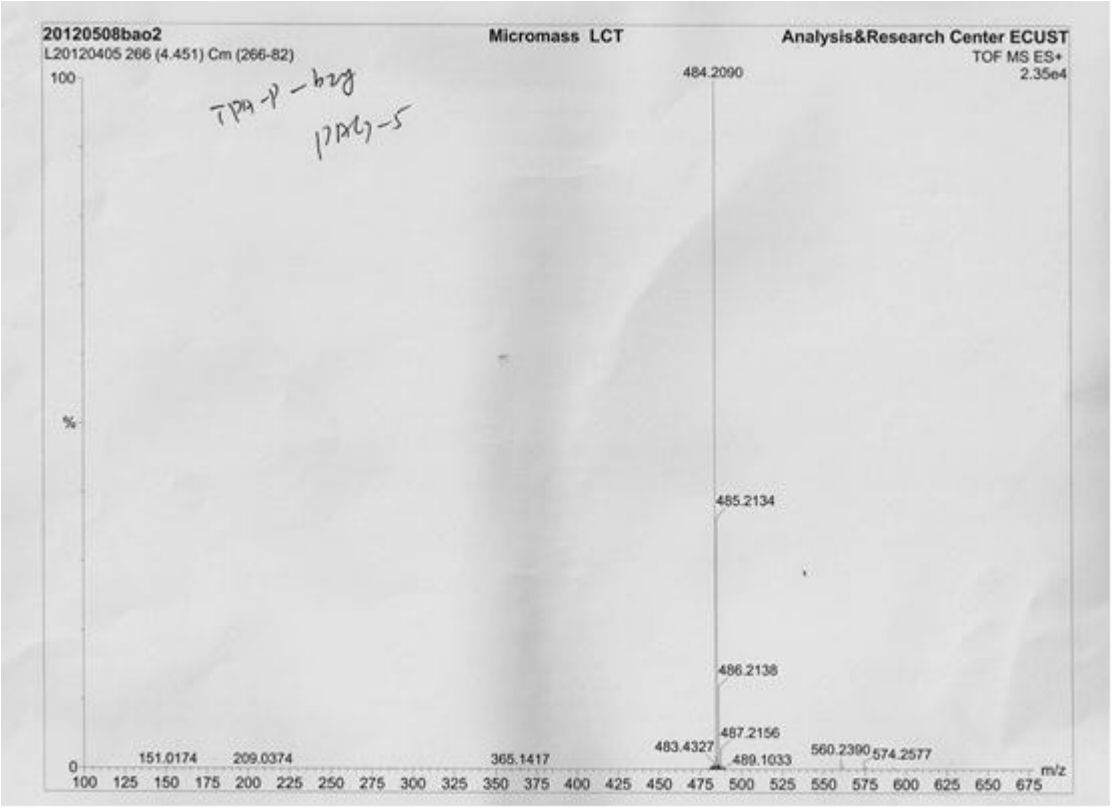
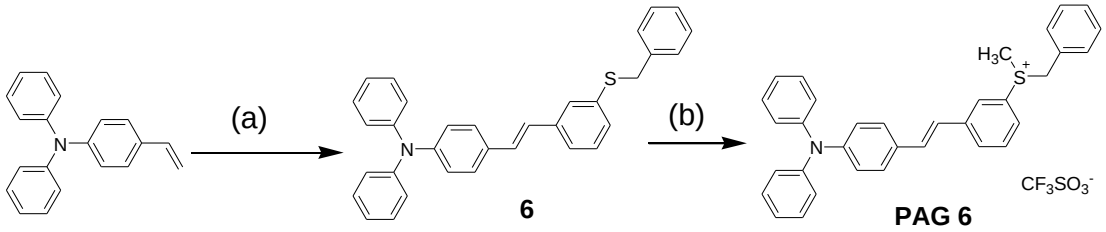


Fig. S8-3. TOF-MS of PAG **5**

Scheme S5:



(a) Compound **2**, $Pd(OAc)_2$, Triethanolamine, 120 ^oC, 24 h; (b) Methyl trifluoromethanesulfonate, CH_2Cl_2, -78 ^oC, 2 h, r.t. 24 h.

(*E*)-4-(N,N-diphenyl)amine-3'-benzylthiostilbene (6):

Compound **4** was prepared with the same method as **5** by 4-(N,N-diphenyl)amine-styrene 1.35g (5.0 mmol, 1 equiv) and compound **2** 1.53g (5.5mmol, 1.1 equiv) and catalyst by $Pd(OAc)_2$ 11.2 mg (0.05 mmol, 0.01 equiv). The product can be purified by column chromatography with DCM/petroleum ether (1/10; v/v) as eluent to give a yellow product (1.36g, 52.0 % yield).

^{1}H NMR (400 MHz, $CDCl_3$, δ_{ppm}): 7.40 (s, 1H); 7.35 (d, *J = 8.6 Hz*, 2H, PhH); 7.29 (d, *J = 6.8 Hz*, 2H, PhH); 7.28~7.24 (m, 7H, PhH and $CDCl_3$); 7.17 (t, *J = 7.6 Hz*, 2H, PhH); 7.10 (d, *J = 8.2 Hz*, 4H, PhH); 7.04 (d, *J = 8.6 Hz*, 4H, PhH); 6.97 (d, *J = 16.2 Hz*, 1H, CH=CH); 6.89 (d, *J = 16.2 Hz*, 1H, CH=CH); 4.10 (s, 2H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$, δ_{ppm}): 147.32; 138.11; 137.33; 136.61; 130.99; 129.20; 128.93; 128.76; 128.69; 128.40; 128.27; 127.32; 127.08; 126.05; 124.40; 124.34; 123.29; 122.98; 38.83. EI-MS (m/z): calcd for $C_{27}H_{23}NS$, 469.2; found, 469.2 $[M]^+$; Anal. calcd for $C_{33}H_{27}NS$: C, 84.40; H, 5.79; N, 2.98; Found: C, 84.45; H, 5.93; N, 3.01.

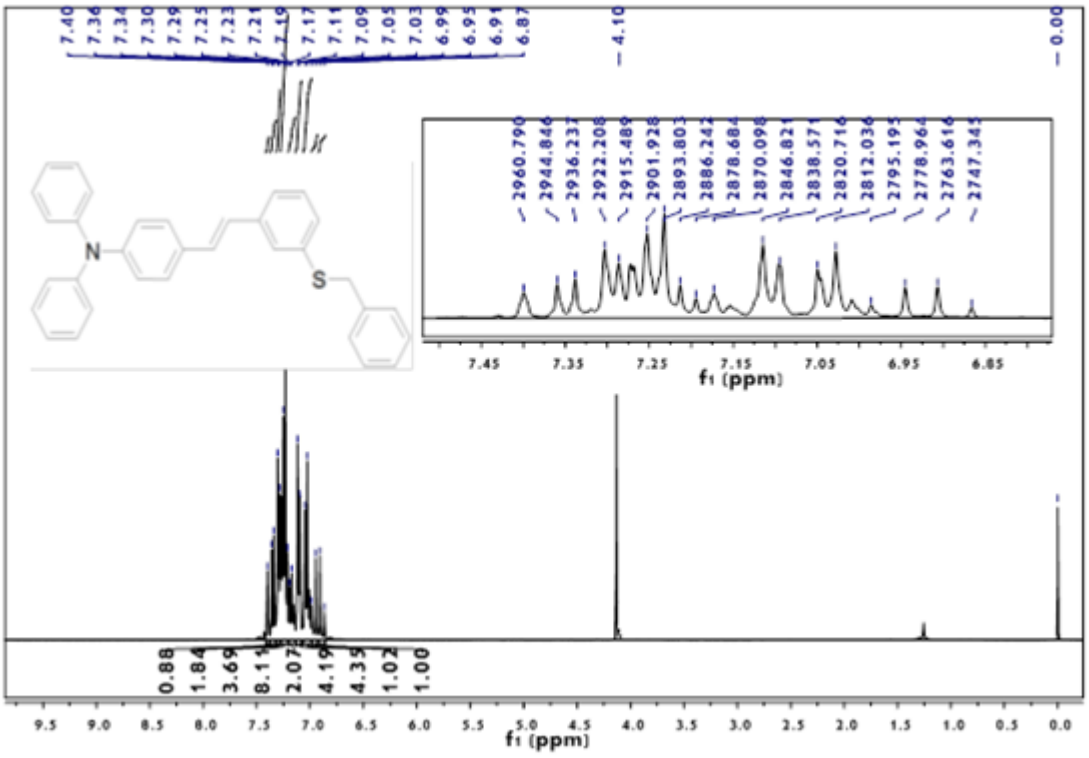


Fig. S9. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **6**.

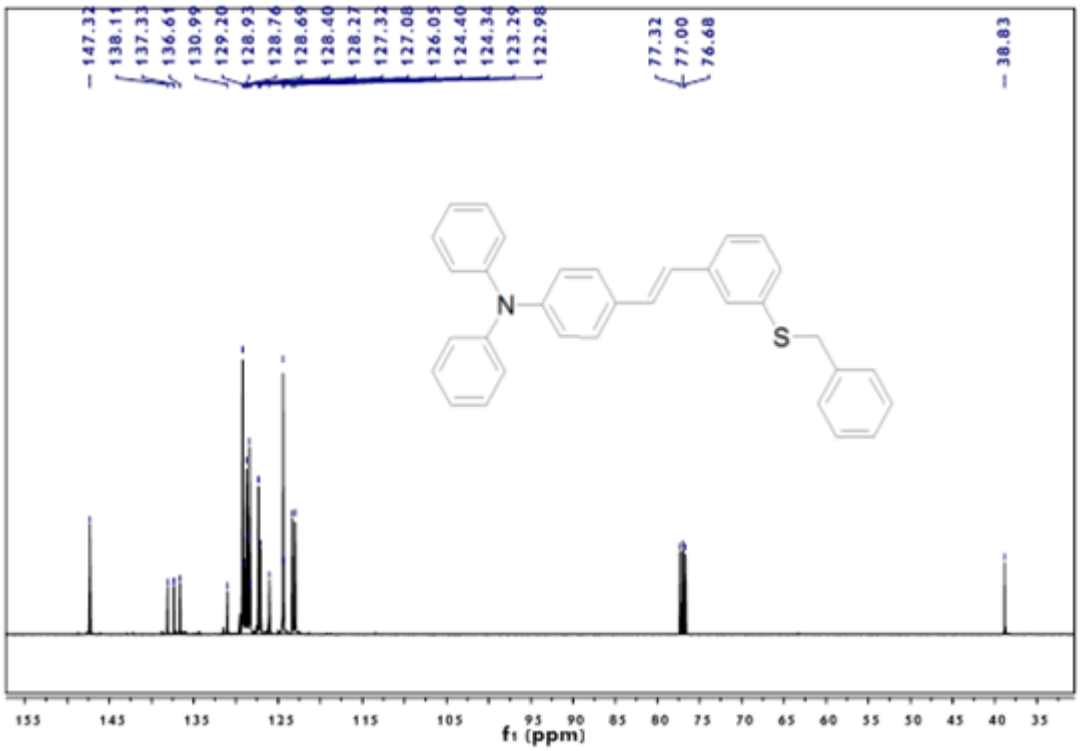


Fig. S9-2. ^{13}C NMR (100 MHz, $CDCl_3$) of compound **6**.

(*E*)-3-(((N,N-diphenyl)amino)-styryl)-phenyl-methyl-benzly-sulfonium trifluoromethanesulfonate (PAG 6):

PAG 6 was prepared by the same method as **PAG 5** by equivalent molar rare materials. And the yellow product was gained (361mg, 57.4 % yield).

^1H NMR (400 MHz, CD_3CN, δ_{ppm}): 7.86 (d, *J = 7.6 Hz*, 1H, PhH); 7.80 (s, 1H, PhH); 7.59 (t, *J =7.6 Hz, 8.8 Hz*, 1H, PhH); 7.51 (d, *J = 8.8 Hz*, 1H, PhH); 7.47 (d, *J = 8.8 Hz*, 2H, PhH); 7.31-7.44 (m, 8H, PhH); 7.23 (m, 3H, PhH); 7.10 (m, 6H, PhH); 7.00 (d, *J = 8.6 Hz*, 2H, PhH); 4.88 (d, *J = 12.8 Hz*, 1H, CH_2); 4.72 (d, J = 12.8 Hz, 1H, CH_2); 3.18 (s, 3H, CH_3). ^{13}C NMR (100 MHz, CD_3CN, δ_{ppm}): 149.11; 148.19; 141.68; 132.98; 132.49; 131.85; 131.62; 131.14; 131.04; 130.47; 130.23; 129.71; 128.87; 128.61; 128.30; 125.69; 124.66; 124.57; 123.96; 123.49; 51.67; 25.41. EI-MS (m/z): calcd for c, 633.1619, found: 484.2093 $[M\text{-}CF_3SO_3^-]^+$; Anal. calcd for 633.1619: C, 66.33; H, 4.77; N, 2.21; Found: C, 66.30; H, 4.66; N, 2.15.

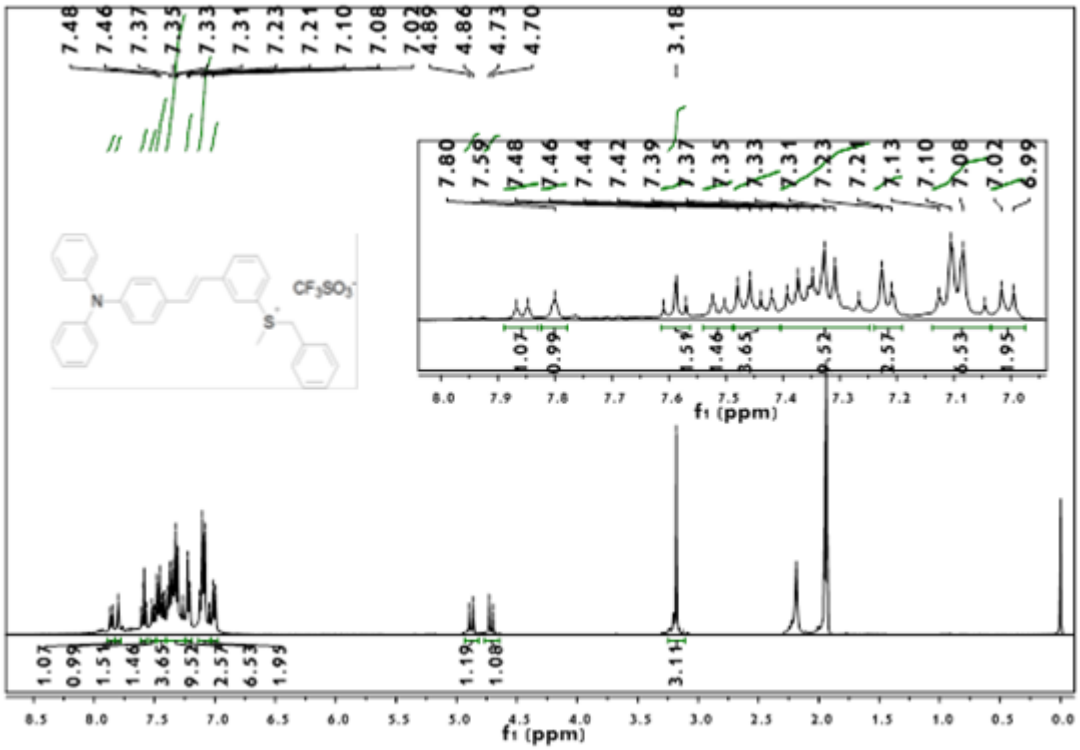


Fig. S10. ^{1}H NMR (400 MHz, CD_3CN) of PAG **6**.

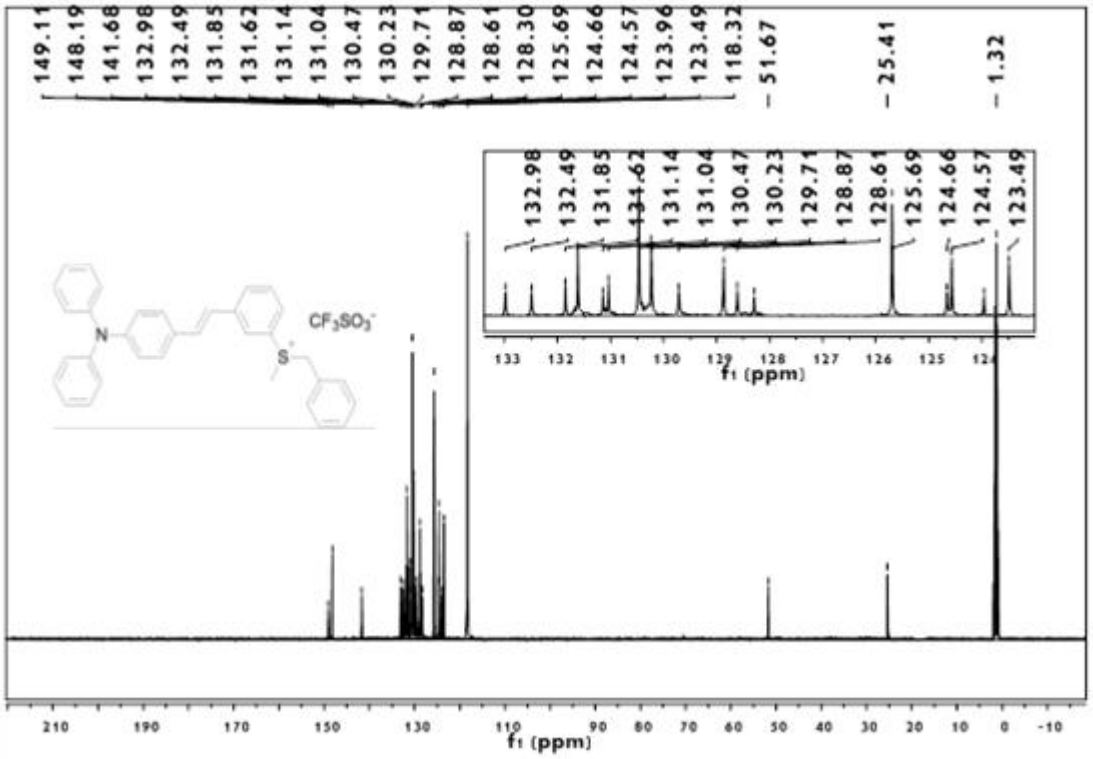


Fig. S10-2. ^{13}C NMR (100 MHz, CD_3CN) of PAG **6**.

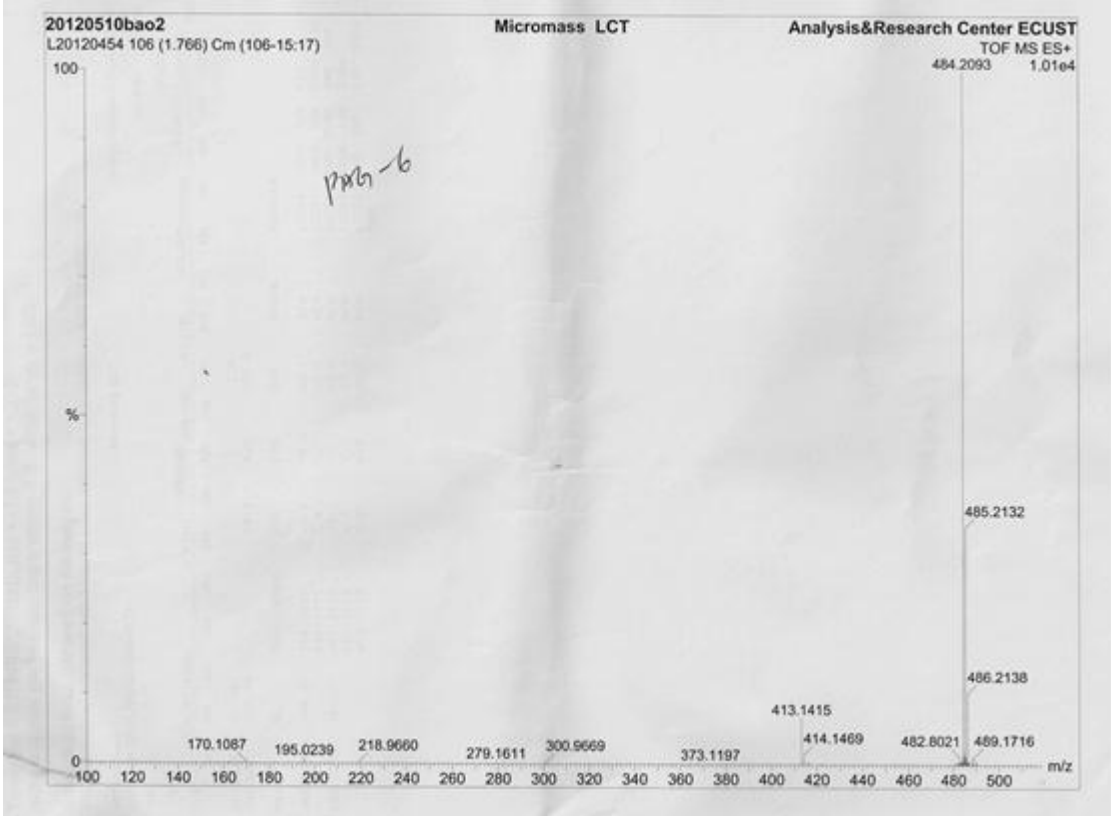


Fig. S10-3. TOF-MS of PAG **6**

II. Photophysical and photochemical characterizations.

Absorption spectra were recorded on a Shimadzu UV-2550 UV-vis spectrometer with 1 cm quartz cuvettes. Steady-state fluorescence spectra were collected from a FluoroMax-4 spectrofluorometer. Emission spectra are spectrally corrected, and fluorescence quantum yields included the correction due to solvent refractive index and were determined relative to quinine bisulfate in 0.05 M sulfuric acid ($\Phi = 0.52$)[3].

The molar extinction coefficients (ε) of PAGs were determined by concentration-dependent maximum absorption ($A = \varepsilon\ c\ l$) by dissolving different amount of samples in acetonitrile, and the uncertainties are estimated to be ca. 3%. One-photon photolytic reaction of **PAG 3-6** were performed by irradiating the solutions in acetonitrile with a LED point source, which equipped with 405 nm channel. Photoacid generation quantum yields were measured by using Rhodamine B base as an acid indicator,[4] which is protonated by acid produced in the photolysis to give a characteristic absorbance at 555 nm in acetonitrile. The acid concentration in acetonitrile was determined by a calibration curve of Rhodamine B titrated with *p*-tolunesulfonic acid in acetonitrile. The photon doses at 405 nm were determined by ferrioxalate actinometry and the uncertainty of the measured dose is ca. 3%.[5] The optical density of the samples was greater than 2.5 at the 405 nm, so all photons incident on the solution could be assumed to be absorbed. The dose rates were kept sufficiently small to ensure the maximum conversion was lower than 15%. The uncertainties in the photoacid generation quantum yields are estimated to be ca. 10%.

The cyclic voltammetry experiments[6] (using a computer-controlled Radiometer Voltalab 6 potentiostat with a three-electrode single-compartment cell; the working electrode was a platinum disk; a saturated calomel electrode (SCE) used as a reference was placed in a separate compartment) were performed at 300 K, in N_2-degassed acetonitrile with a constant concentration (0.1 M) of n-Bu_4NBF_4. Ferrocene was used as an internal reference.

Theoretical calculation methods: The geometrical structures and frontier molecular orbitals of the synthesized sulfonium salts PAGs were optimized by employing the density functional theory at the B3LYP/6-31 level with the Gaussian 03W program package.[7] And the singlet transition natures and the two-photon absorption related parameters of **PAGs 1-4** were calculated by time dependent density functional theory (TD-DFT) at TD CAM-B3LYP/6-31G* and TD LC-BLYP/6-31G*. Molecular orbitals were visualizable using Gaussview.

The two-photon absorption cross sections were measured from 690 – 1080 nm by using open-aperture Z-scan method[8,9] with a femtosecond mode-locked Ti: Sapphire laser (Spectra-Physics, Mai Tai : pulse duration: ~140 fs; repetition rate: 80 MHz; wavelength range: 690-1020 nm). The setup was shown in the following Figure. After passing through a beam expander (x 4), the laser beam is focused using an f = 10 cm lens and passed through a quartz cell (1 mm optical path length). The position of the sample cell is varied along the laser-beam direction (Z-axis) using a Z-step motorized stage controlled by a computer. At constant incident excitation, the local power density within the sample is changed and the corresponding transmitted laser beam, *T(z)*, recorded with a silicon photodetector (Ophir PD300) is monitored in connection

with the z-position of the cell. The on-axis peak intensity of the incident pulses at the focal point, I_0, ranged from 35 to 50 GW cm^{-2}. If we assume that the linear absorption of the sample is negligible at working wavelength and that the laser exhibits a Gaussian beam profile, the nonlinear absorption coefficient β can be calculated from the curve fitting to the experimental transmittance with the following equation:

$$T(z) = 1 - \frac{\beta l I_0}{2\sqrt{2}(1+(\frac{z}{z_0})^2)} \qquad (1)$$

where Z_0 corresponds to the diffraction length of the incident beam, l the optical path length. The 2PA cross-section, δ, (in units of 1 GM: 10^{-50} cm^4 s photon^{-1} molecule^{-1}) is then determined by using the relationship:

$$\beta = \frac{\delta . N_A . d}{h\nu} 10^{-3} \qquad \text{...}(2)$$

Where h is the Planck constant, ν the frequency of the incident laser beam, N_A the Avogadro constant and d is the concentration of the chromospheres (mol. L^{-1}). The rhodamine 6G in methanol[10] (16.2 ± 2.4 GM at 806 nm) was used for the calibration of our measurement technique.

$$T_{MAX} - T_{MIN} = \Delta T \propto \delta . c . I_0 \qquad (3)$$

The slope of the correlation between ΔT vs. I_0 will then be measured. Here, we used a typical 'Z-scan' standard at 806 nm (Rhodamine 6G (R6G) in Methanol $\delta_{806\ nm}$ = 16.2 GM). Therefore, one can easily derive δ from the following ratio:

$$\frac{\Delta T}{\Delta T_0} = \frac{\delta . c}{\delta_0 . c_0} \qquad (4)$$

So, we measured the Z-scan curves of R6G and PAGs **3-6** at different laser intensities (next page) at 806 nm and then the relevant transmittance variation *vs.* excitation power for R6G and PAGs were plotted and linearly fitted, respectively. Then δ values of PAGs can be calculated by the comparison of the relative slopes and concentrations of PAGs and R6G. The Z-scan measurements have been performed at least three times for reproducibility.

Two-photon absorption cross-sections of **PAG 3** were also determined by the method of two-photon excited fluorescence using fluorescein as a standard with known two-photon absorption cross-sections.[10] The 800 nm pump source was from the fundamental of a fs mode-locked Ti:sapphire laser system (output beam ≈ 80 fs duration and 250 kHz repetition rate). The laser was focused on a quartz cuvette with a spot size of 1-mm and an optical path length of 10-mm. The two-photon induced fluorescence was collected with a polychromator (Spectropro-550i, Horiba Jobin Yvon) and detected by a CCD detector. The samples were dissolved in CH_3CN at a concentration of 10^{-4} M, and fluorescein in water (pH = 11) at the concentration of 10^{-5} M. Two-photon absorption cross-section (δ) was obtained as follows:

$$\delta_S = \frac{F_S}{F_R}\left[\frac{\Phi_R C_R n_S}{\Phi_S C_S n_R}\right]\delta_R. \quad (5)$$

Where subscripts *S* and *R* denote the sample and the reference, respectively, *F* represents the integrated area of two-photon induced fluorescence, *Φ* stands for fluorescence quantum yield, *C* for concentration, and *n* for refractive index of the solvents. The experimental errors of δ values are estimated to be ±20%, as a result of variations of laser energies and sample concentrations.

The concentration of generated acid upon two-photon excitation was also titrated using rhodamine B base as an acid indicator. All the experiments were carefully carried out in the dark to avoid photogeneration of acid due to parasite light. Typically, a solution of acetonitrile with the PAG (5×10^{-4} M) was two-photon irradiated for 15 min at the focus of Z-scan measurements. An excess of rhodamine B (2×10^{-5} M) was then added to the sample. The concentration of the photogenerated acid was spectrophotometrically evaluated from the absorbance of protonated rhodamine B base at 555 nm. Each measurement was reproduced three times, which leads to an average value of H^+ concentration.

The photolithography was performed on the Si slide. To increase the adhesion strength, the slide was previously treated with Piranha solution for 3 h at 80 ^oC, and then baked at 90 ^oC for 3 min. Then a 20 wt % SU-8 solution (with 1 wt% PAG **6** compared with SU-8 resin) was spin-coated onto the slides at 2000 rpm for 120 s after being filtered through a syringe filter with a 0.45-μm pore size. Then the slide was prebaked at 100 ^oC for 3 min. The thickness of the films was around 500 nm. Then the obtained film was irradiated under atmospheric conditions with a high pressure Hg lamp with 405 nm filter for 20 s with the light intensity of 10 mW/cm^2. Then the film was post-baked for 3 min at 100 ^oC. After cooling, the photoresist films were treated with developer at room temperature for 120 s and rinsed with isopropanol, and dried with blowing nitrogen; the morphologies were detected with bright-field microscopy.

For two-photon microfabrication, the photoresist was exposed in the pattern of the target structure at 800 nm with tightly focused (0.6 N.A.) 80-fs pulses from a Ti: sapphire laser (250 KHz repetition rate) at an average power of 40 μW and a linear scan speed of 1.0 μm s^{-1}. Others were same as one-photon photolithography.

III. Figures and tables

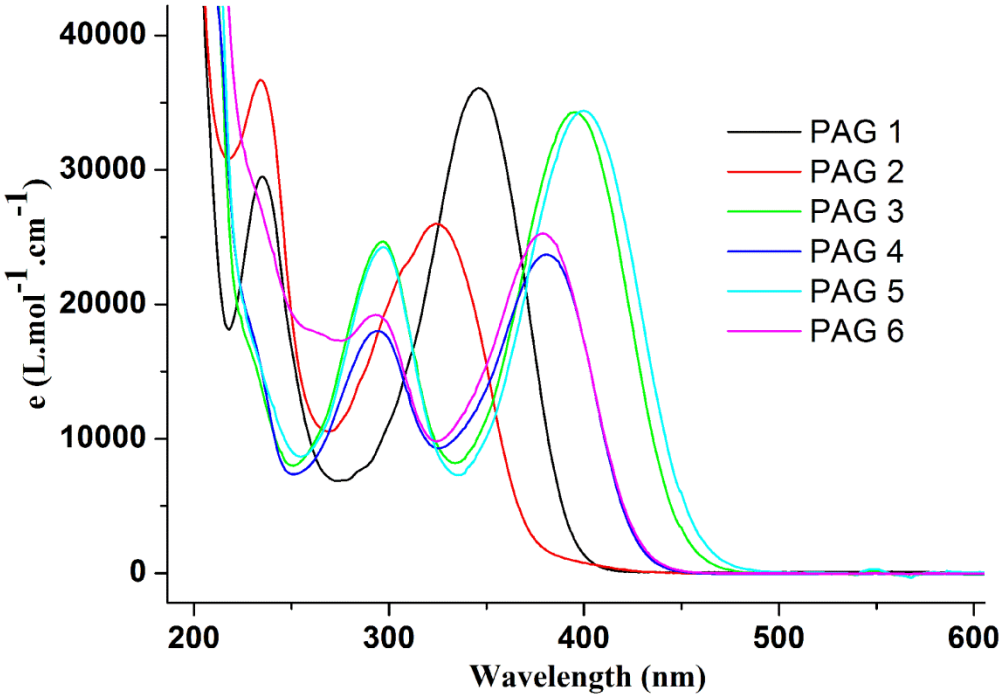


Fig. S11: The UV-vis spectra of PAGs **1-6** in acetonitrile.

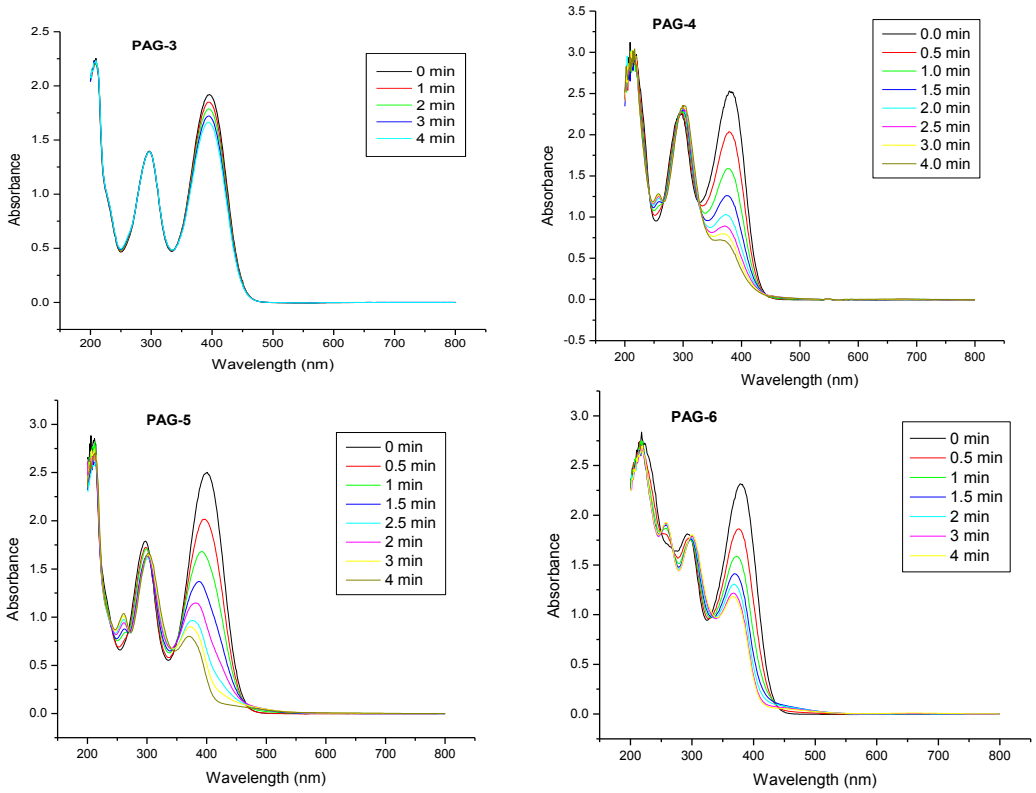


Fig. S12. The UV-Vis spectra of PAGs **3-6** under irradiation of 405 nm light in acetonitrile solution with 0.25 mW/cm^2 light intensity.

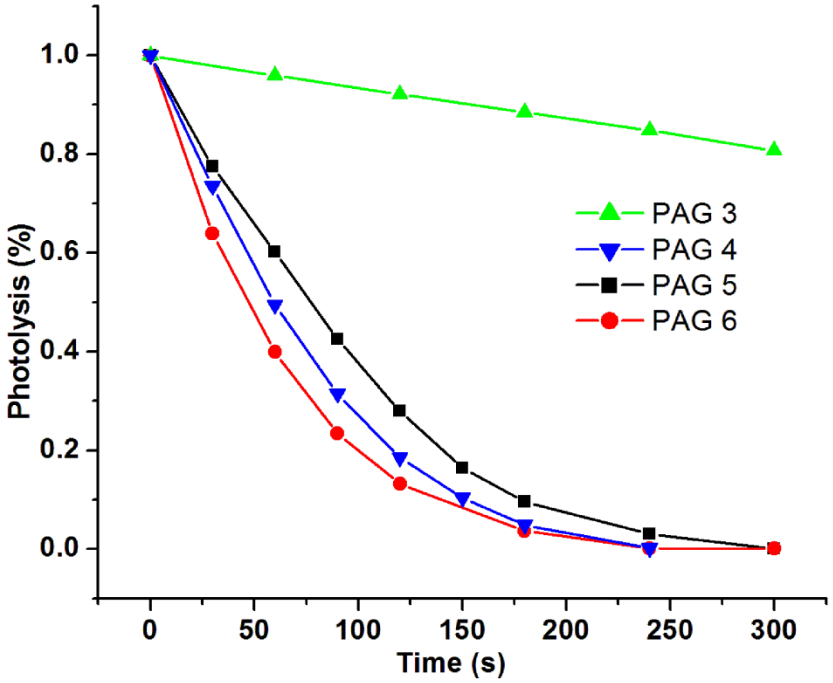


Fig. S13: Time course of single photon photolysis of PAGs **3-6** at 405 nm (0.25 mW/cm^2) irradiation corresponding to Fig. S12.

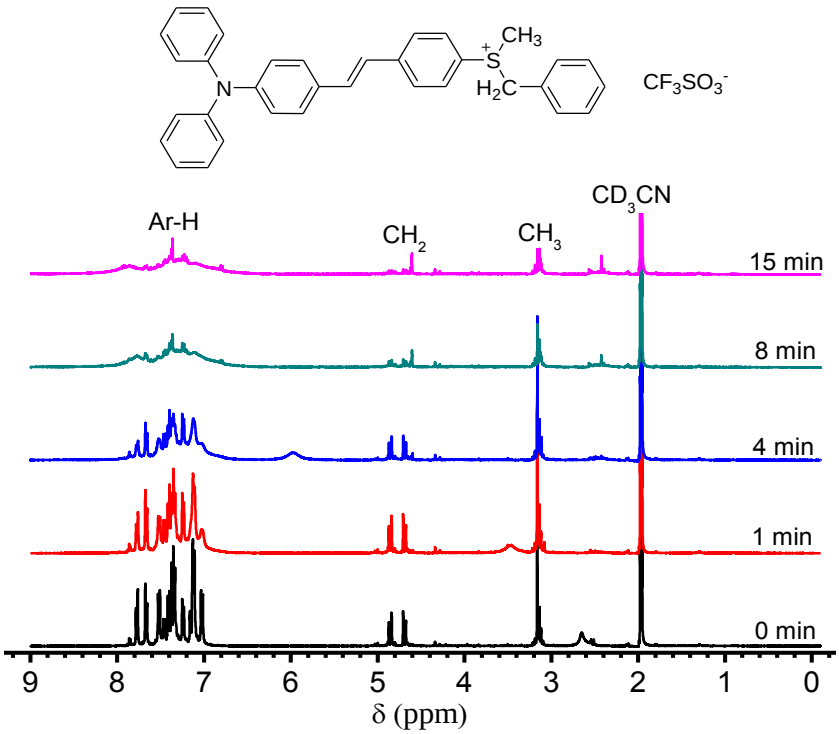


Fig. S14: ^{1}H NMR spectra of PAG **5** in CD_3CN (5 mg/0.6 mL) evolution with the irradiation of 405 nm light with intensity of 2.0 mW/cm^2 for different time.

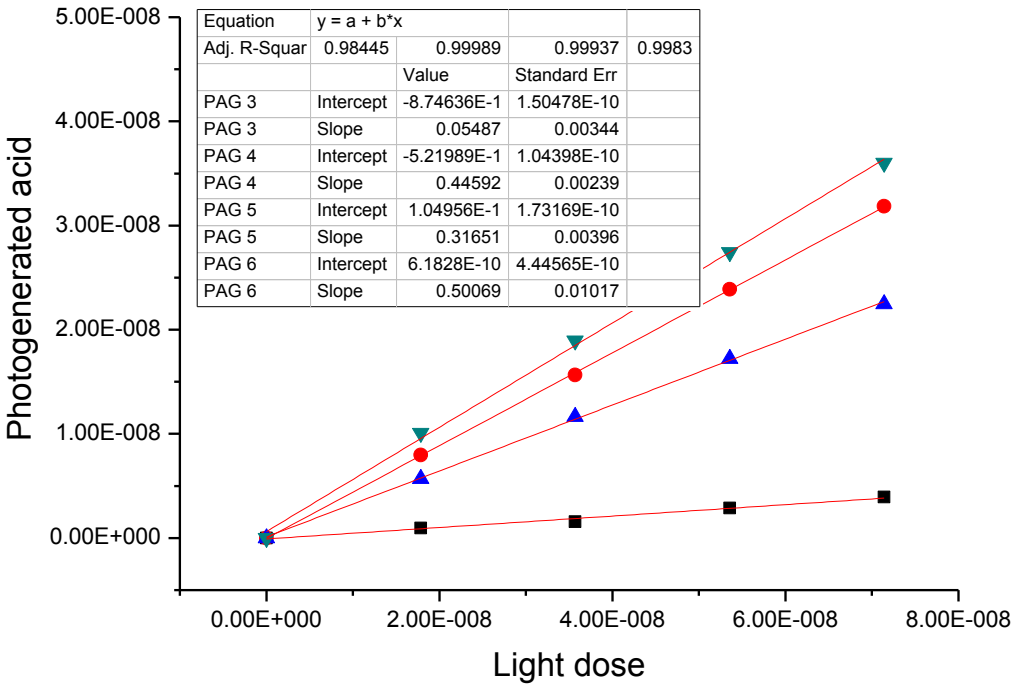


Fig. S15. Number of photogenerated acid as function of the number of the absorbed photon in acetonitrile (Black Squares: PAG **3**; Blue Triangles: PAG **5**; Red Circles: PAG **4**; Cyan Triangles: PAG **6**.). The inset is the linear fitting results.

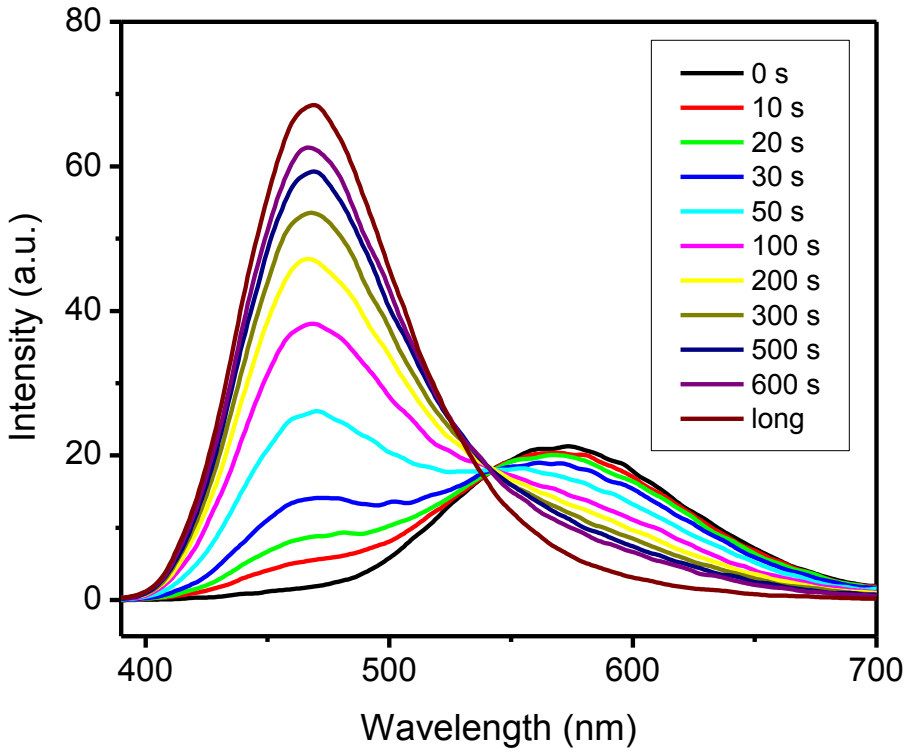


Fig. S16: The emission spectra of PAG **3** (1×10^{-5} M) in ACN under irradiation of 405 nm light with intensity of 2.0 mW/cm^2 at different time.

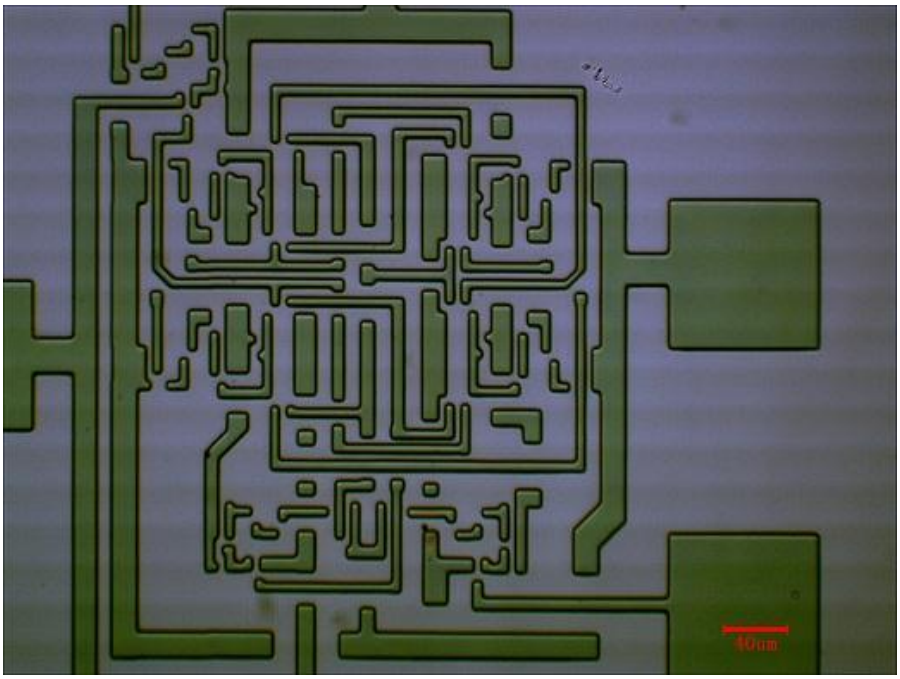


Fig. S17: The microscopy picture of photoresist film of SU-8 resin using PAG **6** as photoacid generators under 405 nm irradiation.

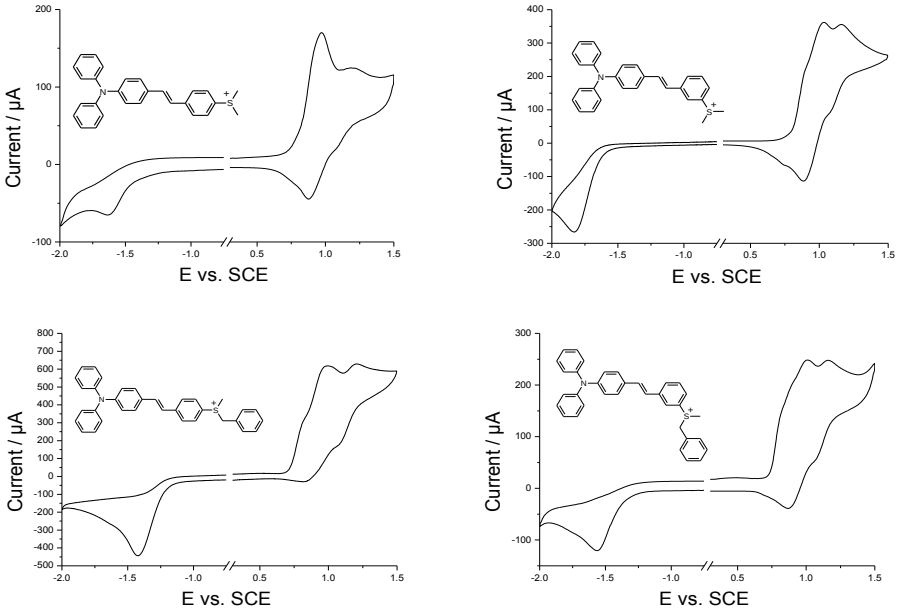


Fig. S18: Cyclic voltamogramm of PAGs **3-6** in acetonitrile + $(nBu)_4NBF_4$ (0.1 M) on platinum electrode at 200 mV s^{-1} ([PAGs]: 3×10^{-3} M).

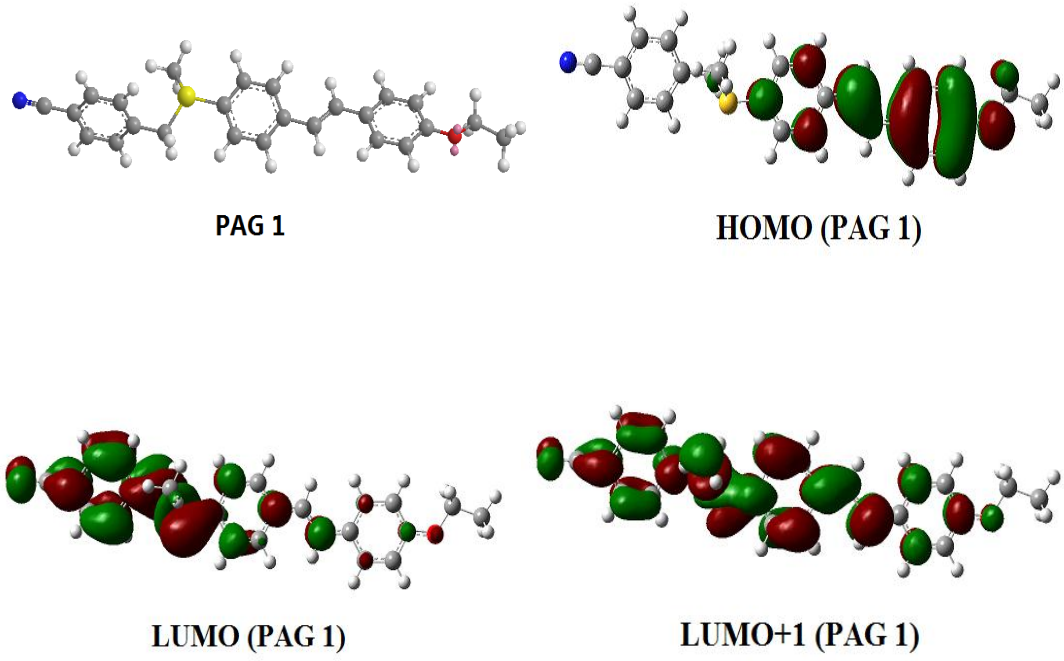


Fig. S19: The frontier orbital plots of the HOMO, LUMO and LUMO+1 of PAG **1**.

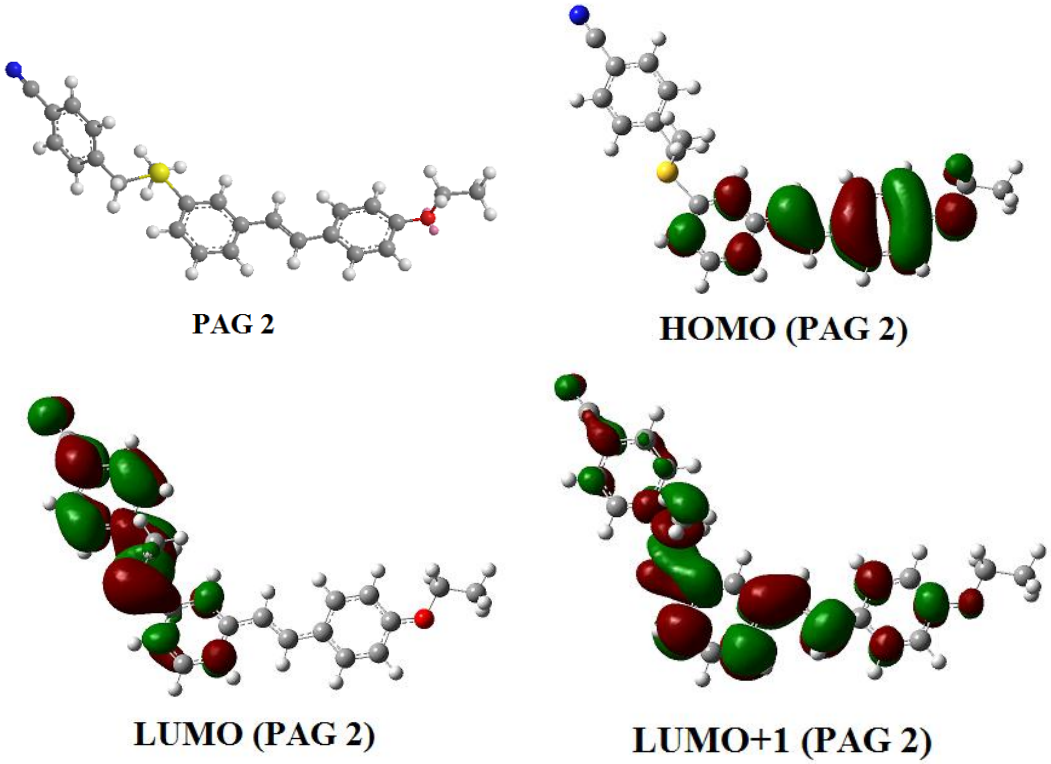


Fig. S20: The frontier orbital plots of the HOMO, LUMO and LUMO+1 of PAG **2**.

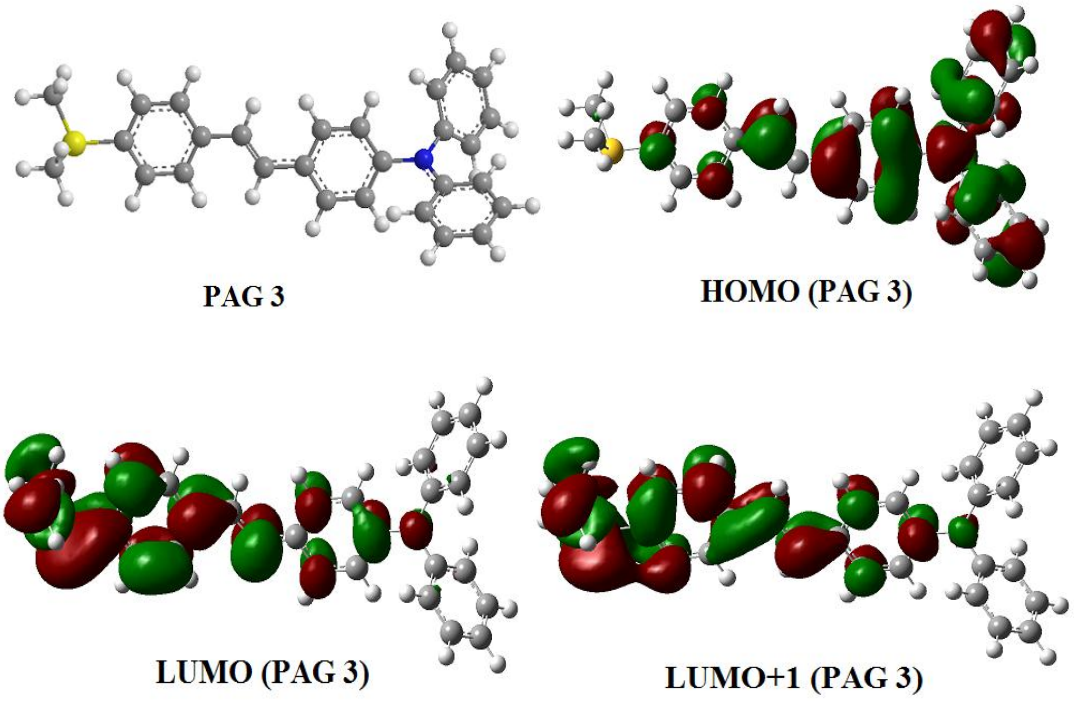


Fig. S21: The frontier orbital plots of the HOMO, LUMO and LUMO+1 of PAG **3**.

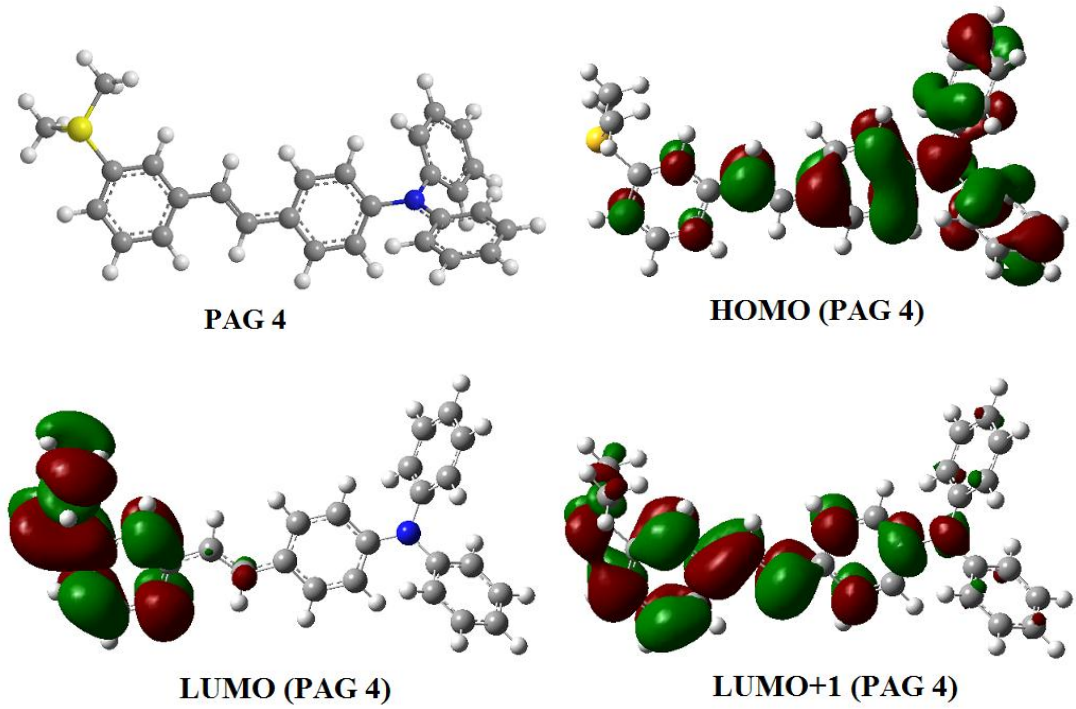


Fig. S22: The frontier orbital plots of the HOMO, LUMO and LUMO+1 of PAG **4**.

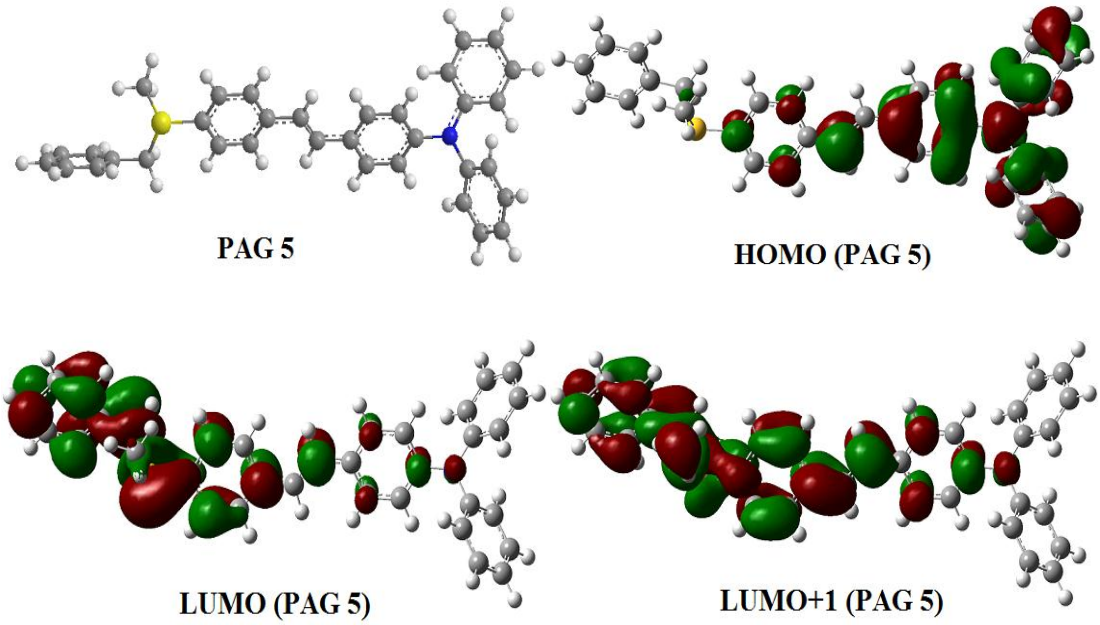


Fig. S23: The frontier orbital plots of the HOMO, LUMO and LUMO+1 of PAG **5**.

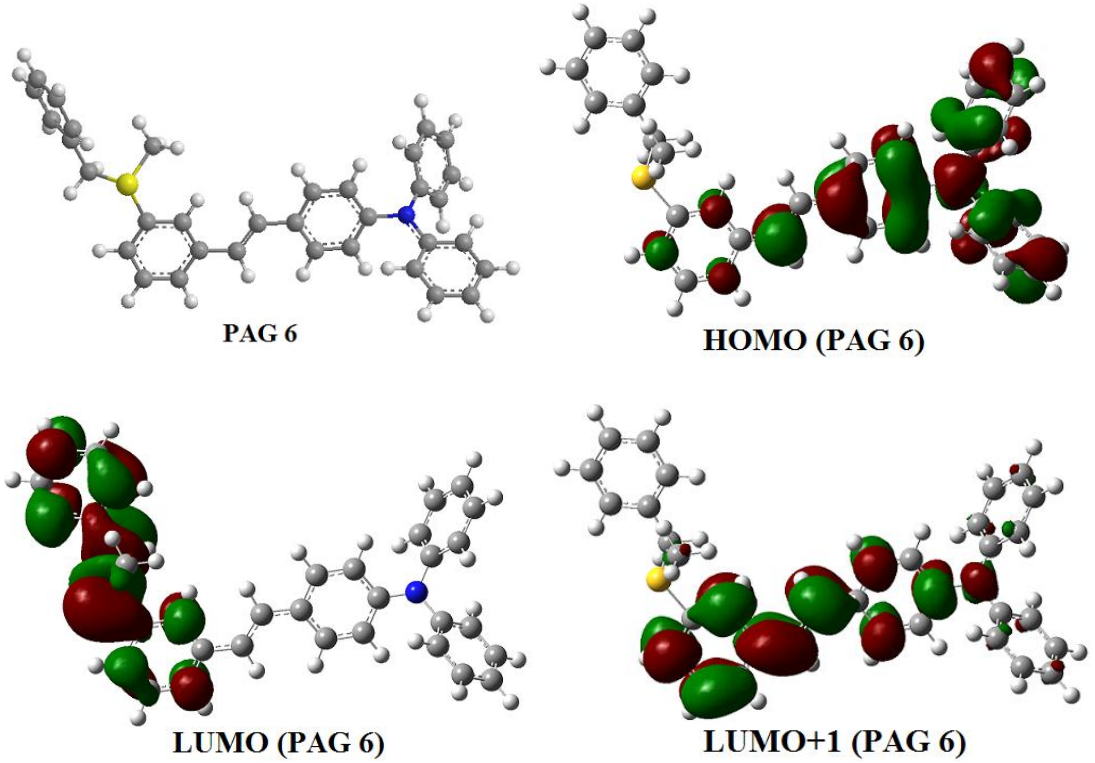


Fig. S24: The frontier orbital plots of the HOMO, LUMO and LUMO+1 of PAG **6**.

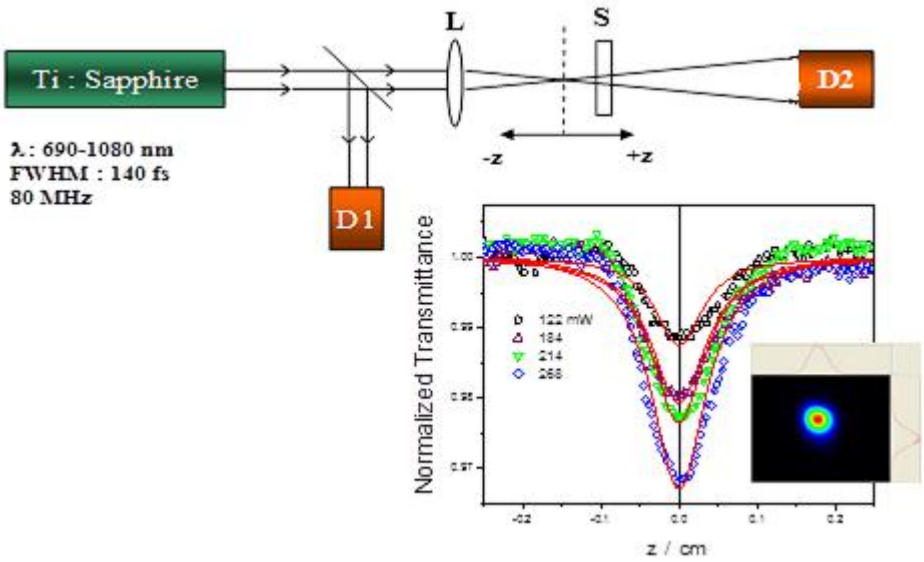


Fig. S25: The Z-Scan setup for the two-photon absorption cross-sections testing. D: detector; L: Lens; S: Cell with sample solution (10^{-3}M); (Insets: Typical Z-scan trace recorded at 806 nm for R6G and laser profile and the profiles of the laser spots).

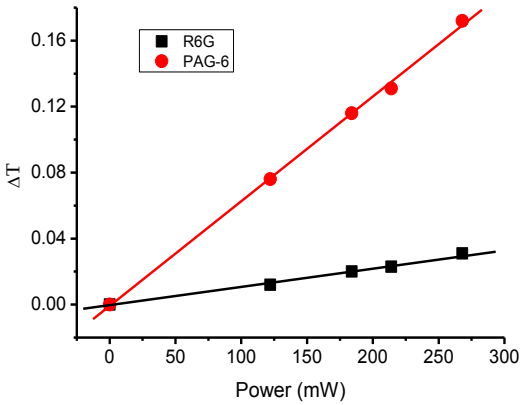


Fig. S26: The transmittance variation (ΔT) *vs*. excitation power of R6G and **PAG 6** with their corresponding fitting curves at different powers based on the equation (1) – (4). (The ΔTs of R6G were in Fig. S25).

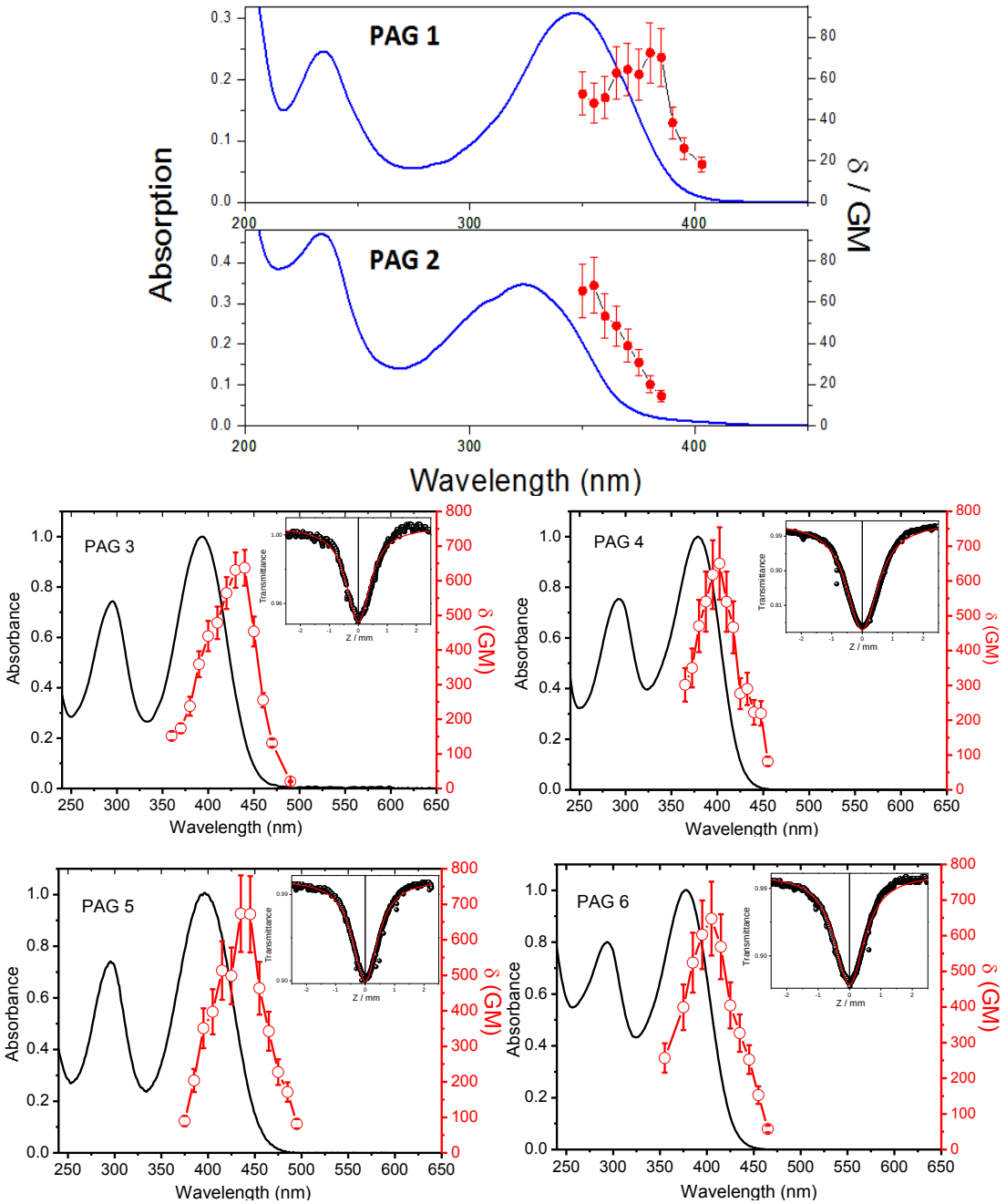


Fig. S27: One and two-photon absorption spectra of sulfonium-based derivatives **PAGs 1-6** in ACN. Insets: Typical Z-scan trace recorded at 800 nm with its corresponding fitting curves (The wavelength of two-photon absorption has been divided by 2 in order to compare with one-photon absorption spectra).

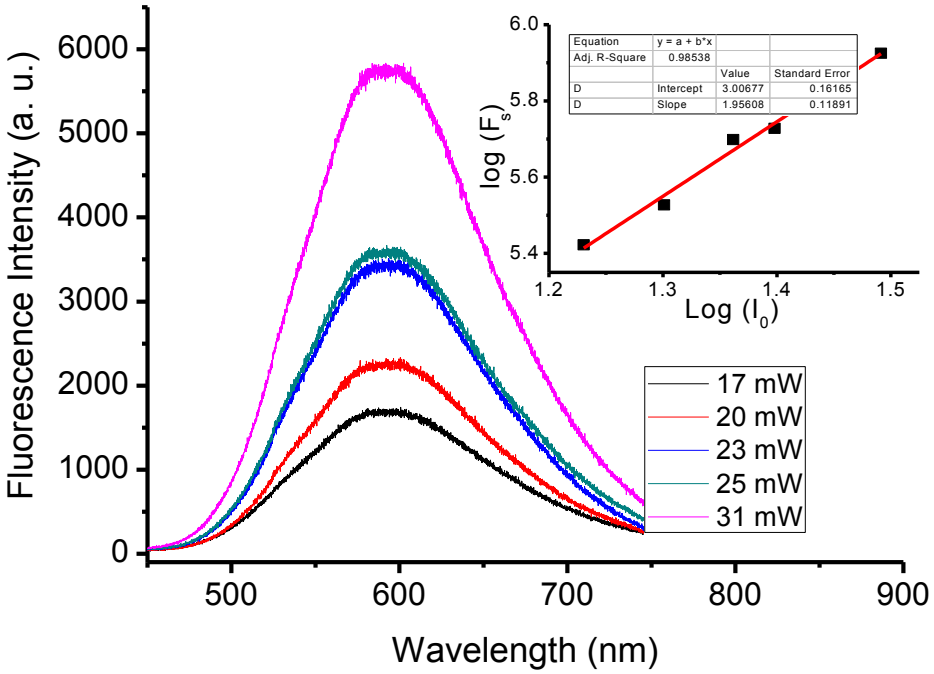


Fig. S28: Two-photon excited fluorescence (TPEF) spectra of **PAG 3** in ACN (ex: 800 nm, C = 1.0×10^{-4} mol L^{-1}). Insets: The squared dependence of induced fluorescence power and incident laser intensity was observed, and the log–log plot of the fluorescence signal vs excited light power provided direct evidence for two-photon excited process, the slope is 1.96.

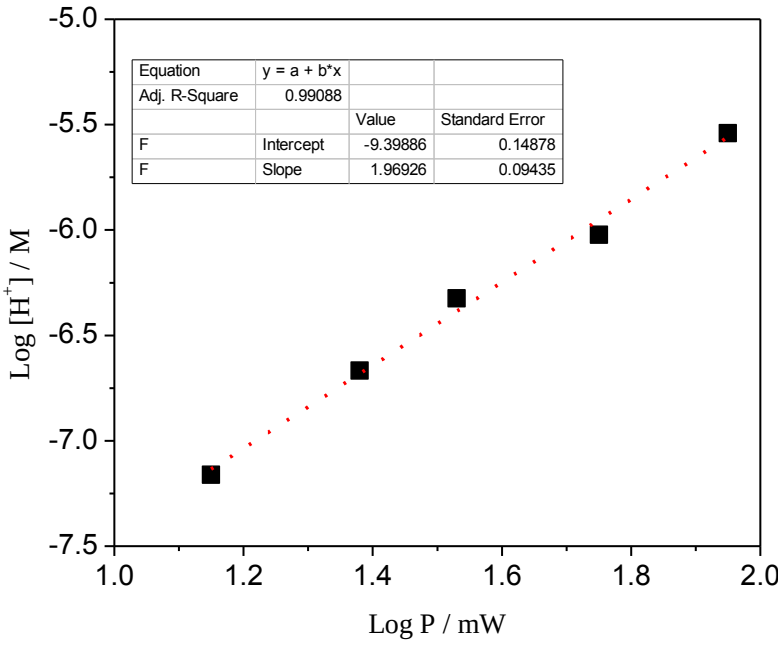


Fig. S29: Plots of log [H^+] vs log [excitation power] irradiated at 800 nm for PAG **6** for 15 min. The concentration of the photogenerated acid, which was determined spectrophotometrically with rhodamine B, increases with the square of the excitation power. This quadratic relationship is consistent with a photochemical reaction, which is two-photon activated. The inset is the result of linear fitting.

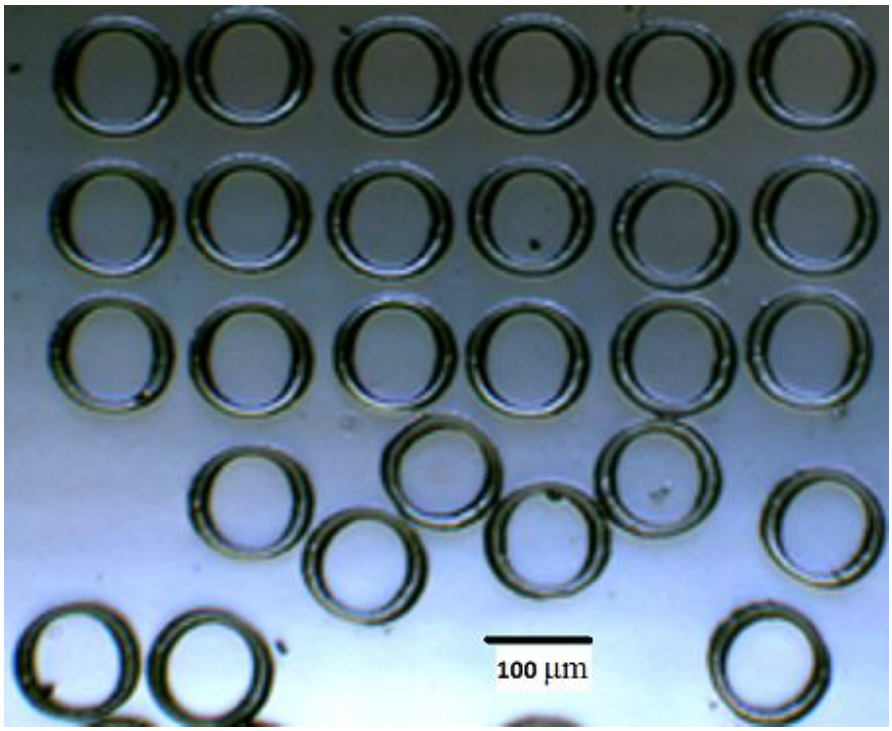


Fig. S30: The microscopy picture of photoresist film of SU-8 resin using **PAG 6** as photoacid generators under 800 nm excitation (two-photon mode), and some polymer rings left the array during the ultrasonic cleaning.

Table S1: The corresponidng parameters for free energy change of photoinduced intramolecular electron transfer of PAG **1-6**

Compounds	E_{ox1} [a] (V)	E_{ox2} [a] (V)	E_{red} [a] (V)	E_{00} [b](eV)	ΔG_{eT} [c] (eV)
PAG 1	1.35	-	-0.92	3.24	-0.97
PAG 2	1.35	-	-0.89	3.50	-1.23
PAG 3	0.97	1.21	-1.64	2.75	-0.14
PAG 4	1.03	1.16	-1.83	2.93	-0.07
PAG 5	0.99	1.21	-1.42	2.76	-0.34
PAG 6	1.00	1.16	-1.57	2.91	-0.32

[a] Peak values vs SCE (200 mV/s scan rate) at the constant concentration of 10^{-3} mol/L of sulfonium salts with 0.1 N tetrabutylammonium tetrafluoroborate as electrolyte.
[b] The energy of singlet excited state.
[c] The estimation of the free energy (ΔG_{eT}) associated to this process. We calculated ΔG_{eT} using Rehm−Weller equation :

$$\Delta G_{eT} = E_{ox} - E_{red} - E_{00} - C ;$$

In this formalism, E_{ox} and E_{red} correspond to the oxidation and reduction potentials of the donor and acceptor, respectively. E_{00} is the energy of singlet excited state, which is calculated by Berlman's method. C is the Coulombic energy term characterizing the interaction of the radical ion pairs. In acetonitrile, this term usually makes a small contribution to the overall energy change for PET and was neglected in the calculation.

Table S2: The absorption and singlet transition natures of PAG **1-4** based on TD CAM-B3LYP/6-31G* and TD LC-BLYP/6-31G* levels.

	TD CAM-B3LYP/6-31G*			TD LC-BLYP/6-31G*		
	λ_{max} /nm	*f*	*Transition nature*	λ_{max}^{o} /nm	*f*	*Transition nature*
PAG 1	S_1 365.8	1.43	H→L 40.8% H→L+1 5.4%	S_1 323.7	1.58	H→L 32.6% H→L+1 6.9%
	S_2 280.2	0.01		S_2 243.2	0.01	
PAG 2	S_1 336.0	0.21	H→L 33.5% H→L+1 11.5%	S_1 293.1	1.23	H→L+1 31.8% H→L+2 5.4%
	S_2 318.0	1.08	H→L 4.3% H→L+1 21.1% H→L+2 20.6%	S_2 266.3	0.16	
PAG 3	S_1 434.8	1.34	H→L 44.2%	S_1 363.4	1.63	H-1→L 6.3% H→L 31.9%
	S_2 306.1	0.04		S_2 255.0	0.01	
PAG 4	S_1 419.6	0.83	H→L 41.9%	S_1 342.9	1.35	H→L 25.1% H→L+1 8.0%
	S_2 340.9	0.45		S_2 271.9	0.12	

Table S3: The two photon absorption cross sections of **PAGs 1-4** calculated by TD LC-BLYP//TD CAM-B3LYP/6-31G* and their corresponding transition natures and maximum two-photon absoption wavelengths.

	λ_{abs}^{T}	δ_{max}/GM	Experiment
PAG 1	S_1 731.5	141.6	73GM(760nm)
	S_2 561.0	46.7	
	S_3 523.1	6.1	
PAG 2	S_1 672.0	9.5	
	S_2 635.8	51.1	68GM(710nm)
	S_3 516.6	1.5	
PAG 3	S_1 870.1	268.3	643GM(880nm)
	S_2 612.3	108.5	
	S_3 571.4	475	
PAG 4	S_1 840.6	168.5	650GM(800nm)
	S_2 681.2	3.22	
	S_3 566.1	349.1	

Table S4: The molecular orbital coefficients of HOMO, LUMO and LUMO+1 in **PAGs 1-4**; and the molecular structures of PAGs were optimized by B3LYP/6-31G* (the atom numbers were shown below)

PAG1			HOMO	LUMO	LUMO+1	PAG2			HOMO	LUMO	LUMO+1	LUMO+2
1	C	1S	0.00008	0.00012	-0.00013	1	C	1S	0.00023	-0.00007	0.00046	-0.06898
		2S	-0.00034	-0.00013	-0.00003			2S	-0.00091	-0.00040	-0.00048	0.00019
		2PX	-0.01505	0.00024	-0.00085			2PX	-0.02110	-0.00012	-0.00053	-0.00043
		2PY	-0.03305	-0.00040	-0.00100			2PY	0.02878	0.00026	-0.00196	-0.00024
		2PZ	-0.18066	-0.00175	-0.00549			2PZ	-0.16892	-0.00026	0.00644	-0.00105
		3S	0.00155	-0.00357	0.00390			3S	0.00353	-0.00125	-0.00739	0.00479
		3PX	-0.01287	0.00302	-0.00265			3PX	-0.01641	-0.00044	-0.00205	-0.01001
		3PY	-0.02598	0.00112	-0.00101			3PY	0.02489	-0.00374	-0.00670	-0.00385
		3PZ	-0.14579	0.00458	-0.01250			3PZ	-0.15102	-0.00294	0.01290	-0.00865
		4XX	-0.00099	-0.00093	0.00073			4XX	0.00072	-0.00008	0.00091	0.00666
		4YY	-0.00279	-0.00098	0.00076			4YY	-0.00383	0.00037	-0.00256	0.00050
		4ZZ	0.00381	0.00192	-0.00149			4ZZ	0.00319	-0.00030	0.00176	-0.00151
		4XY	-0.00205	-0.00137	0.00102			4XY	0.00101	0.00007	0.00013	0.00101
		4XZ	-0.00666	-0.00598	0.00445			4XZ	0.00300	-0.00074	0.00477	0.00019
		4YZ	-0.00852	-0.00297	0.00230			4YZ	0.01251	-0.00118	0.00859	0.00274
2	C	1S	-0.00011	-0.00039	0.00033	2	C	1S	-0.00026	-0.00018	-0.00126	0.00514
		2S	0.00034	0.00081	-0.00063			2S	0.00065	0.00019	0.00303	-0.00110
		2PX	0.00763	0.00567	-0.00374			2PX	0.01834	-0.00181	0.01632	0.00194
		2PY	0.01813	0.01470	-0.01026			2PY	-0.02440	0.00239	-0.01723	0.00965

		2PZ	0.09527	0.07927	-0.05571			2PZ	0.13813	-0.01590	0.10933	-0.00978
		3S	-0.00180	0.00505	-0.00774			3S	-0.00380	-0.00962	0.01510	0.06421
		3PX	0.00516	0.00964	-0.00514			3PX	0.01465	-0.01091	0.00789	0.00514
		3PY	0.01313	0.01311	-0.01060			3PY	-0.01857	0.00047	-0.01652	-0.00710
		3PZ	0.07197	0.07429	-0.05222			3PZ	0.11115	-0.01055	0.10887	-0.01470
		4XX	-0.00203	0.00024	-0.00036			4XX	0.00307	-0.00030	-0.00069	0.07083
		4YY	0.00315	0.00002	0.00020			4YY	0.00025	-0.00001	0.00021	-0.00073
		4ZZ	-0.00117	-0.00030	0.00009			4ZZ	-0.00351	-0.00014	0.00048	0.00010
		4XY	-0.00154	0.00033	-0.00024			4XY	-0.00301	-0.00018	0.00052	0.00017
		4XZ	-0.01333	0.00170	-0.00200			4XZ	0.01600	0.00053	-0.00351	0.00021
		4YZ	0.00991	0.00007	0.00068			4YZ	-0.00052	0.00019	-0.00103	-0.00209
3	C	1S	0.00017	-0.00046	0.00034	3	C	1S	0.00041	-0.00080	-0.00079	-0.00052
		2S	0.00035	0.00063	-0.00042			2S	0.00051	0.00049	0.00095	-0.00217
		2PX	0.02431	-0.00288	0.00315			2PX	0.02905	0.00248	-0.00272	0.00230
		2PY	0.04897	-0.00240	0.00443			2PY	-0.04724	0.00032	0.01070	0.00258
		2PZ	0.27413	-0.00905	0.02091			2PZ	0.27505	0.00298	-0.03882	0.00975
		3S	-0.00595	0.00655	-0.00318			3S	-0.01276	0.02152	0.01125	-0.02691
		3PX	0.01994	-0.00759	0.00079			3PX	0.01824	0.00426	-0.00295	0.03691
		3PY	0.03495	-0.00270	-0.00447			3PY	-0.02906	0.04171	-0.00779	0.00943
		3PZ	0.21244	-0.01357	0.02469			3PZ	0.21278	-0.00063	-0.04509	0.04559
		4XX	0.00118	0.00191	-0.00127			4XX	-0.00115	0.00057	-0.00152	-0.03884
		4YY	0.00022	0.00006	-0.00017			4YY	0.00054	-0.00063	0.00162	-0.00068
		4ZZ	-0.00126	-0.00205	0.00150			4ZZ	0.00088	-0.00020	-0.00022	0.00051
		4XY	0.00127	0.00185	-0.00134			4XY	0.00086	0.00001	0.00057	-0.00047
		4XZ	0.00780	0.01256	-0.00863			4XZ	-0.00818	0.00151	-0.01258	0.00057
		4YZ	0.00011	0.00012	-0.00039			4YZ	-0.00252	0.00112	-0.00886	-0.00770
4	C	1S	0.00033	0.00067	-0.00042	4	C	1S	0.00084	0.00011	0.00154	-0.00534
		2S	-0.00076	-0.00149	0.00068			2S	-0.00210	-0.00166	-0.00294	0.00133
		2PX	0.01327	0.00942	-0.00660			2PX	0.00875	-0.00147	0.00935	-0.00427
		2PY	0.02543	0.01646	-0.01226			2PY	-0.01870	0.00148	-0.02131	0.00521
		2PZ	0.13995	0.08737	-0.06379			2PZ	0.09958	-0.01470	0.09836	-0.01436
		3S	-0.00106	-0.00460	0.00793			3S	-0.00151	0.02600	-0.02481	0.05688
		3PX	0.00524	0.00692	-0.00837			3PX	0.00907	-0.00994	0.01993	0.01238
		3PY	0.01585	0.01416	-0.01743			3PY	0.00083	0.01404	-0.02590	0.00142
		3PZ	0.10306	0.09023	-0.06912			3PZ	0.06827	-0.00890	0.10495	-0.00366
		4XX	-0.00179	0.00032	-0.00025			4XX	0.00119	0.00009	-0.00017	0.06965
		4YY	-0.00289	-0.00018	-0.00005			4YY	-0.00448	0.00025	0.00048	-0.00008
		4ZZ	0.00472	-0.00006	0.00031			4ZZ	0.00339	-0.00012	-0.00031	0.00068
		4XY	-0.00304	0.00020	-0.00022			4XY	0.00090	0.00018	0.00036	-0.00040
		4XZ	-0.01221	0.00091	-0.00114			4XZ	0.00577	0.00008	-0.00111	0.00051
		4YZ	-0.00855	-0.00020	-0.00056			4YZ	0.01455	0.00032	-0.00219	-0.00075
5	C	1S	-0.00012	-0.00033	0.00019	5	C	1S	-0.00031	-0.00011	-0.00075	-0.00135
		2S	0.00014	0.00063	-0.00035			2S	0.00052	0.00079	0.00119	-0.00077
		2PX	-0.01426	-0.00218	0.00116			2PX	-0.01963	0.00057	0.00137	0.00199

		2PY	-0.02930	-0.00208	0.00096			2PY	0.03174	-0.00022	0.00248	0.00202
		2PZ	-0.15849	-0.01125	0.00530			2PZ	-0.17195	0.00246	-0.00542	0.00154
		3S	0.00311	0.00242	-0.00163			3S	0.00621	-0.00957	0.01190	-0.00054
		3PX	-0.01424	-0.00328	0.00051			3PX	-0.00956	0.00292	0.00249	-0.00337
		3PY	-0.02436	-0.00078	0.00262			3PY	0.02456	-0.00661	0.00595	0.00512
		3PZ	-0.13827	-0.01070	0.00494			3PZ	-0.13595	-0.00057	0.00102	-0.00412
		4XX	-0.00136	-0.00098	0.00073			4XX	0.00221	-0.00037	0.00198	0.00072
		4YY	0.00295	0.00117	-0.00093			4YY	0.00113	-0.00013	-0.00022	0.00108
		4ZZ	-0.00162	-0.00028	0.00022			4ZZ	-0.00342	0.00028	-0.00184	-0.00034
		4XY	-0.00089	-0.00089	0.00067			4XY	-0.00227	0.00009	-0.00155	-0.00108
		4XZ	-0.00938	-0.00649	0.00492			4XZ	0.01057	-0.00128	0.00898	-0.00107
		4YZ	0.00924	0.00380	-0.00294			4YZ	-0.00336	-0.00018	0.00056	0.00530
6	C	1S	0.00011	0.00001	0.00002	6	C	1S	0.00028	-0.00009	-0.00002	0.00018
		2S	-0.00018	-0.00007	-0.00006			2S	-0.00045	-0.00018	0.00031	-0.00018
		2PX	-0.01882	-0.00775	0.00586			2PX	-0.02671	0.00202	-0.01402	0.00004
		2PY	-0.04046	-0.01666	0.01247			2PY	0.03872	-0.00303	0.02098	-0.00826
		2PZ	-0.22204	-0.09031	0.06780			2PZ	-0.22348	0.01645	-0.11829	0.01250
		3S	-0.00016	0.00036	0.00032			3S	-0.00004	0.00337	-0.00436	-0.07057
		3PX	-0.01063	-0.00762	0.00613			3PX	-0.01653	0.00719	-0.01458	0.00237
		3PY	-0.02406	-0.01377	0.01297			3PY	0.02011	-0.00499	0.01928	-0.00186
		3PZ	-0.13584	-0.08167	0.06435			3PZ	-0.13698	0.01479	-0.11313	0.01007
		4XX	0.00315	0.00035	-0.00020			4XX	-0.00322	0.00013	-0.00041	-0.06868
		4YY	-0.00057	-0.00028	0.00026			4YY	0.00376	-0.00016	0.00031	-0.00018
		4ZZ	-0.00252	-0.00007	-0.00005			4ZZ	-0.00038	-0.00007	0.00007	0.00007
		4XY	0.00361	0.00030	-0.00018			4XY	0.00146	-0.00014	0.00020	-0.00005
		4XZ	0.02075	0.00230	-0.00137			4XZ	-0.01679	0.00034	-0.00207	-0.00003
		4YZ	-0.00198	-0.00087	0.00079			4YZ	-0.01289	0.00019	-0.00134	-0.00115
7	H	1S	0.00027	0.00007	-0.00001	7	H	1S	0.00070	0.00011	0.00017	-0.00080
		2S	0.00054	0.00008	0.00041			2S	0.00139	0.00114	0.00099	0.00004
8	H	1S	-0.00010	0.00028	-0.00025	8	H	1S	-0.00005	0.00002	0.00094	0.00101
		2S	0.00011	-0.00109	0.00108			2S	0.00085	-0.00002	-0.00643	0.00066
9	H	1S	-0.00059	-0.00077	0.00030	9	H	1S	-0.00152	0.00006	-0.00168	-0.00514
		2S	0.00180	0.00248	0.00146			2S	0.00593	0.00333	-0.00179	-0.00136
10	H	1S	-0.00010	-0.00024	0.00014	10	H	1S	-0.00010	-0.00040	-0.00060	0.00278
		2S	-0.00043	-0.00090	0.00009			2S	-0.00112	-0.00259	-0.00063	-0.00099
11	O	1S	0.00002	-0.00001	0.00000	11	O	1S	-0.00011	-0.00003	-0.00011	-0.00402
		2S	0.00007	0.00000	0.00005			2S	0.00044	-0.00012	0.00009	-0.00014
		2PX	0.02250	0.00422	-0.00308			2PX	0.03152	-0.00105	0.00747	-0.00010
		2PY	0.04843	0.00940	-0.00665			2PY	-0.04606	0.00155	-0.01135	0.00440
		2PZ	0.26557	0.05088	-0.03626			2PZ	0.26758	-0.00933	0.06372	-0.00682
		3S	-0.00062	0.00027	-0.00026			3S	-0.00078	0.00107	0.00113	0.03734
		3PX	0.01845	0.00383	-0.00289			3PX	0.02497	-0.00119	0.00730	0.00268
		3PY	0.03912	0.00866	-0.00655			3PY	-0.03753	0.00218	-0.01062	0.00429
		3PZ	0.21534	0.04721	-0.03435			3PZ	0.21689	-0.00871	0.06062	-0.00548

		4XX	0.00012	0.00037	-0.00029			4XX	-0.00096	0.00003	-0.00085	0.03576
		4YY	0.00245	0.00040	-0.00027			4YY	-0.00175	-0.00001	0.00007	-0.00063
		4ZZ	-0.00248	-0.00077	0.00057			4ZZ	0.00277	-0.00017	0.00061	0.00002
		4XY	0.00080	0.00058	-0.00043			4XY	0.00151	-0.00005	0.00067	0.00025
		4XZ	0.00059	0.00245	-0.00196			4XZ	-0.00441	0.00052	-0.00381	0.00045
		4YZ	0.00739	0.00118	-0.00079			4YZ	0.00582	0.00003	-0.00046	-0.00229
12	C	1S	-0.00003	-0.00005	0.00004	12	C	1S	0.00010	-0.00002	0.00012	-0.00032
		2S	0.00007	0.00010	-0.00006			2S	-0.00027	-0.00009	-0.00020	0.00005
		2PX	-0.00291	0.00021	-0.00022			2PX	-0.00438	-0.00014	0.00020	-0.00023
		2PY	-0.00599	0.00065	-0.00064			2PY	0.00550	0.00007	-0.00065	-0.00001
		2PZ	-0.03293	0.00345	-0.00334			2PZ	-0.03269	-0.00044	0.00438	-0.00035
		3S	0.00006	0.00026	-0.00021			3S	-0.00044	-0.00003	-0.00042	0.00289
		3PX	0.00246	0.00179	-0.00150			3PX	0.00374	0.00010	0.00242	-0.00013
		3PY	0.00583	0.00412	-0.00329			3PY	-0.00512	0.00105	-0.00571	0.00177
		3PZ	0.03128	0.02238	-0.01792			3PZ	0.03176	-0.00392	0.02945	-0.00330
		4XX	-0.00060	-0.00014	0.00010			4XX	0.00206	-0.00011	0.00056	0.01788
		4YY	-0.00415	-0.00085	0.00062			4YY	0.00274	-0.00012	0.00077	0.00030
		4ZZ	0.00475	0.00097	-0.00070			4ZZ	-0.00481	0.00016	-0.00127	0.00045
		4XY	-0.00183	-0.00037	0.00027			4XY	-0.00280	0.00011	-0.00073	-0.00077
		4XZ	-0.00376	-0.00079	0.00054			4XZ	0.01003	-0.00039	0.00269	-0.00043
		4YZ	-0.01271	-0.00258	0.00187			4YZ	-0.00872	0.00032	-0.00228	0.00158
13	C	1S	0.00001	0.00001	-0.00001	13	C	1S	-0.00006	-0.00001	0.00000	-0.00135
		2S	-0.00005	-0.00004	0.00003			2S	0.00009	-0.00004	0.00009	0.00000
		2PX	-0.00023	-0.00013	0.00009			2PX	-0.00013	0.00005	-0.00029	0.00002
		2PY	-0.00076	-0.00048	0.00036			2PY	0.00096	-0.00008	0.00059	-0.00019
		2PZ	-0.00395	-0.00243	0.00180			2PZ	-0.00410	0.00041	-0.00296	0.00032
		3S	0.00008	-0.00002	0.00009			3S	0.00064	0.00050	-0.00071	-0.00177
		3PX	-0.00195	-0.00064	0.00046			3PX	-0.00239	0.00028	-0.00135	-0.00027
		3PY	-0.00421	-0.00149	0.00115			3PY	0.00439	-0.00003	0.00169	-0.00080
		3PZ	-0.02309	-0.00824	0.00627			3PZ	-0.02318	0.00162	-0.01154	0.00112
		4XX	0.00009	-0.00004	0.00003			4XX	0.00004	-0.00001	0.00009	-0.00688
		4YY	-0.00049	-0.00006	0.00004			4YY	0.00049	0.00000	0.00001	0.00005
		4ZZ	0.00040	0.00010	-0.00008			4ZZ	-0.00055	0.00001	-0.00009	0.00001
		4XY	-0.00002	-0.00007	0.00006			4XY	-0.00022	0.00002	-0.00011	-0.00006
		4XZ	0.00060	-0.00029	0.00025			4XZ	0.00028	-0.00006	0.00048	-0.00006
		4YZ	-0.00150	-0.00018	0.00013			4YZ	-0.00154	0.00001	-0.00002	0.00029
14	H	1S	-0.04180	-0.00594	0.00422	14	H	1S	0.04194	-0.00117	0.00801	0.00000
		2S	-0.08975	-0.02990	0.02336			2S	0.09025	-0.00540	0.03931	0.00474
15	H	1S	0.04186	0.00600	-0.00428	15	H	1S	-0.04213	0.00115	-0.00796	0.02363
		2S	0.08973	0.02985	-0.02326			2S	-0.09045	0.00535	-0.03905	-0.00465
16	H	1S	0.00001	-0.00001	0.00000	16	H	1S	-0.00014	-0.00001	-0.00001	-0.02347
		2S	0.00002	-0.00002	0.00000			2S	-0.00024	-0.00003	0.00006	-0.00002
17	H	1S	0.00109	-0.00111	0.00089	17	H	1S	-0.00098	-0.00017	0.00131	0.00002
		2S	0.02041	0.00429	-0.00315			2S	-0.02039	0.00091	-0.00635	0.00081

18	H	1S	-0.00107	0.00114	-0.00090	18	H	1S	0.00097	0.00017	-0.00130	-0.00373
		2S	-0.02038	-0.00423	0.00310			2S	0.02041	-0.00089	0.00636	-0.00079
19	C	1S	0.00018	0.00145	-0.00052	19	C	1S	0.00058	0.00070	0.00217	0.00381
		2S	-0.00102	-0.00305	0.00102			2S	-0.00279	-0.00109	-0.00545	0.00317
		2PX	-0.00921	-0.01363	0.00989			2PX	-0.00988	0.00500	-0.01836	-0.00634
		2PY	-0.01741	-0.02958	0.01808			2PY	0.01404	-0.01136	0.02329	-0.00985
		2PZ	-0.11036	-0.19576	0.12707			2PZ	-0.11432	0.03135	-0.22459	0.00438
		3S	0.00386	-0.01636	0.01559			3S	0.00762	0.01327	-0.03053	-0.13124
		3PX	-0.00622	-0.02043	0.00473			3PX	0.00102	0.07333	-0.05265	-0.01967
		3PY	-0.00932	-0.03675	0.03582			3PY	0.00496	-0.03154	0.05314	0.04611
		3PZ	-0.07733	-0.20288	0.14492			3PZ	-0.07900	0.04952	-0.25673	-0.00076
		4XX	0.00276	-0.00011	0.00037			4XX	-0.00288	0.00083	0.00060	-0.12990
		4YY	-0.00199	0.00019	-0.00023			4YY	0.00222	-0.00023	-0.00023	0.00143
		4ZZ	-0.00071	0.00010	0.00012			4ZZ	0.00084	0.00001	-0.00049	-0.00058
		4XY	0.00240	-0.00019	0.00003			4XY	0.00181	-0.00001	0.00028	-0.00033
		4XZ	0.01828	-0.00289	0.00330			4XZ	-0.02051	-0.00058	0.00757	0.00053
		4YZ	-0.00953	0.00170	-0.00276			4YZ	-0.00265	0.00058	-0.00031	0.00512
20	C	1S	0.00056	0.00012	-0.00063	20	C	1S	0.00154	0.00189	0.00037	0.00056
		2S	-0.00119	0.00005	0.00248			2S	-0.00278	0.00416	-0.00310	0.00192
		2PX	-0.02168	0.00287	-0.00476			2PX	0.00056	-0.00365	0.00711	0.00369
		2PY	-0.02657	0.00866	-0.00701			2PY	0.00958	0.00237	-0.00565	0.00547
		2PZ	-0.23684	0.05531	-0.06613			2PZ	-0.23711	-0.02052	0.12063	0.00404
		3S	-0.00448	-0.00180	-0.01119			3S	-0.01503	-0.09246	0.01695	0.06604
		3PX	-0.01734	0.01585	-0.01182			3PX	-0.00300	0.03486	-0.04062	-0.06639
		3PY	-0.02338	0.00388	0.01097			3PY	0.00785	-0.01757	-0.00122	0.02463
		3PZ	-0.19647	0.06800	-0.08525			3PZ	-0.19945	-0.04001	0.15299	0.00269
		4XX	-0.00031	-0.00270	0.00143			4XX	0.00015	0.00043	-0.00162	0.06536
		4YY	0.00143	0.00203	-0.00156			4YY	0.00113	0.00042	0.00262	-0.00072
		4ZZ	-0.00095	0.00094	-0.00022			4ZZ	-0.00069	0.00048	-0.00083	0.00312
		4XY	0.00031	-0.00003	0.00020			4XY	-0.00033	0.00024	-0.00102	-0.00014
		4XZ	-0.00292	-0.01712	0.01000			4XZ	0.00654	-0.00418	0.02038	-0.00031
		4YZ	0.00604	0.00727	-0.00535			4YZ	-0.00277	0.00143	0.00249	0.01021
21	H	1S	0.00303	-0.00123	0.00116	21	H	1S	0.00770	-0.00320	-0.00265	0.00380
		2S	0.00369	-0.00424	0.01033			2S	0.00975	0.03836	-0.03563	-0.00681
22	H	1S	0.00014	0.00536	-0.00258	22	H	1S	0.00176	-0.00265	0.01234	0.02153
		2S	0.00271	0.01082	-0.01659			2S	0.00643	-0.00097	0.03461	0.00707
23	C	1S	0.00006	0.00002	-0.00094	23	C	1S	0.00015	-0.00128	0.00007	0.03952
		2S	0.00063	0.00148	-0.00006			2S	0.00135	0.00026	0.00598	0.00214
		2PX	0.00289	0.02212	-0.01297			2PX	-0.00235	0.00649	-0.02692	-0.00325
		2PY	0.00376	0.00441	-0.00035			2PY	0.00010	-0.00890	0.03680	-0.02853
		2PZ	0.02968	0.25443	-0.13226			2PZ	0.04414	-0.03144	0.23559	0.02443
		3S	-0.00690	-0.00776	0.03277			3S	-0.01301	0.03585	-0.04928	0.13771
		3PX	0.00403	0.03592	-0.01968			3PX	0.00112	-0.00595	-0.06115	-0.02243
		3PY	0.00788	0.00651	-0.02320			3PY	-0.01270	-0.00552	-0.00403	-0.03797

		3PZ	0.01888	0.26858	-0.14808			3PZ	0.03272	-0.02533	0.27603	0.04637
		4XX	-0.00226	0.00166	-0.00080			4XX	0.00009	0.00243	-0.00022	0.17208
		4YY	0.00010	-0.00009	-0.00029			4YY	-0.00041	0.00357	-0.00128	0.00381
		4ZZ	0.00229	-0.00111	0.00115			4ZZ	0.00071	-0.00606	0.00207	0.00337
		4XY	-0.00153	0.00047	-0.00069			4XY	-0.00010	-0.00388	0.00186	-0.00613
		4XZ	-0.01502	0.00729	-0.00692			4XZ	0.01252	-0.00768	-0.00683	-0.00273
		4YZ	0.00099	-0.00117	-0.00262			4YZ	0.00803	0.01443	-0.01250	-0.01462
24	C	1S	0.00151	-0.00021	-0.00179	24	C	1S	0.00360	-0.00039	-0.00070	0.00836
		2S	-0.00317	0.00109	0.00443			2S	-0.00779	-0.00017	0.00199	0.00091
		2PX	0.00458	-0.00751	0.00126			2PX	-0.00680	-0.03328	0.03316	-0.00205
		2PY	-0.00080	0.00195	-0.00190			2PY	0.02468	0.03632	-0.03555	-0.01667
		2PZ	0.09891	-0.05334	0.08891			2PZ	0.08955	0.20912	-0.17445	0.01441
		3S	-0.00980	0.00457	0.00666			3S	-0.02227	0.00740	0.02906	0.11093
		3PX	0.01612	-0.00755	-0.00646			3PX	-0.01752	-0.04532	0.06612	-0.00801
		3PY	0.00790	0.00872	-0.03810			3PY	-0.01253	0.06105	-0.08065	-0.00898
		3PZ	0.07614	-0.06535	0.11845			3PZ	0.07222	0.24471	-0.21142	0.02724
		4XX	0.00003	0.00252	-0.00114			4XX	-0.00028	0.00152	0.00112	0.14087
		4YY	0.00007	0.00033	-0.00076			4YY	-0.00025	-0.00077	-0.00347	0.00259
		4ZZ	0.00017	-0.00270	0.00137			4ZZ	0.00109	-0.00102	0.00315	-0.00369
		4XY	0.00029	0.00124	-0.00029			4XY	0.00094	-0.00047	0.00100	0.00107
		4XZ	-0.00106	0.01587	-0.00633			4XZ	0.00147	-0.00461	-0.00327	0.00081
		4YZ	0.00233	0.01049	-0.00577			4YZ	-0.00206	-0.00045	-0.01445	-0.00948
25	C	1S	-0.00125	-0.00085	-0.00557	25	C	1S	-0.00307	-0.00152	0.00293	-0.01301
		2S	0.00262	0.00133	0.01041			2S	0.00662	-0.00017	-0.01290	0.00165
		2PX	0.01320	-0.01705	-0.01014			2PX	-0.02495	0.01958	0.01603	0.00356
		2PY	-0.00115	-0.00145	0.00231			2PY	0.01590	-0.02152	-0.00713	0.04048
		2PZ	0.10587	-0.10834	0.05246			2PZ	0.10067	-0.16131	-0.07976	-0.03488
		3S	0.00745	0.00941	0.05540			3S	0.01718	0.04576	0.02248	-0.25182
		3PX	0.00514	-0.01447	-0.01688			3PX	-0.00648	0.06052	0.01241	-0.06229
		3PY	0.00141	-0.01015	0.00332			3PY	0.01693	-0.01935	0.02611	-0.00055
		3PZ	0.09086	-0.12437	0.05451			3PZ	0.09163	-0.22748	-0.09380	-0.07261
		4XX	-0.00046	0.00253	-0.00149			4XX	-0.00014	-0.00101	0.00650	-0.34824
		4YY	-0.00004	-0.00044	-0.00034			4YY	0.00037	-0.00095	-0.00179	-0.00090
		4ZZ	0.00021	-0.00235	0.00092			4ZZ	-0.00102	0.00105	-0.00516	0.00443
		4XY	-0.00021	-0.00115	-0.00114			4XY	-0.00085	0.00097	-0.00291	-0.00191
		4XZ	-0.00127	0.01636	-0.00896			4XZ	-0.00170	0.00875	-0.01973	-0.00133
		4YZ	-0.00243	-0.01096	0.00610			4YZ	0.00158	0.00459	-0.00062	-0.00386
26	C	1S	-0.00069	-0.00014	-0.00107	26	C	1S	-0.00156	-0.00281	-0.00199	0.00575
		2S	0.00083	-0.00175	-0.00610			2S	0.00206	0.00593	0.00340	0.00474
		2PX	0.00270	-0.01555	0.00695			2PX	-0.00359	0.02205	0.02006	-0.00817
		2PY	0.00069	-0.00093	0.00240			2PY	-0.00521	-0.01703	-0.01413	0.01587
		2PZ	0.00284	-0.17404	0.04348			2PZ	-0.00482	-0.08602	-0.07557	-0.02618
		3S	0.01091	0.01547	0.06502			3S	0.02332	0.01973	0.01415	-0.19923
		3PX	0.00941	-0.02721	-0.02692			3PX	-0.01977	0.03654	0.01923	-0.04767

		3PY	-0.00310	0.00389	0.05434			3PY	-0.00687	-0.02689	-0.00685	0.02863
		3PZ	0.01262	-0.23369	0.05888			3PZ	0.00176	-0.11108	-0.10770	-0.03351
		4XX	0.00128	-0.00101	0.00231			4XX	0.00193	0.00482	-0.00500	-0.27254
		4YY	-0.00028	-0.00064	-0.00237			4YY	-0.00071	-0.00186	0.00005	-0.00018
		4ZZ	-0.00123	0.00120	-0.00171			4ZZ	-0.00172	-0.00349	0.00440	0.00046
		4XY	-0.00036	0.00009	-0.00306			4XY	-0.00062	-0.00182	0.00334	0.00066
		4XZ	0.00727	-0.00851	0.00882			4XZ	-0.00661	-0.01663	0.01928	-0.00078
		4YZ	-0.00368	0.00838	-0.00608			4YZ	-0.00125	-0.00328	0.00194	-0.00332
27	H	1S	-0.00139	-0.00051	-0.00223	27	H	1S	-0.00350	0.00014	0.00133	-0.00429
		2S	0.00619	0.00797	-0.02571			2S	0.01285	-0.01924	0.04196	-0.00087
28	C	1S	0.00052	0.00224	0.00665	28	C	1S	0.00129	-0.00650	-0.00837	0.00568
		2S	-0.00113	-0.00496	-0.01428			2S	-0.00288	0.00673	0.00739	0.01303
		2PX	-0.00072	-0.00889	0.02611			2PX	0.00660	0.00678	0.04758	-0.01185
		2PY	0.00074	0.00347	0.02018			2PY	-0.00185	0.00687	-0.03896	-0.06900
		2PZ	0.00819	-0.17226	0.08538			2PZ	-0.02426	0.16537	-0.13499	0.04119
		3S	-0.00499	-0.02558	-0.08644			3S	-0.00745	0.05407	0.09027	0.09869
		3PX	-0.00346	-0.00988	0.01922			3PX	0.00733	0.02762	0.10369	-0.13429
		3PY	-0.00054	0.01188	0.02842			3PY	0.00932	0.05605	-0.03854	-0.15158
		3PZ	0.01229	-0.20013	0.12094			3PZ	-0.01484	0.20721	-0.22045	0.00784
		4XX	0.00125	-0.00134	0.00313			4XX	0.00153	-0.00503	-0.00062	0.09877
		4YY	0.00017	-0.00137	-0.00280			4YY	-0.00196	-0.00385	0.00272	-0.00383
		4ZZ	-0.00134	0.00274	-0.00074			4ZZ	0.00082	0.00664	-0.00526	0.00701
		4XY	0.00031	-0.00055	0.00215			4XY	0.00020	0.00530	-0.00174	0.00214
		4XZ	0.00769	-0.01403	0.00599			4XZ	-0.00458	0.02084	0.00085	-0.00050
		4YZ	0.00337	-0.00753	0.00575			4YZ	-0.00731	-0.00425	0.02043	0.01924
29	H	1S	0.00054	-0.00241	-0.00522	29	H	1S	0.00144	-0.00529	-0.00699	0.01280
		2S	-0.00148	-0.00071	-0.02476			2S	-0.00474	-0.00754	0.03195	0.00638
30	C	1S	0.00019	-0.00365	-0.01352	30	C	1S	0.00022	0.00370	0.00405	0.00789
		2S	-0.00068	0.00377	0.01181			2S	-0.00032	-0.00728	-0.00965	-0.00414
		2PX	-0.01018	-0.00154	-0.07205			2PX	0.01402	0.01637	-0.03740	0.01046
		2PY	-0.00215	0.00205	-0.00584			2PY	-0.01382	-0.00899	0.04894	-0.00157
		2PZ	-0.10915	0.19268	-0.12303			2PZ	-0.09606	-0.16250	0.24195	-0.01290
		3S	0.00258	0.03450	0.13541			3S	-0.00183	-0.05848	-0.02942	0.04855
		3PX	-0.00985	0.00557	-0.12283			3PX	0.01003	0.02898	-0.04855	0.04941
		3PY	-0.00420	0.02686	0.07434			3PY	-0.00382	-0.00608	0.06072	-0.01407
		3PZ	-0.09860	0.24550	-0.17494			3PZ	-0.08727	-0.18180	0.33787	-0.00582
		4XX	0.00053	-0.00437	-0.00186			4XX	0.00038	-0.00175	-0.00099	0.10024
		4YY	-0.00002	-0.00043	-0.00222			4YY	0.00005	-0.00350	0.00076	-0.00315
		4ZZ	-0.00045	0.00361	-0.00118			4ZZ	-0.00039	0.00517	0.00009	-0.00232
		4XY	-0.00012	-0.00145	-0.00296			4XY	-0.00027	0.00069	-0.00145	0.00620
		4XZ	0.00332	-0.02264	0.00560			4XZ	-0.00030	0.00786	0.00495	0.00680
		4YZ	-0.00021	0.00419	0.00281			4YZ	0.00145	-0.01031	0.00453	0.01257
31	H	1S	-0.00089	-0.00204	-0.00942	31	H	1S	-0.00197	-0.00400	-0.00108	-0.01107
		2S	-0.00211	0.00084	0.00363			2S	-0.00330	-0.01076	-0.01008	0.00618

32	H	1S	0.00066	-0.00329	-0.00997	32	H	1S	0.00033	-0.00591	-0.00451	0.02185
		2S	0.00129	-0.00749	-0.01457			2S	-0.00053	-0.01169	-0.00385	0.00959
33	S	1S	-0.00002	-0.00471	-0.01220	33	S	1S	0.00002	-0.00754	-0.00643	0.01718
		2S	0.00012	0.02104	0.05506			2S	-0.00014	0.03388	0.02937	0.00980
		2PX	-0.00027	-0.01127	-0.00922			2PX	0.00147	0.00789	-0.00440	-0.04341
		2PY	-0.00056	-0.01472	-0.03566			2PY	-0.00015	-0.03562	-0.01951	0.01434
		2PZ	0.00045	-0.07506	-0.03022			2PZ	0.00163	-0.08576	-0.01315	0.01829
		3S	-0.00007	-0.05473	-0.14033			3S	0.00007	-0.08720	-0.07305	-0.02876
		3PX	0.00107	0.03063	0.02925			3PX	-0.00462	-0.01997	0.01362	0.11505
		3PY	0.00161	0.04426	0.10870			3PY	0.00057	0.10443	0.05928	-0.03804
		3PZ	0.00129	0.20855	0.09041			3PZ	-0.00314	0.23985	0.03658	-0.06061
		4S	-0.00208	-0.09770	-0.32402			4S	0.00093	-0.16931	-0.18193	0.07246
		4PX	-0.00583	0.05991	-0.04455			4PX	0.00211	-0.04182	0.05652	0.26158
		4PY	0.00206	0.05361	0.15672			4PY	-0.00425	0.15095	0.07473	-0.18969
		4PZ	-0.03423	0.43295	0.07730			4PZ	-0.03468	0.48398	0.12321	-0.00963
		5XX	-0.00243	0.01695	0.01899			5XX	-0.00076	0.01071	-0.00214	0.37815
		5YY	0.00011	-0.00637	-0.01475			5YY	-0.00113	0.01912	-0.00211	-0.00467
		5ZZ	0.00227	-0.00831	-0.00033			5ZZ	0.00183	-0.02627	0.00676	0.01442
		5XY	-0.00072	0.01069	0.01361			5XY	0.00097	-0.03193	-0.00844	-0.01101
		5XZ	-0.01801	0.07624	-0.02282			5XZ	0.00293	-0.03776	0.02869	0.01049
		5YZ	-0.00712	0.05158	-0.00175			5YZ	-0.00504	0.07833	-0.01152	-0.02154
34	C	1S	-0.00483	0.02885	-0.00898	34	C	1S	-0.00108	0.02954	-0.00862	0.06170
		2S	0.00838	-0.05108	0.00371			2S	-0.00052	-0.05440	0.01809	0.02605
		2PX	0.01429	-0.03288	0.02242			2PX	0.00342	-0.00980	-0.01171	-0.02106
		2PY	0.01311	-0.07200	0.02505			2PY	0.00624	-0.07157	0.01873	-0.01116
		2PZ	-0.01710	0.07233	-0.03803			2PZ	-0.00528	0.07699	-0.03194	-0.07310
		3S	0.04002	-0.29182	0.10625			3S	0.01714	-0.30112	0.06532	0.08451
		3PX	0.00009	-0.02718	-0.01680			3PX	0.00113	-0.03101	0.07013	-0.33026
		3PY	0.02059	-0.13563	0.07067			3PY	0.01793	-0.12782	-0.02126	-0.01456
		3PZ	-0.01496	0.08399	-0.10852			3PZ	-0.00891	0.08385	-0.04866	-0.20273
		4XX	-0.00167	0.00544	-0.00364			4XX	-0.00039	0.00257	-0.00037	0.19840
		4YY	0.00050	0.00447	0.00283			4YY	-0.00055	0.00791	0.00171	0.00206
		4ZZ	0.00098	-0.00735	-0.00389			4ZZ	0.00007	-0.00851	-0.00108	0.00706
		4XY	-0.00027	0.00356	-0.00170			4XY	-0.00026	-0.00149	0.00473	0.00158
		4XZ	0.00023	-0.00149	0.00473			4XZ	-0.00002	0.00171	-0.00405	-0.00086
		4YZ	-0.00087	0.00057	-0.00017			4YZ	-0.00027	-0.00201	0.00148	0.00405
35	H	1S	-0.00885	0.02188	-0.01781	35	H	1S	-0.00057	-0.01998	0.00509	-0.00303
		2S	-0.01840	0.07732	-0.06716			2S	-0.00303	0.02358	0.01906	-0.00570
36	H	1S	0.00132	0.01192	0.01467	36	H	1S	-0.00341	0.01709	0.01860	0.01237
		2S	0.00407	0.01036	0.06840			2S	0.00548	0.02853	0.02848	0.00889
37	H	1S	0.00161	-0.01766	-0.00106	37	H	1S	0.00004	0.01871	-0.02266	-0.05786
		2S	-0.00373	0.02043	0.01660			2S	0.00458	0.06807	-0.11525	0.01399
38	C	1S	0.00524	-0.03407	-0.00244	38	C	1S	0.00080	-0.03746	0.00441	0.01913
		2S	-0.00642	0.05293	0.00801			2S	0.00046	0.05919	-0.00777	-0.01681

		2PX	-0.01607	0.06251	0.00858			2PX	-0.00247	-0.02133	0.01245	0.01780
		2PY	-0.01442	0.09909	0.01913			2PY	-0.00802	0.14068	0.00705	0.00503
		2PZ	-0.01741	0.11085	0.04423			2PZ	-0.00422	0.11471	0.01248	0.05701
		3S	-0.05907	0.31650	-0.10315			3S	-0.01120	0.32436	-0.12947	0.01870
		3PX	0.01071	0.05698	0.13444			3PX	0.00159	-0.01542	-0.12782	0.27130
		3PY	-0.02149	0.17572	0.04022			3PY	-0.02225	0.24054	0.12739	0.01017
		3PZ	-0.01603	0.19147	0.13987			3PZ	-0.00411	0.21501	0.04760	0.13290
		4XX	0.00121	-0.00750	-0.00218			4XX	0.00049	-0.00380	0.00034	-0.00616
		4YY	-0.00010	-0.00362	-0.00091			4YY	0.00035	-0.01136	-0.00520	-0.00330
		4ZZ	-0.00085	0.00560	-0.00102			4ZZ	-0.00012	0.00814	0.00058	-0.00078
		4XY	-0.00004	-0.00528	-0.00603			4XY	0.00013	0.00754	0.00156	0.00079
		4XZ	-0.00050	-0.00840	-0.01976			4XZ	0.00003	0.00876	0.00713	-0.00651
		4YZ	-0.00099	-0.00205	-0.00751			4YZ	-0.00046	-0.00701	-0.00749	-0.01169
39	H	1S	-0.00086	0.03028	0.03838	39	H	1S	0.00312	-0.00209	-0.00339	0.01106
		2S	0.00598	0.05570	0.18500			2S	-0.00760	0.04463	0.05093	-0.03002
40	H	1S	-0.00050	-0.00359	0.01080	40	H	1S	0.00045	0.04074	0.01577	-0.02407
		2S	-0.00183	0.03749	0.04908			2S	0.00373	0.09801	0.08599	-0.02261
41	C	1S	-0.00205	0.00687	-0.00290	41	C	1S	0.00002	0.00641	-0.00622	-0.15966
		2S	0.00332	-0.02050	-0.01018			2S	0.00071	-0.02370	-0.00111	0.00023
		2PX	0.01128	-0.03634	0.01063			2PX	-0.00023	0.04272	-0.00683	0.00422
		2PY	0.00361	0.02749	0.08192			2PY	0.00205	0.04456	0.06339	-0.00413
		2PZ	0.00494	0.10809	0.26321			2PZ	0.00141	0.17065	0.13480	-0.07948
		3S	0.02165	-0.03160	0.10189			3S	-0.00393	-0.00575	0.13685	-0.18482
		3PX	0.02753	-0.02383	0.15330			3PX	0.00887	0.01132	-0.15088	0.00586
		3PY	0.00827	0.04501	0.10420			3PY	0.00156	0.09136	0.14015	0.01815
		3PZ	0.00194	0.12662	0.33434			3PZ	0.00174	0.19797	0.15204	-0.10552
		4XX	0.00057	0.00070	0.00155			4XX	0.00019	-0.00278	-0.00013	-0.25320
		4YY	-0.00037	-0.00139	-0.00285			4YY	-0.00012	0.00354	0.00031	0.00046
		4ZZ	-0.00019	-0.00072	-0.00152			4ZZ	0.00017	-0.00286	-0.00244	-0.00111
		4XY	-0.00050	0.00538	0.00419			4XY	0.00029	-0.00705	-0.00382	0.00161
		4XZ	-0.00081	0.00903	0.01115			4XZ	0.00015	-0.01097	-0.00442	0.00071
		4YZ	-0.00007	-0.00094	-0.00068			4YZ	-0.00008	0.00309	0.00141	0.00430
42	C	1S	0.00000	0.00099	0.00111	42	C	1S	0.00037	-0.00333	0.00025	-0.00405
		2S	-0.00045	-0.00083	-0.00463			2S	-0.00059	0.00673	-0.00183	-0.00426
		2PX	-0.00065	-0.00542	-0.00879			2PX	0.00065	-0.00517	-0.00219	0.00610
		2PY	0.00245	-0.02406	-0.04511			2PY	-0.00036	-0.02496	-0.02859	-0.00196
		2PZ	0.00636	-0.09078	-0.14245			2PZ	0.00285	-0.10980	-0.06176	0.04731
		3S	0.00658	-0.02708	0.03520			3S	-0.00258	0.03443	0.03107	0.09021
		3PX	-0.00893	0.00463	-0.04396			3PX	-0.00328	0.02477	0.05125	0.04474
		3PY	-0.00127	-0.02759	-0.10467			3PY	0.00168	-0.03729	-0.02580	0.00318
		3PZ	0.00518	-0.10884	-0.18272			3PZ	0.00128	-0.12467	-0.08844	0.04686
		4XX	0.00026	-0.00101	0.00135			4XX	0.00002	-0.00042	-0.00005	0.14287
		4YY	-0.00036	-0.00046	-0.00505			4YY	0.00004	0.00791	0.00663	-0.00020
		4ZZ	0.00005	0.00161	0.00425			4ZZ	-0.00001	-0.00720	-0.00663	-0.00832

		4XY	0.00000	0.00225	0.00450			4XY	-0.00009	0.00016	-0.00119	0.00781
		4XZ	0.00019	0.00531	0.01558			4XZ	0.00005	-0.00778	-0.00456	0.00193
		4YZ	-0.00015	-0.00436	-0.01016			4YZ	0.00010	0.00906	0.00725	0.00449
43	C	1S	0.00061	-0.00339	0.00116	43	C	1S	-0.00020	0.00113	0.00030	-0.01016
		2S	-0.00209	0.00692	-0.00227			2S	0.00065	-0.00146	-0.00393	-0.00165
		2PX	-0.00276	0.00604	-0.00842			2PX	-0.00095	-0.00145	0.00034	0.00489
		2PY	-0.00082	-0.00849	-0.03910			2PY	0.00059	-0.04823	-0.02650	0.00497
		2PZ	0.00812	-0.08001	-0.12695			2PZ	0.00258	-0.12530	-0.07193	0.03971
		3S	0.00739	0.02769	0.01417			3S	-0.00228	-0.02123	0.05466	0.06583
		3PX	-0.00476	-0.01534	-0.04437			3PX	0.00263	-0.00694	0.00999	-0.01020
		3PY	0.00699	-0.01168	-0.01587			3PY	0.00283	-0.06386	-0.08836	0.00759
		3PZ	0.00466	-0.08708	-0.17707			3PZ	-0.00019	-0.15374	-0.07859	0.08625
		4XX	0.00029	-0.00102	0.00103			4XX	0.00001	-0.00216	-0.00019	0.08836
		4YY	-0.00008	0.00397	0.00731			4YY	-0.00009	0.00043	-0.00088	0.00037
		4ZZ	-0.00028	-0.00277	-0.00797			4ZZ	0.00004	0.00193	0.00129	0.00100
		4XY	0.00017	0.00123	0.00487			4XY	-0.00011	-0.00337	-0.00390	-0.00206
		4XZ	0.00001	0.00783	0.01583			4XZ	-0.00005	-0.01095	-0.00984	0.00701
		4YZ	0.00027	0.00351	0.01070			4YZ	0.00002	-0.00230	-0.00134	0.01463
44	C	1S	-0.00024	0.00075	-0.00018	44	C	1S	-0.00014	0.00292	-0.00082	0.00022
		2S	0.00077	-0.00287	0.00215			2S	0.00027	-0.00595	0.00400	0.00167
		2PX	0.00138	-0.00449	-0.00254			2PX	-0.00053	0.00363	-0.00694	-0.00416
		2PY	-0.00055	-0.01269	-0.04003			2PY	0.00025	-0.04600	-0.03049	0.01152
		2PZ	-0.00236	-0.03918	-0.13312			2PZ	-0.00075	-0.10209	-0.07807	0.03381
		3S	-0.00738	0.00632	-0.04306			3S	0.00304	-0.03635	-0.04290	0.09236
		3PX	-0.00375	0.00751	-0.02239			3PX	-0.00233	0.01434	0.00091	-0.01317
		3PY	0.00039	-0.01911	-0.03578			3PY	0.00075	-0.05802	-0.05990	0.02335
		3PZ	-0.00142	-0.04797	-0.16514			3PZ	-0.00056	-0.12617	-0.09369	0.04442
		4XX	-0.00007	-0.00006	-0.00130			4XX	0.00002	0.00038	0.00099	0.11235
		4YY	0.00007	-0.00269	-0.00620			4YY	-0.00004	0.00155	0.00037	-0.00135
		4ZZ	-0.00016	0.00307	0.00719			4ZZ	-0.00001	-0.00142	-0.00144	-0.00078
		4XY	0.00022	-0.00279	-0.00511			4XY	-0.00008	0.00506	0.00405	0.00205
		4XZ	0.00042	-0.00802	-0.01499			4XZ	-0.00019	0.01341	0.00947	-0.00547
		4YZ	0.00027	-0.00480	-0.01024			4YZ	0.00003	-0.00002	0.00076	-0.01337
45	H	1S	-0.00057	0.00441	0.00078	45	H	1S	-0.00028	0.00577	0.00056	-0.00073
		2S	-0.00082	0.01451	0.03190			2S	-0.00054	0.02886	0.02253	0.00135
46	C	1S	-0.00051	0.00282	-0.00044	46	C	1S	0.00008	0.00081	-0.00065	-0.01560
		2S	0.00144	-0.00616	0.00298			2S	-0.00010	-0.00276	0.00291	0.00014
		2PX	0.00263	-0.01201	-0.00208			2PX	0.00024	-0.00055	-0.00491	-0.00242
		2PY	0.00018	-0.02115	-0.04742			2PY	-0.00026	-0.02835	-0.02637	0.00868
		2PZ	-0.00136	-0.06792	-0.15361			2PZ	-0.00073	-0.06535	-0.07010	0.04794
		3S	-0.00532	-0.02546	-0.03715			3S	0.00043	-0.00357	-0.04472	0.12317
		3PX	0.00032	-0.02107	-0.01504			3PX	0.00033	-0.00987	0.01828	0.01861
		3PY	-0.00371	-0.01996	-0.07289			3PY	-0.00179	-0.03257	-0.02781	-0.00797
		3PZ	-0.00018	-0.08444	-0.19051			3PZ	0.00058	-0.08027	-0.08936	0.05742

		4XX	0.00000	-0.00057	-0.00086			4XX	0.00002	0.00097	-0.00035	0.15215
		4YY	-0.00028	0.00278	0.00532			4YY	0.00010	-0.00816	-0.00585	-0.00048
		4ZZ	0.00007	-0.00172	-0.00432			4ZZ	-0.00007	0.00746	0.00562	0.00795
		4XY	-0.00004	-0.00133	-0.00452			4XY	0.00001	0.00217	0.00114	-0.00740
		4XZ	0.00053	-0.00833	-0.01603			4XZ	-0.00013	0.00702	0.00444	-0.00194
		4YZ	-0.00015	0.00388	0.00914			4YZ	0.00014	-0.01005	-0.00705	-0.00439
47	H	1S	-0.00074	0.00507	0.00160	47	H	1S	-0.00001	0.00514	-0.00019	0.00877
		2S	0.00140	0.01965	0.03324			2S	-0.00261	0.02008	0.01709	0.00261
48	C	1S	-0.00012	0.00050	-0.00008	48	C	1S	0.00002	0.00047	-0.00067	-0.03255
		2S	0.00009	-0.00143	-0.00158			2S	0.00001	-0.00177	0.00019	-0.00064
		2PX	-0.00037	0.00376	0.00899			2PX	-0.00017	0.00931	0.00610	0.00266
		2PY	-0.00248	0.03825	0.07835			2PY	-0.00117	0.07267	0.05317	-0.00742
		2PZ	-0.00748	0.12006	0.25632			2PZ	-0.00260	0.17652	0.13081	-0.06996
		3S	0.00232	-0.00737	0.01688			3S	-0.00034	-0.00500	0.01571	-0.17717
		3PX	0.00536	0.00258	0.03880			3PX	0.00029	0.00853	-0.02269	-0.01655
		3PY	-0.00328	0.04835	0.09611			3PY	-0.00270	0.09053	0.08262	-0.00635
		3PZ	-0.00569	0.13700	0.31153			3PZ	-0.00151	0.20444	0.15497	-0.08422
		4XX	0.00004	-0.00064	-0.00110			4XX	0.00005	0.00037	0.00028	-0.22121
		4YY	-0.00004	0.00051	0.00001			4YY	-0.00004	-0.00212	-0.00239	-0.00113
		4ZZ	0.00000	-0.00014	0.00086			4ZZ	0.00001	0.00137	0.00180	0.00479
		4XY	-0.00006	-0.00173	-0.00476			4XY	0.00000	0.00361	0.00303	-0.00399
		4XZ	-0.00002	-0.00616	-0.01559			4XZ	0.00001	0.00908	0.00710	-0.00292
		4YZ	-0.00005	0.00096	0.00030			4YZ	0.00000	-0.00267	-0.00308	-0.00954
49	H	1S	-0.00042	0.00079	0.00040	49	H	1S	-0.00028	0.00460	-0.00051	0.00569
		2S	-0.00118	0.00652	-0.00428			2S	-0.00039	0.01441	-0.00750	0.00079
50	H	1S	-0.00105	0.00422	0.00070	50	H	1S	0.00022	0.00090	-0.00118	0.00535
		2S	-0.00246	0.01376	-0.00287			2S	0.00049	0.00650	-0.00911	-0.00195
51	C	1S	-0.00012	0.00012	-0.00027	51	C	1S	-0.00001	0.00008	-0.00008	0.00101
		2S	0.00020	-0.00073	0.00005			2S	0.00008	-0.00084	-0.00051	0.00052
		2PX	0.00042	0.00101	0.00457			2PX	-0.00004	0.00209	0.00174	-0.00163
		2PY	0.00033	0.00938	0.02675			2PY	0.00017	0.01992	0.01853	-0.00093
		2PZ	0.00111	0.03079	0.08678			2PZ	0.00040	0.04903	0.04492	-0.02774
		3S	0.00248	0.00148	0.01223			3S	-0.00047	0.00447	0.01229	-0.06566
		3PX	0.00301	-0.00023	0.01527			3PX	0.00075	0.00050	-0.01550	-0.00379
		3PY	0.00047	0.00885	0.02583			3PY	-0.00025	0.01969	0.02653	-0.00864
		3PZ	0.00052	0.02924	0.08235			3PZ	0.00040	0.04622	0.03984	-0.02222
		4XX	0.00002	0.00073	0.00189			4XX	-0.00001	-0.00091	-0.00055	-0.06472
		4YY	-0.00005	0.00044	0.00066			4YY	-0.00005	0.00542	0.00416	0.00128
		4ZZ	0.00005	-0.00123	-0.00253			4ZZ	0.00006	-0.00456	-0.00347	-0.00555
		4XY	-0.00013	0.00320	0.00754			4XY	0.00006	-0.00524	-0.00443	0.00442
		4XZ	-0.00054	0.01059	0.02421			4XZ	0.00016	-0.01383	-0.01079	0.00575
		4YZ	-0.00001	0.00052	0.00104			4YZ	-0.00008	0.00664	0.00513	0.01532
52	N	1S	-0.00002	0.00008	-0.00003	52	N	1S	0.00001	0.00007	-0.00024	-0.00690
		2S	-0.00012	-0.00004	-0.00037			2S	0.00003	-0.00014	-0.00046	-0.00028

2PX	0.00009	-0.00363	-0.00829	2PX	0.00002	-0.00352	-0.00336	-0.00004
2PY	0.00118	-0.02207	-0.05297	2PY	0.00053	-0.04520	-0.03636	0.00403
2PZ	0.00424	-0.07414	-0.17218	2PZ	0.00151	-0.11134	-0.08829	0.05107
3S	0.00177	-0.00210	0.00554	3S	-0.00056	-0.00063	0.01265	0.12295
3PX	0.00052	-0.00408	-0.00675	3PX	0.00014	-0.00328	-0.00609	0.00795
3PY	0.00084	-0.02128	-0.05175	3PY	0.00032	-0.04367	-0.03409	0.00202
3PZ	0.00298	-0.07013	-0.16911	3PZ	0.00107	-0.10634	-0.08731	0.05132
4XX	-0.00004	-0.00015	-0.00042	4XX	0.00001	0.00011	-0.00017	0.12200
4YY	-0.00003	0.00002	-0.00014	4YY	0.00004	-0.00082	-0.00077	-0.00026
4ZZ	-0.00006	0.00021	0.00025	4ZZ	-0.00001	0.00070	0.00023	0.00054
4XY	0.00007	-0.00056	-0.00102	4XY	-0.00003	0.00091	0.00059	-0.00076
4XZ	0.00025	-0.00180	-0.00329	4XZ	-0.00007	0.00223	0.00145	-0.00073
4YZ	0.00001	-0.00006	-0.00011	4YZ	0.00004	-0.00104	-0.00067	-0.00186
								0.00087

PAG3			HOMO	LUMO	LUMO+1		PAG4			HOMO	LUMO	LUMO+1
1	C	1S	0.00276	0.00129	-0.00080		1	C	1S	0.00308	-0.00098	-0.00143
		2S	-0.00579	-0.00292	0.00183				2S	-0.00647	0.00217	0.00304
		2PX	0.00489	0.00273	-0.00186				2PX	0.01698	-0.00336	-0.00461
		2PY	-0.09799	-0.00650	-0.00307				2PY	0.08853	-0.00641	-0.00328
		2PZ	-0.14398	-0.00135	-0.01448				2PZ	-0.13685	0.00639	-0.00419
		3S	-0.03335	-0.00829	0.00347				3S	-0.03466	0.00811	0.01167
		3PX	0.00201	-0.00278	0.00069				3PX	0.01507	0.00112	0.00134
		3PY	-0.09864	-0.00402	-0.00901				3PY	0.08907	-0.00765	-0.00654
		3PZ	-0.11599	0.00688	-0.02552				3PZ	-0.10672	-0.00014	-0.01163
		4XX	-0.00023	0.00024	-0.00021				4XX	-0.00070	0.00003	0.00001
		4YY	-0.00343	-0.00289	0.00177				4YY	-0.00222	0.00115	0.00188
		4ZZ	0.00419	0.00282	-0.00171				4ZZ	0.00349	-0.00129	-0.00203
		4XY	0.00201	0.00300	-0.00170				4XY	-0.00232	0.00246	0.00343
		4XZ	0.00181	0.00683	-0.00392				4XZ	0.00358	-0.00586	-0.00818
		4YZ	-0.00496	-0.00328	0.00203				4YZ	0.00460	-0.00146	-0.00233
2	C	1S	-0.00062	-0.00079	0.00045		2	C	1S	-0.00081	0.00048	0.00069
		2S	0.00095	0.00174	-0.00125				2S	0.00139	-0.00107	-0.00121
		2PX	-0.00145	-0.00025	0.00044				2PX	-0.00409	0.00191	0.00285
		2PY	0.02555	0.04042	-0.01943				2PY	-0.02451	0.02811	0.03665
		2PZ	0.04636	0.09284	-0.04519				2PZ	0.04971	-0.06954	-0.09144
		3S	0.00969	0.00627	-0.00006				3S	0.00980	-0.00494	-0.01164
		3PX	-0.00486	-0.00318	0.00185				3PX	-0.00794	0.00556	0.00623
		3PY	0.02700	0.03688	-0.01246				3PY	-0.02120	0.02833	0.04603
		3PZ	0.03335	0.08935	-0.03798				3PZ	0.02993	-0.06850	-0.10720
		4XX	0.00046	-0.00006	0.00007				4XX	-0.00049	0.00006	0.00005
		4YY	0.00382	0.00004	0.00096				4YY	0.00579	0.00023	0.00123

		4ZZ	-0.00443	-0.00014	-0.00092			4ZZ	-0.00548	-0.00024	-0.00121
		4XY	0.00659	-0.00055	0.00109			4XY	-0.00521	-0.00020	-0.00058
		4XZ	0.01153	-0.00188	0.00282			4XZ	0.00889	0.00098	0.00225
		4YZ	0.00489	0.00016	0.00098			4YZ	-0.00701	-0.00035	-0.00172
3	C	1S	0.00003	-0.00004	0.00003		3	C	1S	-0.00001	-0.00002	-0.00001
		2S	0.00010	-0.00010	0.00028				2S	-0.00009	-0.00015	-0.00025
		2PX	-0.00058	0.00002	-0.00007				2PX	0.00054	-0.00033	-0.00076
		2PY	0.07230	-0.00652	0.01420				2PY	-0.06506	-0.00627	-0.02051
		2PZ	0.20202	-0.01060	0.03219				2PZ	0.20093	0.01266	0.04921
		3S	-0.00068	0.00198	-0.00390				3S	0.00035	0.00231	0.00266
		3PX	0.00157	-0.00198	0.00517				3PX	-0.00260	-0.00304	-0.00343
		3PY	0.06572	-0.00798	0.00887				3PY	-0.05935	-0.00518	-0.02514
		3PZ	0.16276	-0.01556	0.01561				3PZ	0.16169	0.00584	0.07413
		4XX	0.00006	0.00000	0.00003				4XX	-0.00007	-0.00007	-0.00014
		4YY	-0.00040	0.00074	-0.00089				4YY	0.00010	0.00154	0.00219
		4ZZ	0.00042	-0.00074	0.00086				4ZZ	-0.00010	-0.00147	-0.00207
		4XY	-0.00086	-0.00534	0.00224				4XY	0.00090	-0.00349	-0.00455
		4XZ	-0.00244	-0.01394	0.00593				4XZ	-0.00279	0.01008	0.01291
		4YZ	-0.00052	0.00085	-0.00096				4YZ	-0.00010	-0.00215	-0.00298
4	C	1S	0.00067	0.00069	-0.00029		4	C	1S	0.00076	-0.00058	-0.00083
		2S	-0.00113	-0.00139	0.00066				2S	-0.00122	0.00140	0.00173
		2PX	0.00232	0.00123	-0.00121				2PX	0.00063	0.00054	0.00034
		2PY	0.02580	0.04003	-0.02227				2PY	-0.02478	0.02817	0.03581
		2PZ	0.04753	0.09048	-0.05041				2PZ	0.04752	-0.07046	-0.08992
		3S	-0.00812	-0.00841	0.00452				3S	-0.01076	0.00240	0.00877
		3PX	0.00530	0.00501	-0.00461				3PX	0.00338	-0.00216	-0.00194
		3PY	0.02234	0.04135	-0.02788				3PY	-0.02695	0.02347	0.03689
		3PZ	0.02746	0.09084	-0.05321				3PZ	0.03431	-0.06432	-0.09565
		4XX	-0.00013	0.00004	-0.00001				4XX	-0.00110	-0.00007	-0.00004
		4YY	-0.00470	-0.00003	-0.00101				4YY	-0.00184	0.00000	-0.00063
		4ZZ	0.00499	0.00009	0.00103				4ZZ	0.00313	-0.00008	0.00053
		4XY	0.00613	-0.00024	0.00045				4XY	-0.00632	-0.00055	-0.00132
		4XZ	0.01013	-0.00119	0.00138				4XZ	0.01239	0.00183	0.00399
		4YZ	-0.00559	-0.00006	-0.00119				4YZ	0.00361	-0.00017	0.00058
5	C	1S	-0.00270	-0.00129	0.00077		5	C	1S	-0.00312	0.00100	0.00144
		2S	0.00570	0.00284	-0.00166				2S	0.00646	-0.00229	-0.00306
		2PX	-0.00913	-0.00335	0.00221				2PX	0.00120	0.00147	0.00252
		2PY	-0.09422	-0.00945	0.00309				2PY	0.09439	-0.00393	0.00055
		2PZ	-0.13522	-0.00840	-0.00001				2PZ	-0.14439	-0.00207	-0.01725
		3S	0.03184	0.01011	-0.00758				3S	0.03597	-0.00570	-0.00993
		3PX	-0.00714	0.00299	-0.00208				3PX	0.00663	-0.00208	-0.00336
		3PY	-0.09330	-0.01001	0.00520				3PY	0.09466	-0.00030	0.00470
		3PZ	-0.10523	-0.00125	-0.00573				3PZ	-0.11648	-0.00977	-0.02875
		4XX	0.00041	-0.00011	0.00010				4XX	-0.00019	0.00031	0.00042

		4YY	0.00307	0.00248	-0.00160			4YY	0.00366	-0.00257	-0.00379
		4ZZ	-0.00399	-0.00250	0.00155			4ZZ	-0.00407	0.00242	0.00359
		4XY	0.00224	0.00318	-0.00195			4XY	-0.00166	0.00184	0.00243
		4XZ	0.00249	0.00705	-0.00436			4XZ	0.00088	-0.00474	-0.00635
		4YZ	0.00473	0.00276	-0.00170			4YZ	-0.00533	0.00328	0.00483
6	C	1S	-0.00006	0.00002	-0.00003		6	C	1S	0.00011	0.00001	0.00003
		2S	0.00017	0.00006	-0.00015				2S	-0.00037	0.00009	0.00011
		2PX	-0.00028	-0.00011	-0.00018				2PX	-0.00123	-0.00036	-0.00052
		2PY	-0.03173	-0.04052	0.02436				2PY	0.02781	-0.02841	-0.04076
		2PZ	-0.11842	-0.10437	0.06221				2PZ	-0.12015	0.07996	0.11367
		3S	0.00099	-0.00141	0.00342				3S	-0.00131	-0.00164	-0.00215
		3PX	-0.00166	-0.00109	0.00236				3PX	0.00856	-0.00234	-0.00321
		3PY	-0.06586	-0.04519	0.03024				3PY	0.06393	-0.03234	-0.04916
		3PZ	-0.06811	-0.10004	0.06735				3PZ	-0.07084	0.07844	0.11718
		4XX	0.00054	0.00012	-0.00007				4XX	-0.00244	0.00041	0.00057
		4YY	0.00042	-0.00024	0.00052				4YY	-0.00067	-0.00041	-0.00073
		4ZZ	-0.00095	0.00012	-0.00043				4ZZ	0.00309	-0.00001	0.00016
		4XY	-0.00248	0.00052	-0.00063				4XY	0.00161	0.00046	0.00096
		4XZ	-0.02579	-0.00306	0.00090				4XZ	-0.02512	0.00210	0.00182
		4YZ	0.00140	-0.00006	0.00044				4YZ	0.00520	-0.00018	0.00002
7	H	1S	0.00921	0.00070	-0.00034		7	H	1S	0.00911	-0.00054	-0.00057
		2S	-0.01187	-0.00414	0.00164				2S	-0.01170	0.00403	0.00602
8	H	1S	-0.00651	-0.00070	0.00036		8	H	1S	-0.00688	0.00062	0.00075
		2S	-0.00659	-0.00397	0.00331				2S	-0.00828	0.00038	0.00096
9	H	1S	0.00666	0.00077	-0.00041		9	H	1S	0.00677	-0.00053	-0.00067
		2S	0.00783	0.00173	0.00252				2S	0.00700	-0.00324	-0.00446
10	H	1S	-0.00910	-0.00074	0.00029		10	H	1S	-0.00924	0.00054	0.00058
		2S	0.01153	0.00505	-0.00432				2S	0.01168	-0.00272	-0.00432
11	C	1S	-0.00014	-0.00001	0.00009		11	C	1S	0.00016	-0.00008	-0.00010
		2S	0.00040	0.00000	0.00000				2S	-0.00047	0.00008	0.00034
		2PX	0.00025	0.00054	-0.00044				2PX	0.00010	-0.00034	-0.00033
		2PY	-0.01377	-0.08267	0.03173				2PY	0.01414	-0.05645	-0.06506
		2PZ	-0.03286	-0.21226	0.08051				2PZ	-0.03688	0.15828	0.18145
		3S	-0.00263	-0.00058	-0.00137				3S	0.00282	0.00134	-0.00095
		3PX	0.00006	-0.00086	0.00232				3PX	0.00106	-0.00098	-0.00428
		3PY	-0.01255	-0.08794	0.05670				3PY	0.01314	-0.06629	-0.06693
		3PZ	-0.01745	-0.22223	0.14160				3PZ	-0.02055	0.18902	0.17778
		4XX	0.00003	0.00004	-0.00002				4XX	0.00008	0.00006	0.00010
		4YY	-0.00304	0.00097	-0.00245				4YY	0.00156	0.00090	0.00127
		4ZZ	0.00295	-0.00103	0.00254				4ZZ	-0.00159	-0.00098	-0.00139
		4XY	-0.00516	0.00131	-0.00128				4XY	0.00486	0.00105	0.00287
		4XZ	-0.01336	0.00337	-0.00331				4XZ	-0.01369	-0.00292	-0.00796
		4YZ	-0.00377	0.00131	-0.00321				4YZ	-0.00206	-0.00132	-0.00191
12	C	1S	0.00036	0.00012	-0.00004		12	C	1S	-0.00036	0.00010	0.00002

		2S	-0.00070	-0.00025	0.00008			2S	0.00071	-0.00004	-0.00029
		2PX	0.00068	0.00024	-0.00017			2PX	0.00033	0.00036	0.00048
		2PY	-0.05681	0.02379	-0.03305			2PY	0.05175	0.02208	0.03612
		2PZ	-0.14449	0.06324	-0.08689			2PZ	-0.14225	-0.06392	-0.10392
		3S	-0.00043	0.00046	-0.00018			3S	0.00010	-0.00189	0.00408
		3PX	-0.00313	-0.00057	0.00121			3PX	0.00446	0.00075	-0.00111
		3PY	-0.05313	0.02711	-0.04880			3PY	0.04830	0.02823	0.03536
		3PZ	-0.12628	0.07829	-0.13604			3PZ	-0.12483	-0.08433	-0.11161
		4XX	0.00009	0.00001	0.00004			4XX	-0.00011	0.00017	0.00018
		4YY	0.00164	0.00406	-0.00442			4YY	-0.00137	0.00290	0.00030
		4ZZ	-0.00162	-0.00402	0.00436			4ZZ	0.00137	-0.00302	-0.00046
		4XY	0.00013	0.00719	-0.00192			4XY	-0.00044	0.00530	0.00515
		4XZ	0.00031	0.01881	-0.00496			4XZ	0.00125	-0.01478	-0.01439
		4YZ	0.00216	0.00509	-0.00557			4YZ	0.00203	-0.00407	-0.00041
13	H	1S	0.00019	-0.00023	0.00018	13	H	1S	-0.00009	-0.00017	-0.00026
		2S	-0.00396	-0.00146	0.00223			2S	0.00410	-0.00006	-0.00286
14	H	1S	-0.00059	0.00021	-0.00014	14	H	1S	0.00058	-0.00012	-0.00007
		2S	0.00313	0.00264	-0.00284			2S	-0.00317	0.00181	0.00221
15	C	1S	-0.00009	0.00003	-0.00003	15	C	1S	0.00009	-0.00003	0.00004
		2S	0.00018	0.00000	0.00004			2S	-0.00016	-0.00007	-0.00003
		2PX	-0.00042	0.00017	-0.00014			2PX	0.00037	0.00154	0.00146
		2PY	-0.00009	0.10116	-0.01202			2PY	-0.00325	0.06726	0.06219
		2PZ	-0.00074	0.26484	-0.03167			2PZ	0.00868	-0.18714	-0.17351
		3S	0.00125	-0.00065	0.00059			3S	-0.00147	0.00123	-0.00096
		3PX	-0.00153	0.00022	0.00090			3PX	0.00081	0.00239	0.00289
		3PY	0.00229	0.10949	-0.01194			3PY	-0.00482	0.07823	0.07822
		3PZ	-0.00404	0.28222	-0.02549			3PZ	0.00308	-0.21542	-0.21430
		4XX	0.00002	0.00000	-0.00002			4XX	-0.00013	-0.00002	-0.00021
		4YY	-0.00029	0.00002	-0.01580			4YY	0.00128	0.01022	-0.01004
		4ZZ	0.00024	-0.00002	0.01583			4ZZ	-0.00112	-0.01023	0.01023
		4XY	0.00368	-0.00312	0.00185			4XY	-0.00318	-0.00080	-0.00551
		4XZ	0.00933	-0.00826	0.00493			4XZ	0.00881	0.00284	0.01516
		4YZ	-0.00033	0.00003	-0.02044			4YZ	-0.00176	-0.01438	0.01398
16	C	1S	0.00010	0.00004	-0.00001	16	C	1S	-0.00004	0.00003	0.00002
		2S	-0.00028	-0.00010	0.00009			2S	0.00015	-0.00011	-0.00004
		2PX	0.00031	0.00014	0.00013			2PX	-0.00056	-0.00192	0.00105
		2PY	0.02126	-0.02473	0.11527			2PY	-0.02051	-0.08650	0.04341
		2PZ	0.05657	-0.06469	0.30187			2PZ	0.05777	0.24013	-0.12165
		3S	0.00077	0.00023	-0.00122			3S	-0.00124	0.00002	-0.00024
		3PX	-0.00109	-0.00086	0.00071			3PX	0.00017	-0.00302	-0.00014
		3PY	0.01964	-0.02990	0.15901			3PY	-0.01859	-0.10561	0.05543
		3PZ	0.04576	-0.08097	0.42071			3PZ	0.04654	0.29251	-0.15300
		4XX	0.00003	-0.00001	-0.00001			4XX	-0.00002	-0.00006	-0.00025
		4YY	0.00042	0.00766	-0.00057			4YY	-0.00058	0.00586	0.00639

		4ZZ	-0.00040	-0.00764	0.00056			4ZZ	0.00056	-0.00582	-0.00613
		4XY	0.00048	-0.00589	-0.00447			4XY	-0.00031	-0.00135	-0.00598
		4XZ	0.00137	-0.01538	-0.01175			4XZ	0.00094	0.00395	0.01686
		4YZ	0.00050	0.00988	-0.00068			4YZ	0.00076	-0.00823	-0.00897
17	C	1S	-0.00007	-0.00002	-0.00001	17	C	1S	0.00001	-0.00001	-0.00009
		2S	0.00017	0.00007	0.00001			2S	-0.00006	0.00008	0.00021
		2PX	-0.00013	-0.00005	-0.00014			2PX	-0.00047	0.00042	-0.00289
		2PY	0.02339	-0.04353	-0.07339			2PY	-0.02036	0.02817	-0.11973
		2PZ	0.06162	-0.11361	-0.19239			2PZ	0.05687	-0.07941	0.33374
		3S	-0.00078	-0.00068	0.00072			3S	0.00123	-0.00067	-0.00026
		3PX	0.00129	0.00018	-0.00070			3PX	-0.00166	0.00165	-0.00372
		3PY	0.02139	-0.04926	-0.11353			3PY	-0.01930	0.03145	-0.15765
		3PZ	0.05409	-0.12966	-0.29724			3PZ	0.05212	-0.08718	0.44122
		4XX	-0.00002	-0.00004	0.00004			4XX	0.00001	-0.00029	-0.00007
		4YY	-0.00058	-0.00612	0.00033			4YY	0.00064	-0.00397	-0.00420
		4ZZ	0.00056	0.00614	-0.00036			4ZZ	-0.00062	0.00426	0.00424
		4XY	0.00054	-0.00693	0.00479			4XY	-0.00011	-0.00701	-0.00070
		4XZ	0.00146	-0.01809	0.01248			4XZ	0.00039	0.01940	0.00178
		4YZ	-0.00073	-0.00788	0.00045			4YZ	-0.00087	0.00552	0.00590
18	C	1S	-0.00005	-0.00002	-0.00002	18	C	1S	0.00003	-0.00001	-0.00002
		2S	0.00010	-0.00001	-0.00002			2S	-0.00005	-0.00002	0.00000
		2PX	-0.00017	-0.00022	-0.00013			2PX	0.00007	-0.00030	-0.00207
		2PY	0.00300	-0.06606	-0.09060			2PY	-0.00094	-0.00953	-0.08535
		2PZ	0.00769	-0.17307	-0.23723			2PZ	0.00245	0.02648	0.23762
		3S	0.00049	0.00095	0.00065			3S	-0.00029	0.00072	0.00086
		3PX	-0.00105	-0.00063	0.00026			3PX	0.00065	-0.00048	-0.00394
		3PY	0.00445	-0.08889	-0.13071			3PY	-0.00222	-0.01379	-0.11683
		3PZ	0.01419	-0.23235	-0.34419			3PZ	0.00778	0.03970	0.32506
		4XX	0.00000	0.00002	-0.00003			4XX	0.00006	0.00033	-0.00003
		4YY	-0.00110	0.00503	-0.00086			4YY	0.00055	0.00375	0.00266
		4ZZ	0.00108	-0.00506	0.00089			4ZZ	-0.00060	-0.00408	-0.00263
		4XY	-0.00171	0.00396	-0.00835			4XY	0.00157	0.00800	-0.00121
		4XZ	-0.00452	0.01035	-0.02185			4XZ	-0.00439	-0.02208	0.00349
		4YZ	-0.00140	0.00650	-0.00111			4YZ	-0.00074	-0.00518	-0.00376
19	H	1S	-0.00012	-0.00007	-0.00002	19	H	1S	0.00008	-0.00005	-0.00009
		2S	0.00116	0.00046	-0.00076			2S	-0.00087	-0.00064	-0.00031
20	C	1S	0.00001	0.00001	0.00001	20	C	1S	0.00000	0.00004	0.00004
		2S	-0.00005	-0.00006	0.00004			2S	-0.00001	-0.00005	-0.00021
		2PX	0.00007	-0.00023	0.00014			2PX	0.00010	-0.00153	0.00109
		2PY	0.00439	-0.06717	0.07589			2PY	0.00272	-0.06589	0.04760
		2PZ	0.01141	-0.17578	0.19867			2PZ	-0.00773	0.18344	-0.13336
		3S	-0.00023	0.00023	-0.00029			3S	0.00015	-0.00035	0.00056
		3PX	0.00060	-0.00018	0.00009			3PX	-0.00012	-0.00151	0.00187
		3PY	0.00475	-0.07958	0.12974			3PY	0.00213	-0.08394	0.06936

		3PZ	0.01408	-0.20685	0.33911			3PZ	-0.00406	0.23388	-0.19633
		4XX	0.00000	0.00004	0.00002			4XX	0.00006	-0.00008	0.00044
		4YY	0.00146	-0.00589	0.00058			4YY	-0.00186	-0.01438	-0.00181
		4ZZ	-0.00145	0.00586	-0.00061			4ZZ	0.00179	0.01449	0.00135
		4XY	-0.00170	0.00528	0.00550			4XY	0.00143	-0.00175	0.01019
		4XZ	-0.00448	0.01384	0.01439			4XZ	-0.00407	0.00424	-0.02851
		4YZ	0.00188	-0.00761	0.00075			4YZ	0.00261	0.02025	0.00259
21	H	1S	0.00002	-0.00001	-0.00002	21	H	1S	0.00001	-0.00006	0.00008
		2S	-0.00024	0.00002	-0.00029			2S	0.00018	-0.00007	-0.00044
22	C	1S	0.00000	0.00000	-0.00002	22	C	1S	0.00000	-0.00006	-0.00001
		2S	-0.00001	0.00004	0.00002			2S	-0.00001	0.00013	0.00006
		2PX	-0.00010	0.00029	-0.00007			2PX	0.00052	0.00224	0.00076
		2PY	-0.02375	0.07785	-0.02159			2PY	0.02062	0.09112	0.03103
		2PZ	-0.06209	0.20381	-0.05644			2PZ	-0.05740	-0.25361	-0.08659
		3S	0.00028	-0.00026	0.00010			3S	-0.00013	0.00015	-0.00023
		3PX	-0.00022	0.00073	0.00037			3PX	0.00058	0.00346	0.00137
		3PY	-0.02372	0.10045	-0.05245			3PY	0.02036	0.12493	0.04428
		3PZ	-0.05967	0.26365	-0.13898			3PZ	-0.05517	-0.34743	-0.12661
		4XX	0.00000	0.00006	0.00001			4XX	0.00000	0.00006	0.00015
		4YY	0.00005	0.00096	0.01765			4YY	0.00041	-0.00447	0.01098
		4ZZ	-0.00004	-0.00102	-0.01767			4ZZ	-0.00041	0.00439	-0.01112
		4XY	-0.00091	0.00863	0.00235			4XY	0.00008	0.00137	0.00360
		4XZ	-0.00243	0.02254	0.00610			4XZ	-0.00024	-0.00403	-0.00950
		4YZ	0.00007	0.00123	0.02277			4YZ	-0.00056	0.00626	-0.01536
23	H	1S	-0.00009	-0.00003	0.00003	23	H	1S	0.00007	-0.00005	-0.00006
		2S	-0.00038	-0.00014	-0.00005			2S	0.00026	0.00005	-0.00014
24	N	1S	0.00005	0.00000	-0.00005	24	N	1S	-0.00040	0.00006	0.00006
		2S	0.00016	0.00024	0.00001			2S	0.00080	-0.00013	-0.00017
		2PX	0.00000	0.00000	0.00000			2PX	0.02676	-0.00308	-0.00384
		2PY	0.00001	-0.00004	0.00004			2PY	0.02345	-0.00061	-0.00122
		2PZ	0.00002	-0.00017	-0.00014			2PZ	0.35333	-0.04713	-0.05750
		3S	0.00066	-0.02313	-0.02274			3S	0.00155	-0.00061	-0.00048
		3PX	0.00170	-0.06034	-0.05923			3PX	0.02244	-0.00437	-0.00593
		3PY	-0.00001	0.00001	0.00010			3PY	0.01030	-0.00635	-0.01061
		3PZ	-0.00005	0.00048	0.00037			3PZ	0.30942	-0.04779	-0.05926
		4XX	-0.00126	0.06394	0.06234			4XX	-0.00049	-0.00032	-0.00056
		4YY	-0.00325	0.16681	0.16236			4YY	0.00046	0.00069	0.00110
		4ZZ	-0.00004	0.00034	-0.00103			4ZZ	-0.00012	-0.00038	-0.00059
		4XY	-0.00014	0.00121	0.00174			4XY	-0.00122	-0.00210	-0.00338
		4XZ	-0.00940	0.15214	0.21340			4XZ	0.00024	0.00382	0.00594
		4YZ	-0.02459	0.39690	0.55547			4YZ	0.00008	-0.00059	-0.00091
25	C	1S	0.00003	-0.00021	0.00000	25	C	1S	-0.00085	-0.00220	-0.00351
		2S	-0.00336	0.03529	0.03557			2S	0.00327	0.00389	0.00618
		2PX	0.00334	-0.03510	-0.03554			2PX	-0.06450	-0.00225	-0.00698

		2PY	0.00414	-0.02707	-0.00309			2PY	-0.03279	-0.00956	-0.01640
		2PZ	0.01090	-0.07107	-0.00841			2PZ	-0.09110	-0.00320	-0.00858
		3S	-0.00432	0.04532	0.04569			3S	0.00390	0.02572	0.04153
		3PX	0.00337	-0.03346	-0.02380			3PX	-0.07446	0.00056	-0.00437
		3PY	-0.00591	0.05347	0.01572			3PY	-0.04085	-0.00571	-0.01198
		3PZ	0.00840	-0.03900	-0.01097			3PZ	-0.03417	-0.00951	-0.01812
		4XX	-0.01279	0.11076	0.08332			4XX	0.00254	-0.00086	-0.00135
		4YY	-0.00632	0.04998	0.02812			4YY	-0.00328	0.00031	0.00033
		4ZZ	-0.02870	0.35000	0.33775			4ZZ	0.00101	-0.00002	0.00007
		4XY	-0.00167	-0.01546	-0.16148			4XY	-0.00381	0.00055	0.00081
		4XZ	-0.01738	0.20017	0.21434			4XZ	0.00739	-0.00090	-0.00104
		4YZ	-0.00405	0.06306	0.05337			4YZ	-0.01958	0.00306	0.00400
26	C	1S	0.00103	-0.00607	-0.00006		26	C	1S	0.00928	-0.00133	-0.00170
		2S	-0.00054	-0.00305	-0.01127				2S	-0.01795	0.00273	0.00345
		2PX	-0.00037	0.00420	-0.00006				2PX	-0.11991	0.01328	0.01862
		2PY	-0.00033	0.00430	-0.00060				2PY	-0.01714	0.00176	0.00309
		2PZ	0.00001	0.00059	-0.00033				2PZ	-0.03316	0.00703	0.01163
		3S	-0.00061	0.00454	0.00427				3S	-0.06477	0.01259	0.01753
		3PX	0.00545	-0.02587	0.01186				3PX	-0.08728	0.01028	0.01524
		3PY	0.01324	-0.10117	0.08816				3PY	-0.03021	0.01068	0.01691
		3PZ	-0.00049	-0.00972	-0.03445				3PZ	-0.02087	0.00882	0.01557
		4XX	-0.00261	0.00547	-0.02972				4XX	-0.00496	-0.00017	-0.00053
		4YY	-0.00139	0.01651	0.00481				4YY	0.00255	-0.00004	0.00002
		4ZZ	0.00237	-0.01441	-0.03440				4ZZ	0.00470	-0.00001	0.00024
		4XY	-0.00338	0.03354	0.02381				4XY	0.00007	0.00016	0.00023
		4XZ	0.00594	-0.05357	-0.01584				4XZ	0.00095	0.00004	0.00009
		4YZ	-0.00848	0.03945	0.01121				4YZ	0.00105	0.00031	0.00062
27	C	1S	0.00527	-0.04891	-0.04321		27	C	1S	-0.00881	0.00078	0.00091
		2S	-0.01326	0.11128	0.07653				2S	0.01794	-0.00122	-0.00162
		2PX	0.02877	-0.35089	-0.33741				2PX	-0.10458	0.01442	0.01954
		2PY	0.00166	0.01588	0.16134				2PY	-0.06870	0.00673	0.00866
		2PZ	0.01019	-0.10650	-0.12380				2PZ	-0.02996	0.00073	0.00123
		3S	-0.01471	0.18117	0.18223				3S	0.06798	-0.00752	-0.00857
		3PX	-0.00103	0.00611	0.00006				3PX	-0.09118	0.01331	0.01972
		3PY	-0.00006	0.00372	0.00991				3PY	-0.03129	0.01395	0.02148
		3PZ	0.00097	-0.00488	0.00139				3PZ	-0.01502	-0.00618	-0.00812
		4XX	0.00025	-0.00281	0.00021				4XX	0.00162	-0.00028	-0.00036
		4YY	-0.00020	0.00326	-0.00065				4YY	0.00133	0.00072	0.00115
		4ZZ	-0.00016	-0.00368	-0.00601				4ZZ	-0.00489	0.00003	-0.00027
		4XY	0.00139	-0.01653	-0.00493				4XY	0.00387	0.00046	0.00097
		4XZ	-0.00235	0.01442	0.03452				4XZ	-0.00146	-0.00017	-0.00031
		4YZ	0.00049	0.00974	0.03449				4YZ	-0.00037	0.00031	0.00047
28	C	1S	0.00263	-0.00528	0.02934		28	C	1S	-0.00349	0.00044	0.00055
		2S	0.00032	0.00006	-0.00001				2S	0.00716	-0.00045	-0.00040

		2PX	-0.00067	-0.00016	0.00015			2PX	0.04251	-0.00086	0.00028
		2PY	-0.00519	-0.00081	0.00045			2PY	0.00118	0.00125	0.00213
		2PZ	-0.00809	0.00199	-0.00053			2PZ	0.01913	-0.00031	0.00054
		3S	0.35271	0.06489	-0.03129			3S	0.02294	-0.01009	-0.01516
		3PX	-0.00112	-0.00030	0.00020			3PX	0.03284	-0.00230	-0.00205
		3PY	-0.00442	-0.00122	0.00102			3PY	-0.00705	0.00525	0.00823
		3PZ	0.00355	-0.00596	0.00398			3PZ	0.01366	0.00055	0.00209
		4XX	0.30837	0.06555	-0.03375			4XX	-0.00140	0.00020	0.00023
		4YY	0.00013	-0.00012	0.00017			4YY	0.00512	-0.00071	-0.00107
		4ZZ	-0.00010	0.00020	-0.00008			4ZZ	-0.00477	0.00058	0.00092
		4XY	0.00007	-0.00009	0.00002			4XY	0.00677	-0.00079	-0.00121
		4XZ	0.00147	-0.00296	0.00213			4XZ	-0.00236	0.00045	0.00075
		4YZ	0.00015	-0.00496	0.00333			4YZ	0.00214	-0.00045	-0.00076
29	H	1S	0.00005	0.00015	-0.00003		29	H	1S	0.00581	0.00030	0.00043
		2S	-0.00113	0.00266	-0.00188				2S	-0.00100	-0.00104	-0.00238
30	C	1S	0.00385	-0.00450	0.00315		30	C	1S	0.00309	-0.00031	-0.00040
		2S	-0.04890	0.00002	-0.00253				2S	-0.00606	0.00114	0.00161
		2PX	0.04325	-0.01200	0.01023				2PX	0.03135	0.00329	0.00651
		2PY	-0.09572	0.00405	-0.00604				2PY	0.02531	0.00039	0.00160
		2PZ	0.00531	-0.03249	0.02308				2PZ	0.01582	0.00303	0.00544
		3S	-0.05995	-0.00389	-0.00212				3S	-0.02891	-0.00410	-0.00726
		3PX	0.05405	-0.00587	0.00772				3PX	0.01813	0.00453	0.00862
		3PY	-0.04157	0.01283	-0.01128				3PY	0.02946	0.00357	0.00717
		3PZ	0.00226	0.00099	-0.00067				3PZ	0.00884	0.00456	0.00763
		4XX	-0.00246	-0.00019	0.00006				4XX	-0.00758	0.00110	0.00169
		4YY	0.00041	-0.00010	0.00007				4YY	0.00401	-0.00075	-0.00108
		4ZZ	0.00142	0.00009	-0.00014				4ZZ	0.00435	-0.00047	-0.00076
		4XY	0.01165	0.00225	-0.00114				4XY	0.00451	-0.00062	-0.00085
		4XZ	0.01742	0.00378	-0.00203				4XZ	-0.00013	0.00002	0.00001
		4YZ	0.00951	0.00193	-0.00103				4YZ	0.00334	-0.00030	-0.00046
31	H	1S	-0.01833	-0.00397	0.00216		31	H	1S	-0.00794	0.00117	0.00100
		2S	-0.10877	-0.01633	0.00940				2S	0.00272	-0.00630	-0.00992
32	C	1S	0.04050	0.00552	-0.00357		32	C	1S	0.00014	-0.00047	-0.00074
		2S	-0.03772	-0.00954	0.00694				2S	-0.00078	0.00088	0.00137
		2PX	-0.06518	-0.01822	0.01018				2PX	0.09770	-0.01005	-0.01572
		2PY	-0.07415	-0.00931	0.00475				2PY	0.04184	-0.00510	-0.00781
		2PZ	0.04716	0.01603	-0.01078				2PZ	0.09078	-0.00960	-0.01449
		3S	-0.02502	-0.01179	0.00982				3S	0.00172	0.00321	0.00571
		3PX	-0.00453	0.00030	-0.00044				3PX	0.08029	-0.01097	-0.01816
		3PY	0.00221	0.00004	0.00006				3PY	0.03181	-0.00729	-0.01188
		3PZ	0.00473	-0.00001	0.00023				3PZ	0.07416	-0.01057	-0.01683
		4XX	0.00203	0.00016	-0.00002				4XX	0.00046	0.00022	0.00040
		4YY	0.00005	0.00007	-0.00008				4YY	-0.00057	-0.00017	-0.00030
		4ZZ	-0.00107	0.00039	-0.00040				4ZZ	0.00010	-0.00013	-0.00020

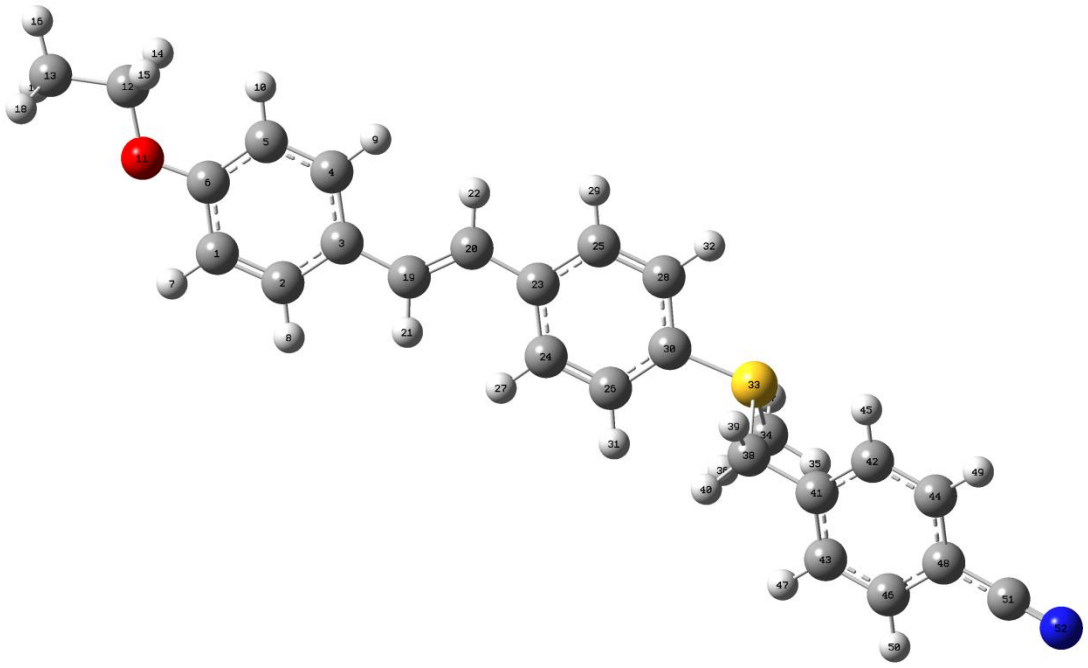
		4XY	-0.00896	-0.00135	0.00076			4XY	-0.00072	-0.00003	-0.00008
		4XZ	0.01812	0.00244	-0.00175			4XZ	0.00068	-0.00006	-0.00008
		4YZ	-0.08169	-0.01547	0.00889			4YZ	-0.00158	-0.00008	-0.00020
33	H	1S	0.08890	0.01364	-0.00772		33	H	1S	-0.01051	0.00038	0.00023
		2S	-0.03673	-0.00236	0.00204				2S	-0.01404	0.00036	-0.00030
34	H	1S	0.06790	0.01196	-0.00508		34	H	1S	0.01034	-0.00159	-0.00216
		2S	-0.07726	-0.01321	0.00886				2S	0.01318	-0.00377	-0.00601
35	H	1S	0.04844	0.02187	-0.01461		35	H	1S	0.00047	-0.00034	-0.00052
		2S	-0.02103	0.00620	-0.00184				2S	0.00149	-0.00075	-0.00144
36	C	1S	0.00014	0.00044	-0.00024		36	C	1S	0.00104	0.00211	0.00338
		2S	0.00281	-0.00103	0.00079				2S	-0.00355	-0.00367	-0.00584
		2PX	-0.00500	-0.00001	-0.00031				2PX	0.03713	-0.00162	-0.00034
		2PY	-0.00353	0.00011	-0.00024				2PY	-0.05419	-0.00961	-0.01769
		2PZ	-0.00077	0.00027	-0.00013				2PZ	-0.09703	-0.00297	-0.00850
		3S	0.00011	0.00042	-0.00027				3S	-0.00501	-0.02501	-0.04082
		3PX	-0.00363	-0.00067	0.00035				3PX	0.05031	-0.00367	-0.00246
		3PY	0.00753	0.00080	-0.00030				3PY	-0.06395	-0.00499	-0.01251
		3PZ	0.04111	0.00160	0.00066				3PZ	-0.04245	-0.00938	-0.01859
		4XX	-0.00999	0.00162	-0.00187				4XX	-0.00112	0.00056	0.00099
		4YY	0.02198	0.00028	0.00127				4YY	0.00401	-0.00035	-0.00043
		4ZZ	0.02349	0.01384	-0.00913				4ZZ	-0.00308	0.00033	0.00035
		4XY	0.03354	0.00463	-0.00126				4XY	0.00102	-0.00030	-0.00037
		4XZ	-0.00008	0.00630	-0.00534				4XZ	0.01419	-0.00206	-0.00262
		4YZ	0.01602	-0.00075	0.00211				4YZ	0.01543	-0.00248	-0.00328
37	C	1S	-0.00343	-0.00057	0.00031		37	C	1S	-0.00946	0.00138	0.00177
		2S	0.00706	0.00121	-0.00081				2S	0.01827	-0.00285	-0.00363
		2PX	-0.00472	-0.00076	0.00055				2PX	0.10038	-0.01082	-0.01465
		2PY	-0.00420	-0.00061	0.00043				2PY	-0.05870	0.00623	0.00915
		2PZ	-0.00238	-0.00064	0.00048				2PZ	-0.04306	0.00791	0.01269
		3S	-0.00228	-0.00054	0.00040				3S	0.06555	-0.01301	-0.01833
		3PX	0.00550	-0.00047	0.00031				3PX	0.06604	-0.00439	-0.00558
		3PY	-0.00097	0.00121	-0.00191				3PY	-0.05988	0.01331	0.02042
		3PZ	0.00314	0.00053	-0.00033				3PZ	-0.02741	0.00906	0.01572
		4XX	-0.00615	-0.00169	0.00110				4XX	0.00394	0.00024	0.00058
		4YY	0.02253	-0.00368	0.00299				4YY	-0.00161	-0.00004	-0.00010
		4ZZ	-0.03061	0.00058	-0.00101				4ZZ	-0.00468	0.00001	-0.00022
		4XY	0.01738	-0.00378	0.00280				4XY	-0.00313	0.00003	-0.00012
		4XZ	-0.02924	0.00377	-0.00315				4XZ	-0.00063	-0.00012	-0.00027
		4YZ	0.00862	-0.00390	0.00317				4YZ	-0.00102	-0.00031	-0.00061
38	C	1S	-0.03188	0.00449	-0.00426		38	C	1S	0.00894	-0.00096	-0.00119
		2S	0.01056	-0.00621	0.00404				2S	-0.01803	0.00174	0.00248
		2PX	-0.00841	-0.00157	0.00104				2PX	0.06672	-0.00996	-0.01370
		2PY	0.00479	0.00113	-0.00069				2PY	-0.10207	0.01170	0.01563
		2PZ	0.00443	0.00062	-0.00047				2PZ	-0.03824	0.00207	0.00326

		3S	-0.00085	-0.00008	-0.00002			3S	-0.06813	0.00824	0.00974
		3PX	-0.00153	-0.00023	0.00016			3PX	0.06909	-0.00770	-0.01144
		3PY	-0.00317	-0.00040	0.00029			3PY	-0.06101	0.01775	0.02748
		3PZ	-0.00800	-0.00123	0.00004			3PZ	-0.02397	-0.00455	-0.00548
		4XX	0.00099	0.00799	-0.00550			4XX	0.00059	0.00030	0.00053
		4YY	0.00014	0.00055	-0.00037			4YY	-0.00367	-0.00081	-0.00141
		4ZZ	-0.00070	-0.00104	0.00069			4ZZ	0.00511	0.00006	0.00044
		4XY	0.07844	0.01044	-0.00747			4XY	0.00299	-0.00011	0.00003
		4XZ	-0.05755	-0.00870	0.00604			4XZ	-0.00056	-0.00025	-0.00037
		4YZ	0.09531	0.01323	-0.00887			4YZ	0.00040	-0.00023	-0.00036
39	C	1S	0.00133	-0.00339	0.00273		39	C	1S	0.00359	-0.00047	-0.00059
		2S	0.06467	0.01084	-0.00835				2S	-0.00744	0.00051	0.00048
		2PX	-0.04455	-0.01150	0.00866				2PX	-0.03786	0.00108	0.00020
		2PY	0.07781	0.01442	-0.01057				2PY	0.01706	0.00109	0.00260
		2PZ	0.00054	-0.00026	0.00020				2PZ	0.02398	-0.00015	0.00113
		3S	-0.00066	0.00019	-0.00019				3S	-0.02373	0.01026	0.01545
		3PX	0.00014	0.00016	-0.00005				3PX	-0.03244	0.00394	0.00463
		3PY	0.00039	0.00009	-0.00001				3PY	0.00572	0.00428	0.00754
		3PZ	0.00107	0.00003	0.00002				3PZ	0.01789	0.00040	0.00220
		4XX	0.00145	-0.00009	0.00011				4XX	0.00399	-0.00044	-0.00059
		4YY	-0.01072	-0.00065	0.00016				4YY	-0.00814	0.00102	0.00156
		4ZZ	-0.01446	-0.00092	0.00001				4ZZ	0.00521	-0.00066	-0.00106
		4XY	0.01039	0.00208	-0.00116				4XY	0.00214	-0.00018	-0.00031
		4XZ	0.01335	0.00480	-0.00352				4XZ	-0.00278	0.00055	0.00090
		4YZ	0.00057	0.00038	-0.00023				4YZ	-0.00151	0.00029	0.00047
40	H	1S	0.00160	0.00079	-0.00066		40	H	1S	-0.00570	-0.00032	-0.00045
		2S	0.00095	-0.00276	0.00197				2S	0.00131	0.00108	0.00261
41	C	1S	-0.00348	0.00476	-0.00350		41	C	1S	-0.00314	0.00038	0.00051
		2S	0.05490	-0.00078	0.00284				2S	0.00614	-0.00126	-0.00179
		2PX	0.03787	-0.01204	0.00956				2PX	-0.01720	-0.00246	-0.00448
		2PY	-0.09431	0.00399	-0.00583				2PY	0.03466	0.00099	0.00278
		2PZ	-0.00414	0.03308	-0.02281				2PZ	0.01773	0.00294	0.00519
		3S	0.06509	0.00310	0.00250				3S	0.02916	0.00332	0.00597
		3PX	0.04937	-0.00596	0.00698				3PX	-0.00377	-0.00207	-0.00361
		3PY	-0.03910	0.01251	-0.00979				3PY	0.03361	0.00421	0.00831
		3PZ	-0.00244	-0.00110	0.00082				3PZ	0.00986	0.00449	0.00741
		4XX	0.00231	0.00020	-0.00003				4XX	0.00820	-0.00113	-0.00169
		4YY	-0.00011	0.00018	-0.00023				4YY	-0.00498	0.00084	0.00117
		4ZZ	0.00230	0.00030	-0.00021				4ZZ	-0.00403	0.00043	0.00070
		4XY	0.01005	0.00187	-0.00089				4XY	-0.00165	0.00031	0.00053
		4XZ	-0.01833	-0.00395	0.00213				4XZ	-0.00289	0.00033	0.00049
		4YZ	-0.00951	-0.00191	0.00097				4YZ	-0.00286	0.00024	0.00038
42	H	1S	0.01839	0.00390	-0.00199		42	H	1S	0.00801	-0.00086	-0.00052
		2S	0.11305	0.01697	-0.01007				2S	-0.00121	0.00605	0.00972

43	C	1S	0.03106	0.00415	-0.00306		43	C	1S	-0.00012	0.00043	0.00068
		2S	-0.03580	-0.00937	0.00721				2S	0.00062	-0.00080	-0.00125
		2PX	0.06521	0.01781	-0.00927				2PX	-0.06451	0.00626	0.00992
		2PY	0.07856	0.01101	-0.00691				2PY	0.07307	-0.00808	-0.01253
		2PZ	0.04023	0.01514	-0.01077				2PZ	0.09838	-0.01012	-0.01534
		3S	-0.02401	-0.01194	0.01029				3S	-0.00123	-0.00282	-0.00491
		3PX	0.00476	-0.00025	0.00035				3PX	-0.05353	0.00620	0.01045
		3PY	-0.00241	-0.00008	0.00004				3PY	0.05749	-0.01036	-0.01703
		3PZ	-0.00472	0.00000	-0.00021				3PZ	0.08043	-0.01101	-0.01757
		4XX	0.00128	0.00018	-0.00005				4XX	-0.00049	-0.00017	-0.00030
		4YY	0.00040	0.00002	0.00000				4YY	0.00084	0.00013	0.00027
		4ZZ	0.00105	-0.00038	0.00034				4ZZ	-0.00036	0.00010	0.00013
		4XY	0.00902	0.00121	-0.00050				4XY	-0.00004	0.00012	0.00018
		4XZ	-0.01830	-0.00201	0.00083				4XZ	0.00130	0.00001	0.00007
		4YZ	0.08978	0.01715	-0.00987				4YZ	0.00125	0.00007	0.00016
44	H	1S	0.08153	0.01202	-0.00614		44	H	1S	0.01071	-0.00042	-0.00029
		2S	-0.03449	-0.00180	0.00095				2S	0.01437	-0.00049	0.00007
45	H	1S	-0.06858	-0.01161	0.00398		45	H	1S	-0.01040	0.00155	0.00210
		2S	0.08237	0.01505	-0.00844				2S	-0.01331	0.00370	0.00586
46	H	1S	0.04223	0.02052	-0.01280		46	H	1S	-0.00052	0.00029	0.00045
		2S	-0.01850	0.00720	-0.00400				2S	-0.00146	0.00061	0.00119
47	H	1S	-0.00062	-0.00047	0.00034		47	H	1S	0.00000	0.00000	0.00000
		2S	-0.00226	0.00102	-0.00085				2S	0.00002	-0.00035	-0.00044
48	S	1S	0.00491	0.00007	0.00016		48	S	1S	0.00000	0.00005	-0.00004
		2S	-0.00378	0.00030	-0.00044				2S	0.00001	-0.00018	0.00021
		2PX	-0.00101	0.00027	-0.00024				2PX	0.00001	0.00094	-0.00036
		2PY	-0.00012	-0.00044	0.00031				2PY	0.00024	0.02443	-0.01421
		2PZ	0.00362	0.00065	-0.00032				2PZ	-0.00069	-0.06877	0.04004
		3S	-0.00747	-0.00076	0.00026				3S	0.00002	0.00066	-0.00035
		3PX	-0.04162	-0.00172	0.00030				3PX	0.00001	-0.00264	0.00109
		3PY	-0.00611	0.00154	-0.00110				3PY	-0.00065	-0.06740	0.04122
		3PZ	0.02052	0.00054	0.00012				3PZ	0.00187	0.18961	-0.11600
		4S	-0.02338	-0.01356	0.00867				4S	-0.00040	0.00051	-0.00184
		4PX	-0.03312	-0.00430	0.00221				4PX	-0.00026	-0.00573	-0.00009
		4PY	0.00310	0.00645	-0.00435				4PY	-0.00331	-0.17574	0.05640
		4PZ	0.01485	-0.00050	0.00094				4PZ	0.00985	0.49678	-0.15909
		5XX	0.00281	0.00048	-0.00027				5XX	-0.00001	0.00204	-0.00122
		5YY	-0.00636	-0.00111	0.00074				5YY	-0.00060	0.00692	-0.01106
		5ZZ	0.00465	0.00074	-0.00052				5ZZ	0.00060	-0.00894	0.01231
		5XY	-0.00527	-0.00079	0.00056				5XY	-0.00001	0.03359	-0.02045
		5XZ	-0.00225	-0.00060	0.00047				5XZ	-0.00003	-0.09394	0.05652
		5YZ	0.00238	0.00059	-0.00046				5YZ	0.00084	-0.00887	0.01482
49	C	1S	-0.00546	0.00046	-0.00027		49	C	1S	0.00041	-0.03536	0.02566
		2S	0.00036	-0.00138	0.00141				2S	-0.00226	0.05045	-0.05377

		2PX	-0.00317	-0.00048	0.00023			2PX	0.00056	-0.09781	0.05362
		2PY	0.00624	0.00160	-0.00092			2PY	0.00333	0.00087	0.01849
		2PZ	-0.02598	0.00403	-0.00410			2PZ	0.00075	0.09593	-0.05385
		3S	-0.02900	0.00060	-0.00175			3S	0.00060	0.39094	-0.24849
		3PX	0.01729	-0.00402	0.00385			3PX	-0.00855	-0.18925	-0.00796
		3PY	0.02940	-0.00405	0.00412			3PY	-0.00134	0.03271	-0.04232
		3PZ	-0.01243	0.00485	-0.00551			3PZ	0.00038	0.16542	-0.10273
		4XX	-0.03132	0.00439	-0.00519			4XX	-0.00015	-0.00964	0.00506
		4YY	0.01044	-0.00647	0.00518			4YY	-0.00018	-0.00328	0.00029
		4ZZ	0.00822	0.00157	-0.00104			4ZZ	-0.00026	0.00551	-0.00577
		4XY	-0.00457	-0.00110	0.00068			4XY	0.00038	0.00000	0.00392
		4XZ	-0.00448	-0.00063	0.00046			4XZ	0.00009	0.00074	-0.00043
		4YZ	-0.00224	-0.00037	0.00018			4YZ	-0.00002	-0.00190	0.00088
50	H	1S	-0.00092	-0.00013	0.00008		50	H	1S	-0.00231	-0.01778	-0.00569
		2S	0.00323	0.00041	-0.00027				2S	0.00277	0.00975	0.04954
51	H	1S	0.00781	0.00150	-0.00059		51	H	1S	-0.00079	0.01566	-0.01857
		2S	-0.00184	-0.00830	0.00572				2S	-0.00164	-0.02236	-0.01280
52	H	1S	-0.00014	-0.00059	0.00043		52	H	1S	0.00181	-0.02045	0.02841
		2S	0.00074	0.00110	-0.00078				2S	0.00786	-0.06912	0.16720
53	C	1S	-0.08551	-0.01149	0.00800		53	C	1S	-0.00042	0.03549	-0.02589
		2S	-0.05059	-0.00786	0.00538				2S	0.00223	-0.05075	0.05395
		2PX	0.09344	0.01312	-0.00875				2PX	-0.00051	0.09590	-0.05209
		2PY	-0.00167	0.00362	-0.00366				2PY	-0.00308	-0.06271	0.02036
		2PZ	-0.07038	-0.01216	0.00906				2PZ	-0.00159	0.07655	-0.05577
		3S	-0.03884	-0.01053	0.00792				3S	-0.00026	-0.39167	0.25150
		3PX	0.07619	0.01437	-0.01061				3PX	0.00851	0.18523	0.01010
		3PY	-0.00054	0.00029	-0.00028				3PY	0.00065	-0.13404	0.09812
		3PZ	0.00059	-0.00020	0.00017				3PZ	0.00109	0.11290	-0.05564
		4XX	-0.00006	-0.00018	0.00017				4XX	0.00015	0.00961	-0.00496
		4YY	0.00051	0.00006	-0.00005				4YY	0.00023	0.00143	0.00138
		4ZZ	0.00092	0.00005	-0.00002				4ZZ	0.00020	-0.00364	0.00392
		4XY	-0.00153	0.00010	-0.00014				4XY	-0.00035	-0.00062	-0.00264
		4XZ	0.01063	0.00062	-0.00012				4XZ	-0.00017	0.00103	-0.00310
		4YZ	0.01436	0.00084	0.00017				4YZ	-0.00005	0.00458	-0.00328
54	H	1S	-0.01041	-0.00212	0.00124		54	H	1S	0.00074	-0.01586	0.01828
		2S	-0.01335	-0.00482	0.00367				2S	0.00175	0.02182	0.01440
55	H	1S	-0.00052	-0.00043	0.00031		55	H	1S	0.00232	0.01769	0.00576
		2S	-0.00155	-0.00093	0.00093				2S	-0.00295	-0.01164	-0.05093
56	H	1S	-0.00546	0.02590	-0.01182		56	H	1S	-0.00181	0.02074	-0.02842
		2S	-0.01326	0.10146	-0.08764				2S	-0.00780	0.07076	-0.16718

PAG 1:



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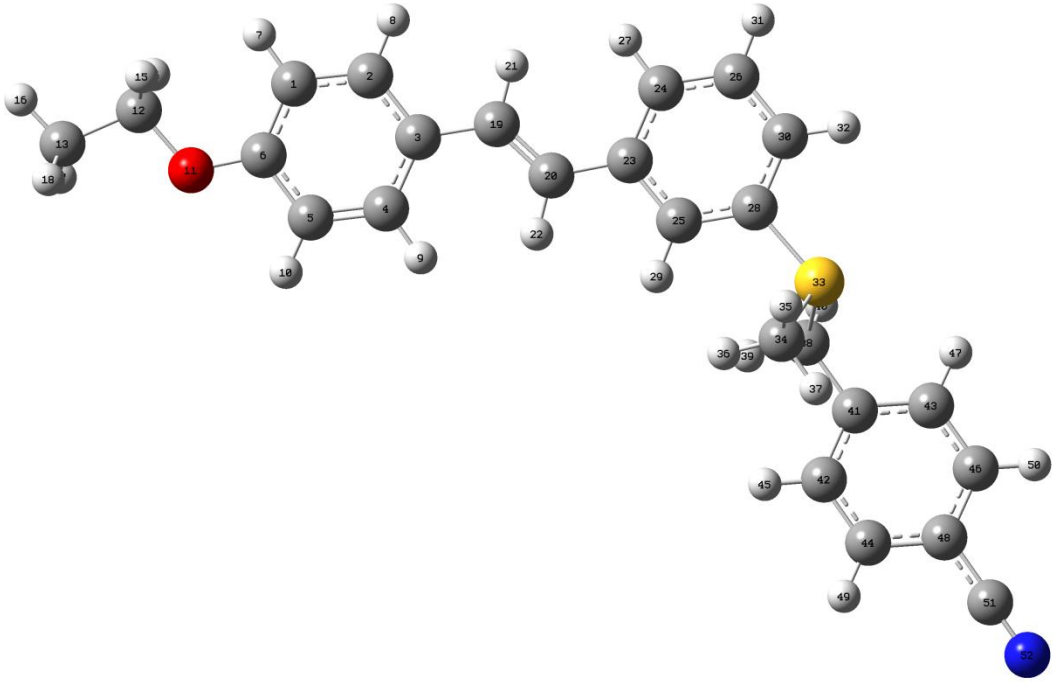

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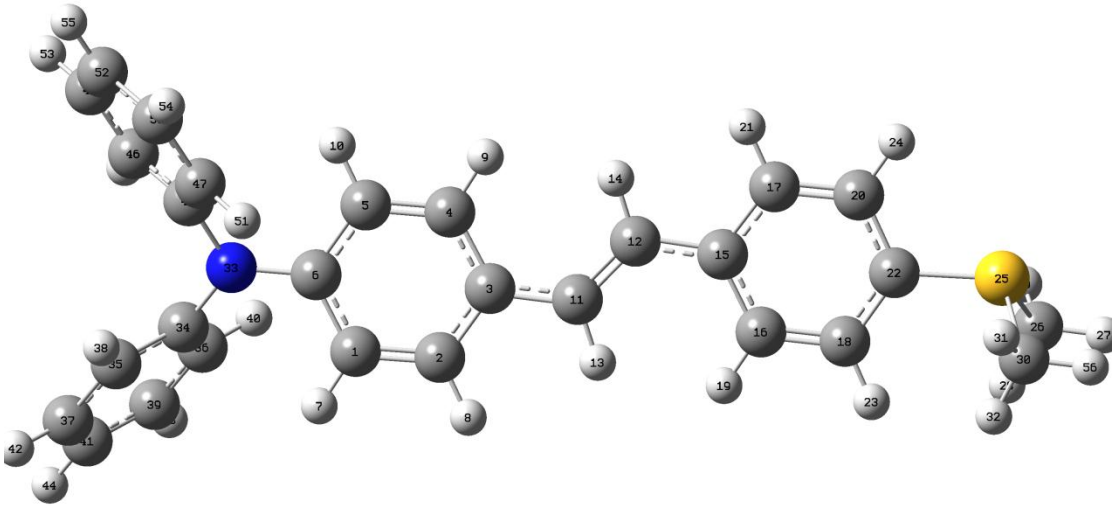

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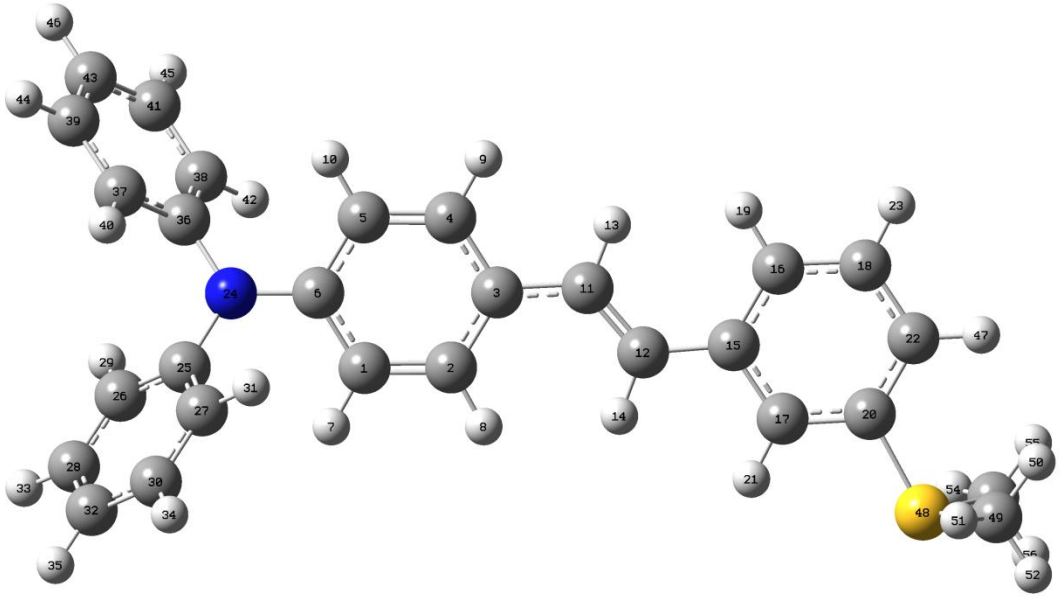

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