SUPPORTING INFORMATION

Syntheses of rod-shaped fluorescent 1,3,2-benzodiazaboroles with phosphonium, and phosphane chalcogenide acceptor functions

Lothar Weber,*[a] Henry Kuhtz,[a] Lena Böhling,[a] Andreas Brockhinke,[a] Anna Chrostowska,[b] Alain Dargelos,[b] Audrey Mazière, [b] Hans-Georg Stammler,[a] and Beate Neumann[a].

Supporting information for this article: Details for the requisition of UV/Vis and photoluminescence (PL) spectra. Selected spectroscopic data of compounds **2-11**.

Experimental Setup:

All experiments were performed under an atmosphere of dry oxygen-free argon using Schlenk techniques. All solvents were dried with the usual drying agents and freshly distilled prior use. The compounds 4-bromo-phenyl-diphenylphosphane[38], 5-bromo-2-diphenylphosphanyl-thiophene[39], 2-bromo-1,3-diethyl-1,3,2-benzodiazaborole **1**[23] and tetrahydrothiophene-gold(I)chloride[40] were prepared according to literature methods.

Oxone ($2KHSO_5 \cdot KHSO_4 \cdot K2SO_4$) was purchased from Alfa Aeser Johnson Matthey Comp., Karlsruhe (Germany). A 1.6M pentane solution of *tert.* butyllithium and a 1.6M hexane solution of *n*-butyllithium were obtained from Aldrich.

NMR spectra were recorded in C_6D_6 or $CDCl_3$ at room temperature on a Bruker AM Avance DRX500 spectrometer (^1H, ^{11}B, ^{13}C) with $SiMe_4$ (^1H, ^{13}C) and $BF_3 \cdot OEt_2$ (^{11}B) as external standards. Some expected ^{13}C peaks corresponding to the boron- bound carbon atoms were not detected above the noise levels. Mass spectra were obtained with a VG Autospec sector field mass spectrometer (Micromass). Absorption spectra were measured with a UV/VIS double-beam spectrometer (Shimadzu UV-2550).

For all solution state measurements, samples were contained in quartz cuvettes of 10 × 10 mm (Hellma type 111-QS, suprasil, optical precision). All solvents were dried by standard methods prior to use. Concentrations varied from 10 to 50 µM according to their optical density.

Absorption was measured with a UV/VIS double-beam spectrometer (Shimadzu UV-2550), using the solvent as a reference. The setup used to acquire excitation-emission spectra (EES) was similar to that employed in commercial static fluorimeters: The output of a continuous

Xe-lamp (75 W, LOT Oriel) was wavelength-separated by a first monochromator (Spectra Pro ARC-175, 1800 l/mm grating, Blaze 250 nm) and then used to irradiate a sample. The fluorescence was collected by mirror optics at right angles and imaged on the entrance slit of a second spectrometer while compensating astigmatism at the same time. The signal was detected by a back-thinned CCD camera (RoperScientific, 1024 \ 256 pixels) in the exit plane of the spectrometer. The resulting images were spatially and spectrally resolved. As the next step, one averaged fluorescence spectrum was calculated from the raw images and stored in the computer. This process was repeated for different excitation wavelengths. The result is a two-dimensional fluorescence pattern with the *y*-axis corresponding to the excitation, and the *x*-axis to the emission wavelength. Figure **S1** shows a sample spectrum obtained with this technique. Here, the wavelength range is λ_{ex} = 230-430 nm (in 1 nm increments) for the UV light and λ_{em} = 205-794 nm for the detector. The time to acquire a complete EES is typically less than 15 min. Post-processing of the EES includes subtraction of the dark current background, conversion of pixel to wavelength scales, and multiplication with a reference file to take the varying lamp intensity as well as grating and detection efficiency into account. The quantum yields were determined against POPOP (*p*-bis-5-phenyl-oxazolyl(2)-benzene) (Φ = 0.93) as the standard.

Stokes shifts were calculated from excitation and emission maxima, which were extracted from spectra that were converted from wavelength to wavenumbers beforehand.

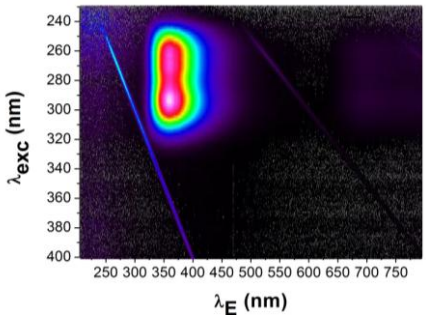


Figure S1: Sample EES spectrum

X-Ray crystallography

Single crystals were coated with a layer of hydrocarbon oil and attached to a glass fiber. Cristallographic data were collected with a Nonius KappaCCD diffractometer with MO-Kα radiation (graphite monochromator, λ = 0.71073 Å) at 100 K for **2**, **4**, **5**, **6**, **7**, **8**, **9** and **11** and 200 K for **3**. Crystallographic programs used for structure solution and refinement were from SHELX-97.[54] The structures were solved by direct methods and were refined by using fullmatrix least squares on F^2 of all unique reflections with anisotropic thermal parameters for all non-hydrogen atoms, except disordered atoms in **8** and **12**. All hydrogen atoms were

refined using a riding model with U(H) = 1.5 U_{eq} for CH_3 groups and U(H) = 1.2 U_{eq} for all others. CCDC XXXXXX contains supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.ac.uk/data_requesst/cif.

UV-Data:

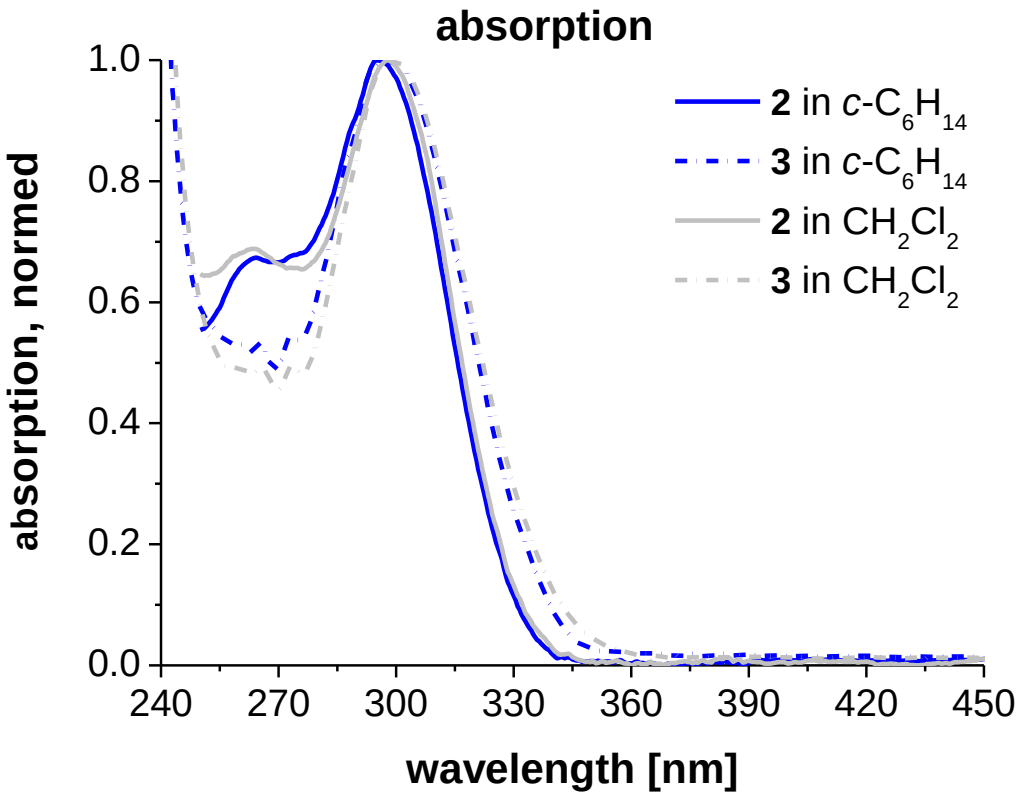


Figure 2S: Absorption spectra of **2** and **3** in *c*-C_6H_{14} and CH_2Cl_2.

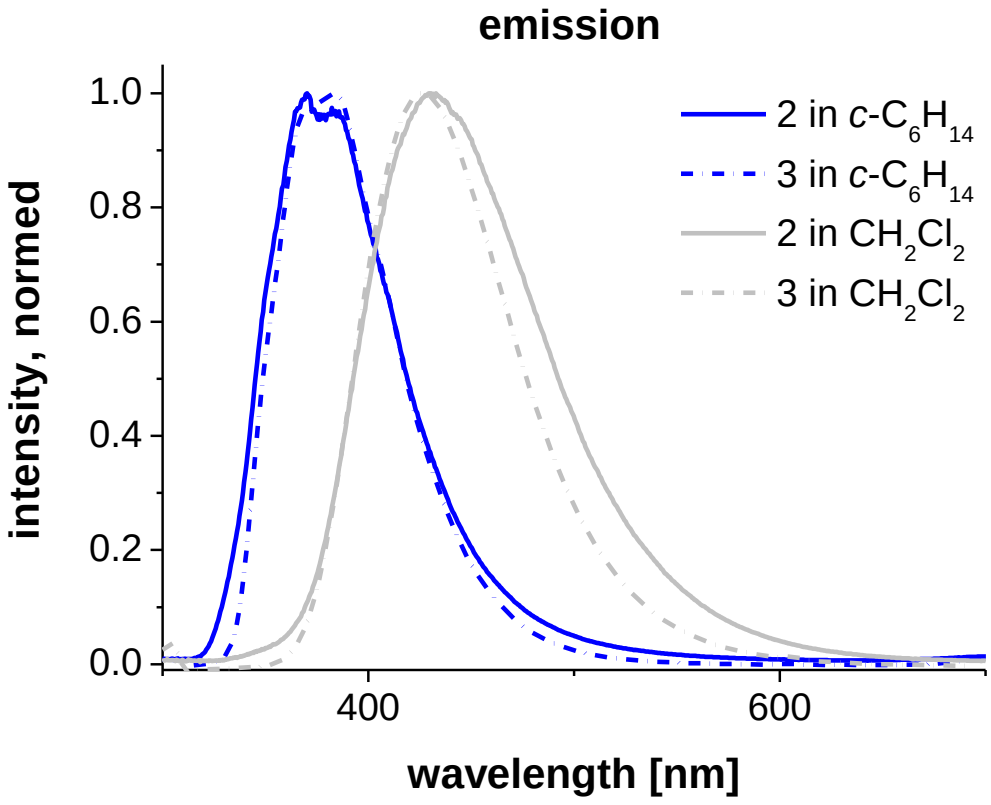


Figure 3S: Emission spectra of **2** and **3** in *c*-C_6H_{14} and CH_2Cl_2.

NMR-Data:

4-Diphenylphosphanyl)-1- (1',3'-diethyl-1',3',2'-benzodiazaborol-2'yl)-benzene (2)

^{1}H-NMR(500 MHz, $CDCl_3$): δ: 1.34 (t, ^{3}J= 7.2 H, 6H, $CH_2C\mathbf{H}_3$), 3.79 (q, ^{3}J= 7.2 Hz, 4H, $C\mathbf{H}_2CH_3$), 7.07 (m, 2H, H-benzodiazaborole), 7.14 (m, 2H, H-benzodiazaborole), 7.34 -7.47 (m, 12 H, H-phenyl and P-C(C**H**-)$_2$), 7.57 (d, 2H, ^{3}J= 7.5 Hz, BC(C**H**)$_2$); ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$): δ: 16.4 (s, $CH_2\mathbf{C}H_3$), 37.8 (s, $\mathbf{C}H_2CH_3$), 109.1 (s, CH-benzodiazaborole), 119.1 (s, CH-benzodiazaborole), 128.7 (d, $^{3}J_{P,C}$= 7.0 Hz, *m*-CH-phenyl), 129.0 (s, *p*-CH-phenyl), 133.1 (d, $^{2}J_{P,C}$= 18.7 Hz, (CH-phenyl), 133.7 (d, $^{3}J_{P,C}$= 6.6 Hz, CH-phenylene), 134.1 (d, $^{2}J_{P,C}$= 19.6 Hz, *o*-CH-phenyl), 137.2 (s, C-benzodiazaborole).
^{11}B{^{1}H}NMR(160 MHz, $CDCl_3$): δ= 29.1 (s); ^{31}P{^{1}H}NMR(202 MHz, $CDCl_3$) δ= -5.2 (s).
MS/EI: m/z = 434 [M^+] 100%

4-(Diphenyl-oxo-phosphanyl)-1-(1',3'-diethyl-1',3',2'-benzodiazaborol-2'-yl)-benzene (3)

^{1}H-NMR(500 MHz, $CDCl_3$): δ: 1.31 (t, ^{3}J= 7.2 H, 6H, $CH_2C\mathbf{H}_3$), 3.72 (q, ^{3}J= 7.2 Hz, 4H, $C\mathbf{H}_2CH_3$), 7.07 (m, 2H, H-benzodiazaborole), 7.13 (m, 2H, H-benzodiazaborole), 7.44 -7.60 (m, 12 H, H-phenyl and P-C(C**H**-)$_2$), 7.57 (d, 2H, ^{3}J= 7.5 Hz, BC(C**H**)$_2$); ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$): δ: 16.4 (s, $CH_2\mathbf{C}H_3$), 37.8 (s, $\mathbf{C}H_2CH_3$), 109.2 (s, CH-benzodiazaborole), 119.0 (s, CH-benzodiazaborole), 128.7 (d, $^{3}J_{P,C}$= 12.1 Hz, *m*-CH-phenyl), 131.5(d, $^{2}J_{P,C}$= 9.6 Hz, CH-phenylene), 132.2 (d, $^{4}J_{P,C}$= 2.6 Hz, *p*-CH-phenylene), 132.3 (d, $^{2}J_{P,C}$= 9.9 Hz, *o*-CH-phenyl), 132.5 (d, $^{1}J_{P,C}$= 104.4 Hz, *i*-C-phenyl), 132.7 (d, $^{1}J_{P,C}$= 103.6 Hz, *i*-C-phenylene), 133.6 (d, $^{3}J_{P,C}$= 11.8 Hz, CH-phenylene), 137.1 (s, C-benzodiazaborole).
^{11}B{^{1}H}NMR(160 MHz, $CDCl_3$): δ= 29.7 (s); ^{31}P{^{1}H}NMR(202 MHz, $CDCl_3$) δ= 29.5 (s).
MS/EI: m/z = 450 [M^+] 100%.

4-(Diphenyl-thiophosphanyl)-1-(1',3',-diethyl-1',3',2',-benzodiazaborol-2'-yl)-benzene (4)

^{1}H-NMR(300 MHz, $CDCl_3$): δ: 1.31 (t, ^{3}J= 7.2 H, 6H, $CH_2C\mathbf{H}_3$), 3.78 (q, ^{3}J= 7.2 Hz, 4H, $C\mathbf{H}_2CH_3$), 7.06 (m, 2H, H-benzodiazaborole), 7.13 (m, 2H, H-benzodiazaborole), 7.50 (m, 6H, H-phenyl/ phenylene), 7.64 (dd, ^{3}J= 8.1, ^{4}J=3.2 Hz, 2 H, H-phenylene), 7.79 (m, 6H, H-phenyl); ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$): δ: 16.3 (s, $CH_2\mathbf{C}H_3$), 37.7 (s, $\mathbf{C}H_2CH_3$), 109.0 (s, CH-benzodiazaborole), 118.9 (s, CH-benzodiazaborole), 128.7 (d, $^{3}J_{P,C}$= 12.5 Hz, *m*-CH-phenyl), 131.6 (d, $^{3}J_{P,C}$= 10.3 Hz, CH-phenylene), 131.8 (d, $^{4}J_{P,C}$= 3.0 Hz, *p*-CH-phenyl), 132.5 (d, $^{2}J_{P,C}$= 10.8 Hz, *o*-CH-phenyl), 132.6 (d, $^{1}J_{P,C}$= 72.0 Hz, *i*-C-phenylene), 132.9 (d,

$^{1}J_{P,C}$= 85.3 Hz, *i*-C-phenyl), 133.7 (d, $^{2}J_{P,C}$= 12.2 Hz, CH-phenylene), 137.1 (s, C-benzodiazaborole). $^{11}B\{^{1}H\}$NMR(160 MHz, $CDCl_3$): δ= 28.9 (s); $^{31}P\{^{1}H\}$NMR(202 MHz, $CDCl_3$) δ= 43.4 (s). MS/EI: m/z= 466 [M^+] 100%

4-(Diphenyl-selenophosphanyl)-1-(1',3'-diethyl-1',3',2'-benzodiazaborol-2'-yl)-benzene (5)

^{1}H-NMR(500 MHz, $CDCl_3$): δ: 1.32 (t, ^{3}J= 7.14 H, 6H, $CH_2C\mathbf{H}_3$), 3.78 (q, ^{3}J= 7.1 Hz, 4H, $C\mathbf{H}_2CH_3$), 7.07 (m, 2H, H-benzodiazaborole), 7.15 (m, 2H, H-benzodiazaborole), 7.50 (m, 6H, H-phenyl/ phenylene), 7.65 (m, 2 H, H-phenylene), 7.80 (m, 6H, H-phenyl); $^{13}C\{^{1}H\}$NMR (125 MHz, $CDCl_3$): δ: 16.3 (s, $CH_2\mathbf{C}H_3$), 37.7 (s, $\mathbf{C}H_2CH_3$), 109.1 (s, CH-benzodiazaborole), 119.0 (s, CH-benzodiazaborole), 128.6 (d, $^{3}J_{P,C}$= 12.5 Hz, *m*-CH-phenyl), 131.6 (d, $^{1}J_{P,C}$= 76.8 Hz, *i*-C-phenyl), 131.7 (d, $^{4}J_{P,C}$= 3.0 Hz, *p*-CH-phenyl), 131.9 (d, $^{3}J_{P,C}$= 10.4 Hz, CH-phenylene) 132.0 (d, $^{1}J_{P,C}$= 76.6 Hz, *i*-C-phenylene), 132.8(d, $^{2}J_{P,C}$= 10.9 Hz, *o*-CH-phenyl), 133.6 (d, $^{2}J_{P,C}$= 12.1 Hz, CH-phenylene), 137.0 (s, C-benzodiazaborole). $^{11}B\{^{1}H\}$NMR(160 MHz, $CDCl_3$): δ= 27.7 (s); $^{31}P\{^{1}H\}$NMR(202 MHz, $CDCl_3$) δ= 35.4 (s) $^{1}J_{(P\text{-}Se)}$= 364.4 Hz). MS/EI: m/z= 514[M^+] 100%.

[κ-P{4-diphenylphosphanyl)-1-(1',3'-diethyl-1',3',2'-benzodiazaborol-2'-yl)-benzene}-gold(I) chloride] (6)

^{1}H-NMR(300 MHz, $CDCl_3$): δ: 1.33 (t, ^{3}J= 7.1 Hz, 6H, $CH_2C\mathbf{H}_3$), 3.78 (q, ^{3}J= 7.1 Hz, 4H, $C\mathbf{H}_2CH_3$), 7.07 (m, 2H, H-benzodiazaborole), 7.14 (m, 2H, H-benzodiazaborole), 7.48-77.69 (m, 14H, H-phenyl/ phenylene);

$^{13}C\{^{1}H\}$NMR (75.5 MHz, $CDCl_3$): δ: 16.5 (s, $CH_2\mathbf{C}H_3$), 37.8 (s, $\mathbf{C}H_2CH_3$), 109.3 (s, CH-benzodiazaborole), 119.1 (s, CH-benzodiazaborole), 128.7 (d, $^{1}J_{P,C}$= 62.4 Hz, *i*-C-phenyl), 129.0 (d, $^{1}J_{P,C}$= 61.9 Hz, *i*-C-phenylene), 129.3 (d, $^{3}J_{P,C}$= 11.9 Hz, *m*-CH-phenyl), 132.2 (d, $^{4}J_{P,C}$= 2.6 Hz, *p*-CH-phenyl), 133.5 (d, $^{2}J_{P,C}$= 13.2 Hz, CH-phenylene) 134.2 (d, $^{3}J_{P,C}$= 11.5 Hz, CH-phenylene), 137.0 (s, C-benzodiazaborole). $^{11}B\{^{1}H\}$NMR(96.3 MHz, $CDCl_3$): δ= 29.1 (s); $^{31}P\{^{1}H\}$NMR(111.9 MHz, $CDCl_3$) δ= 33.5 (s). A reliable mass spectrum could not be obtaind.

[4-(Methyldiphenylphosphonio)-1-(-(1',3'-diethyl-1',3',2'-benzodiazaborol-2'-yl)-benzene]-monomethylsulfate (7)

^{1}H-NMR(300 MHz, $CDCl_3$): δ: 1.33 (t, ^{3}J= 7.1 Hz, 6H, $CH_2C\mathbf{H}_3$), 3.15 (d, $^{2}J_{P,H}$= 13.2 Hz, 3H, P-$C\mathbf{H}_3$), 3.70 (s, 3H, $OC\mathbf{H}_3$), 3.78 (q, ^{3}J= 7.1 Hz, 4H, $C\mathbf{H}_2CH_3$), 7.12 (m, 4H, H-

benzodiazaborole), 7.80 (m, 14H, H-phenyl/ phenylene); $^{13}C\{^{1}H\}$NMR (75.5 MHz, $CDCl_3$): δ: 9.8 (d, $^{1}J_{P,C}$= 57.9Hz, PC**H**$_3$), 16.6 (s, CH_2**C**H_3), 37.9 (s, **C**H_2CH_3), 54.4 (s, O**C**H_3), 109.7 (s, CH-benzodiazaborole), 119.5 (s, CH-benzodiazaborole), 119.5 (d, $^{1}J_{P,C}$= 88.7 Hz, *i*-C-phenyl/phenylene), 130.7 (d, $^{3}J_{P,C}$= 12.9 Hz, *m*-CH-phenyl), 132.6(d, $^{2}J_{P,C}$= 10.3 Hz, CH-phenylene), 133.5 (d, $^{2}J_{P,C}$= 10.7 Hz, *o*-CH-phenyl), 135.3 (d, $^{3}J_{P,C}$= 12.5 Hz, CH-phenylene), 135.3 (d, $^{4}J_{P,C}$= 3.2 Hz, *p*-CH-phenyl), 136.8 (s, C-benzodiazaborole). $^{11}B\{^{1}H\}$NMR(96.3 MHz, $CDCl_3$): δ= 28.9 (s); $^{31}P\{^{1}H\}$NMR(111.9 MHz, $CDCl_3$) δ= 22.1 (s). MS/ ESI positive m/z= 449 [M^+]

5-(Diphenylphosphanyl)-2-(1',3'diethyl-1',3',2'-benzodiazaborol-2'-yl)thiophene (8)

^{1}H-NMR(300 MHz, $CDCl_3$): δ: 1.34 (t, ^{3}J= 7.2 Hz, 6H, CH_2C**H**$_3$), 3.91 (q, ^{3}J= 7.2 Hz, 4H, C**H**$_2CH_3$), 7.03-7.10 (m, 4H, H-benzodiazaborole), 7.36- 7.46 (m,12H, H-phenyl/ thiophene). $^{13}C\{^{1}H\}$NMR (75.5 MHz, $CDCl_3$): δ: 16.4 (s, CH_2**C**H_3), 38.1 (s, **C**H_2CH_3), 109.1 (s, CH-benzodiazaborole), 119.1 (s, CH-benzodiazaborole), 128.7 (d, $^{3}J_{P,C}$= 7.1 Hz, *m*-H-phenyl), 129.2 (s, *p*-H-phenyl), 133.4 (d, $^{2}J_{P,C}$= 19.8 Hz, *o*-H-phenyl), 134.8 (d, $^{3}J_{P,C}$= 6.8 Hz, CH-thiophene), 137.0 (s, C-benzodiazaborole), 137.1 (d, $^{1}J_{P,C}$= 21.8 Hz, *i*-C-phenyl), 138.1 (d. $^{2}J_{P,C}$= 5.9 Hz, CH-thiophene), 143.0 (d, $^{1}J_{P,C}$= 26.5 Hz, C-thiophene).
$^{11}B\{^{1}H\}$NMR(96.3 MHz, $CDCl_3$): δ= 26.6 (s); $^{31}P\{^{1}H\}$NMR(111.9 MHz, $CDCl_3$) δ= -20.4 (s). MS/EI m/z= 440 [M^+] 100%.

5-(Diphenyl-thiophosphanyl)-2-(1',3',diethyl-1',3',2'-benzodiazaborol-2'-yl)-thiophene 9

^{1}H-NMR(300 MHz, $CDCl_3$): δ: 1.34 (t, ^{3}J= 7.2 Hz, 6H, CH_2C**H**$_3$), 3.90 (q, ^{3}J= 7.2 Hz, 4H, C**H**$_2CH_3$), 7.05-7.15 (m, 4H, H-benzodiazaborole), 7.50 (m,8H, H-phenyl), 7.84 (m, 4H, H-phenyl/ thiophene). $^{13}C\{^{1}H\}$NMR (75.5 MHz, $CDCl_3$): δ: 16.4 (s, CH_2**C**H_3), 38.1 (s, **C**H_2CH_3), 109.2 (s, CH-benzodiazaborole), 119.3 (s, CH-benzodiazaborole), 131.9 (d, $^{4}J_{P,C}$= 4.5 Hz, *p*-CH-phenyl), 131.9 (d, $^{3}J_{P,C}$= 11.3 Hz, *m*-CH-phenyl), 133.8 (d, $^{1}J_{P,C}$= 89.2 Hz, *i*-C-phenyl), 134.6 (d, $^{2}J_{P,C}$= 14.6 Hz, CH-thiophene), 137.1 (s, C-benzodiazaborole), 138.0 (d, $^{3}J_{P,C}$= 10.2 Hz, CH-thiophene), 139.8 (d, $^{1}J_{P,C}$= 91.6 Hz, C-thiophene). $^{11}B\{^{1}H\}$NMR(96.3 MHz, $CDCl_3$): δ= 25.7 (s); $^{31}P\{^{1}H\}$NMR(111.9 MHz, $CDCl_3$) δ= 33.2 (s). MS/EI m/z= 472 [M^+] 100%.

5-(Diphenyl-selenophosphanyl)-2-(1',3'-diethyl-1',3',2'-benzodiazaborol-2'-yl)-thiophene (10)

^{1}H-NMR(300 MHz, $CDCl_3$): δ: 1.34 (t, ^{3}J= 7.2 Hz, 6H, $CH_2C\mathbf{H}_3$), 3.89 (q, ^{3}J= 7.2 Hz, 4H, $C\mathbf{H}_2CH_3$), 7.06 (m, 2H, H-benzodiazaborole), 7.13 (m, 2H, H-benzodiazaborole), 7.50 (m,7H, H-phenyl), 7.58 (dd, 4H, ^{3}J= 7.80; ^{3}J=3.5 Hz, 1H, H-thiophene), 7.83 (m, 4H, H-phenyl). ^{13}C{^{1}H}NMR (75.5 MHz, $CDCl_3$): δ: 15.3 (s, $CH_2\mathbf{C}H_3$), 36.9 (s, $\mathbf{C}H_2CH_3$), 108.1 (s, CH-benzodiazaborole), 118.1 (s, CH-benzodiazaborole), 127,6 (d, $^{3}J_{P,C}$= 13.0 Hz, *m*-H-phenyl), 130.8 (d, $^{4}J_{P,C}$= 3.1 Hz, *p*-CH-phenyl), 131.2 (d, $^{2}J_{P,C}$= 11.6 Hz, *o*-CH-phenyl), 131.6 (d, $^{1}J_{P,C}$= 80.5 Hz, *i*-C-phenyl), 133.5 (d, $^{2}J_{P,C}$= 14.6 Hz, CH-thiophene), 135.9 (s, C-benzodiazaborole), 137.2 (d, $^{1}J_{P,C}$= 82.7 Hz, C-thiophene), 137.4 (d, $^{3}J_{P,C}$= 10.0 Hz, CH-thiophene). ^{11}B{^{1}H}NMR(96.3 MHz, $CDCl_3$): δ= 28.8 (s); ^{31}P{^{1}H}NMR(111.9 MHz, $CDCl_3$) δ= 21.6 (s, $^{1}J_{P,Se}$= 381.5 Hz). MS/EI m/z= 520 [M^+].

[5-(Methyldiphenylphosphonio)-2-(1',3'-diethyl-1',3',2'-benzodiazaborol-2'-yl)-thiophene]- monomethylsulfate (11)

^{1}H-NMR(300 MHz, $CDCl_3$): δ: 1.33 (t, ^{3}J= 7.2 Hz, 6H, $CH_2C\mathbf{H}_3$), 3.12 (d, $^{2}J_{P,H}$= 13.5 Hz, 3H, P-$C\mathbf{H}_3$), 3.63 (s, 3H, $OC\mathbf{H}_3$), 3.86 (q, ^{3}J= 7.2 Hz, 4H, $C\mathbf{H}_2CH_3$), 7.10 (m, 4H, H-benzodiazaborole), 7.76 (m, 11H, H-phenyl/ thiophene) 8.15 (dd, ^{3}J= 3.7; ^{3}J= 7.8 Hz, 1H, H-thiophene). ^{13}C{^{1}H}NMR (75.5 MHz, $CDCl_3$): δ: 11.2 (d, $^{1}J_{P,C}$= 59.1 Hz, $P\mathbf{C}H_3$), 16.5 (s, $CH_2\mathbf{C}H_3$), 38.1 (s, $\mathbf{C}H_2CH_3$), 54.5 (s, $O\mathbf{C}H_3$), 109.6 (s, CH-benzodiazaborole), 119.7 (s, CH-benzodiazaborole), 120.2 (d, $^{1}J_{P,C}$= 91.6 Hz, *i*-C-phenyl), 121.5 (d, $^{1}J_{P,C}$= 101.1 Hz, C-thiophene), 130.5 (d, $^{2}J_{P,C}$= 13.32 Hz, *o*-CH-phenyl), 133.0 (d, $^{3}J_{P,C}$= 11.4 Hz, *m*-CH-phenyl), 135.4 (d, $^{4}J_{P,C}$= 3.1 Hz, *p*-CH-phenyl), 135.4 (d, $^{4}J_{P,C}$= 3.1 Hz, *p*-CH-phenyl), 136.0 (s, C-benzodiazaborol), 143.1 (d, $^{2}J_{P,C}$= 15.9 Hz, C-thiophene). ^{11}B{^{1}H}NMR(96.3 MHz, $CDCl_3$): δ= 25.4 (s); ^{31}P{^{1}H}NMR(111.9 MHz, $CDCl_3$) δ= 15.3 (s). MS/ ESI positive m/z= 455 [M^+].

Compound	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**11**
Empirical formula	$C_{28}H_{28}BN_2P$	$C_{28}H_{28}BN_2OP$ x0.5 H_2O	$C_{28}H_{28}BN_2PS$	$C_{28}H_{28}BN_2PSe$	$C28H28AuBCl_2N_2P$, C_5H_{12}	$C_{30}H_{34}BN_2O_4PS$	$C_{26}H_{26}BN_2PS$	$C_{26}H_{26}BN_2PS_2$	$C_{28}H_{32}BN_2O_4PS_2$
M [g mol^{-1}]	434.30	459.31	466.36	513.26	738.87	560.43	440.33	472.39	566.46
Crystal dimensions [mm]	030 × 0.22 × 0.16	0.30 × 0.20 × 0.11	0.30 × 0.26 × 0.12	0.30 × 0.16 × 0.16	0.12 × 0.08 × 0.04	0.30 × 0.26 × 0.16	0.27 × 0.15 × 0.10	0.25 × 0.20 × 0.06	0.30 × 0.26 × 0.08
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	*C*2/*c*	*C*2/*c*	*C*2/*c*	$P2_1/c$	$P\bar{1}$	$P2_1/c$	$P2_1/c$
a [Å]	9.9777(2)	9.0888(2)	10.14690(10)	10.0975(1)	33.195(7)	19.6129(3)	8.7717(3)	18.8093(7)	18.9789(4)
b [Å]	10.8375(2)	9.2706(2)	15.2300(2)	15.3800(1)	9.7525(16)	8.41430(10)	10.1929(4)	8.1110(3)	8.33800(10)
c[Å]	12.8536(2)	32.2486(6)	32.2144(3)	32.4025(3)	22.556(3)	18.1021(2)	13.9611(5)	17.4215(6)	18.3001(3)
α [°]	103.8797(11)	92.2206(11)	90	90	90	90	102.719(3)	90	90
β [°]	101.0244(11)	94.3510(10)	97.0472(5)	97.9366(5)	128.270(17)	110.7219(7)	91.738(2)	116.3641(19)	109.0221(9)
γ [°]	112.4832(10)	112.3154(11)	90	90	90	90	109.672(2)	90	90
V [$Å^3$]	1183.10(4)	2499.75(9)	4940.72(9)	4983.89(7)	5733.0(17)	2794.11(6)	1139.12(7)	2381.42(15)	2737.78(8)
Z	2	4	8	8	8	4	2	4	4
ζ_{calc} [g cm^{-1}]	1.219	1.220	1.254	1.368	1.712	1.332	1.284	1.318	1.374
μ [mm]	0.134	0.135	0.215	1.590	5.308	0.212	0.229	0.308	0.291
F (000)	460	972	1968	2112	2944	1184	464	992	1192
Θ [°]	2.9-27.5	2.9- 27.5	2.9- 30.0	2.9-30.0	3.1- 27.5	3.0- 30.0	2.9- 30.0	3.3- 27.5	2.9- 30.0
No refl. collected	36873	38832	44387	58689	26951	75053	29176	57086	54160
No refl. unique	5392	11204	7175	7227	6552	8133	6632	5415	7975
R (int)	0.035	0.061	0.043	0.049	0.0453	0.050	0.046	0.093	0.049
Nor refl. [$I > 2\sigma(I)$]	4571	7626	5759	5990	5205	6417	5216	4190	6236
Refined parameters	291	616	300	300	308	356	282	291	359
GOF	1.047	1.037	1.160	1.021	1.037	1.046	1.018	1.037	1.043
R_f [$I > 2\sigma(I)$]	0.0362	0.0747	0.0352	0.0285	0.0317	0.0363	0.0408	0.0466	0.0361

wR_F2 (all data)	0.0947	0.2264	0.0989	0.0724	0.0592	0.0975	0.1093	0.1220	0.0946
$\Delta\zeta_{max/min}$ [e Å^{-3}]	0.271/ -0.283	0.779/ -0.515	0.364/ -0.316	0.398/ -0.406	0.837/ -0.843	0.388/ -0.441	0.302/ -0.374	0.638/ -0.463	0.398/ -0.0:573
Remarks					Disorder of C(7)/C(8) on two positions (61:39) C_5H_{12} was squeezed[55]				Disorder O(2), O(3), O(4) on two positions (92:8)

Table S1: Crystallographic data for **2-9** and **11**.

Atomic coordinates for [B3LYP/6-311G(d,p)] optimized geometry, value of total energy for:

Compound 2

15	3.357119	-0.497333	-1.200807
7	-3.837720	-0.681615	-0.894845
7	-3.461633	0.733094	0.885088
5	-2.797754	-0.036351	-0.135791
6	-5.070500	-0.318500	-0.346746
6	-4.840079	0.558565	0.739176
6	-5.905394	1.084191	1.463849
1	-5.739288	1.758291	2.295714
6	-7.204072	0.722684	1.095975
1	-8.044473	1.122257	1.651796
6	-7.431381	-0.142069	0.024695
1	-8.446967	-0.407911	-0.245118
6	-6.366653	-0.674081	-0.707247
1	-6.553585	-1.347024	-1.535514
6	-3.720281	-1.655302	-1.974655
1	-2.738054	-1.526834	-2.431533
1	-4.461553	-1.419565	-2.745990
6	-3.883090	-3.106034	-1.509544
1	-3.100710	-3.367948	-0.793245
1	-3.808842	-3.788157	-2.361451
1	-4.850508	-3.265533	-1.028507
6	-2.890245	1.653284	1.861396
1	-1.843000	1.380354	1.998845
1	-3.386300	1.499784	2.826076
6	-2.986477	3.124496	1.444476
1	-2.435529	3.295748	0.516538
1	-2.559846	3.767484	2.219876
1	-4.023152	3.427701	1.283293
6	-1.253349	-0.150131	-0.371004
6	-0.393010	-0.634430	0.627810
1	-0.803642	-0.945380	1.583792
6	0.981675	-0.742531	0.425214
1	1.609025	-1.126045	1.221137
6	1.553542	-0.366633	-0.795236
6	0.704559	0.105947	-1.806096
1	1.121947	0.387789	-2.767831
6	-0.665481	0.218539	-1.593968
1	-1.289148	0.601603	-2.395836
6	4.019622	-1.473807	0.229382
6	4.005473	-2.870573	0.104020
1	3.613472	-3.322610	-0.801435
6	4.491931	-3.683444	1.123937
1	4.468977	-4.761769	1.011209
6	5.020858	-3.111575	2.279854
1	5.409771	-3.742739	3.071097
6	5.055387	-1.725206	2.409287
1	5.471193	-1.273408	3.303391

6	4.556427	-0.910941	1.393556
1	4.590377	0.165935	1.507151
6	3.971411	1.213656	-0.835490
6	5.241913	1.548642	-1.325804
1	5.810517	0.812790	-1.885297
6	5.779908	2.813749	-1.108228
1	6.765692	3.053549	-1.491258
6	5.046393	3.773923	-0.413144
1	5.459254	4.763430	-0.251579
6	3.777186	3.458153	0.065707
1	3.198942	4.202164	0.602911
6	3.243367	2.186745	-0.140497
1	2.255053	1.953529	0.237081

Compound 3

15	3.225778	-0.178881	0.953074
7	-3.776932	1.162942	-0.004540
7	-3.829487	-1.142545	0.006260
5	-2.945417	-0.008930	0.098613
6	-5.102986	0.746625	-0.145728
6	-5.134214	-0.667553	-0.148112
6	-6.338449	-1.349005	-0.297436
1	-6.372096	-2.431585	-0.310077
6	-7.513911	-0.604685	-0.424388
1	-8.459964	-1.121077	-0.538877
6	-7.485611	0.790167	-0.399101
1	-8.410210	1.348211	-0.491267
6	-6.279308	1.481318	-0.261378
1	-6.267472	2.564449	-0.249691
6	-3.407632	2.571263	0.083735
1	-2.410050	2.622921	0.523369
1	-4.086776	3.071099	0.783512
6	-3.419675	3.301228	-1.263543
1	-2.701921	2.854375	-1.955776
1	-3.149897	4.352143	-1.125187
1	-4.404411	3.262165	-1.733600
6	-3.512541	-2.566392	0.002337
1	-2.444170	-2.664527	-0.198056
1	-4.035912	-3.041966	-0.834900
6	-3.862306	-3.284082	1.310230
1	-3.305265	-2.859697	2.148859
1	-3.609669	-4.345702	1.236584
1	-4.926249	-3.203240	1.541657
6	-1.389783	-0.042726	0.282148
6	-0.531355	0.659835	-0.581045
1	-0.947703	1.230366	-1.404469
6	0.850904	0.641029	-0.412596
1	1.478113	1.212943	-1.087369

6	1.423460	-0.090489	0.632910
6	0.586422	-0.787308	1.511455
1	1.023882	-1.325983	2.344197
6	-0.792800	-0.764129	1.330973
1	-1.418643	-1.300775	2.036036
6	3.928050	1.399343	0.337553
6	4.049894	2.439899	1.266921
1	3.753056	2.269200	2.295213
6	4.569785	3.670231	0.875915
1	4.664211	4.470114	1.601728
6	4.976583	3.870773	-0.442293
1	5.384841	4.828695	-0.744689
6	4.869732	2.835588	-1.368398
1	5.199607	2.983958	-2.390566
6	4.350602	1.601563	-0.980759
1	4.294104	0.794757	-1.702392
6	3.883747	-1.493707	-0.142167
6	3.293218	-1.862227	-1.355906
1	2.380178	-1.381326	-1.687382
6	3.863202	-2.866872	-2.135533
1	3.398662	-3.149869	-3.073515
6	5.019910	-3.513499	-1.705330
1	5.459999	-4.297277	-2.311748
6	5.603569	-3.160826	-0.489615
1	6.495866	-3.672089	-0.146281
6	5.038114	-2.157063	0.291560
1	5.473003	-1.891969	1.248228
8	3.538813	-0.422878	2.398848

Compound 4

15	3.157625	-0.130937	0.849302
7	-3.892556	1.168072	0.078643
7	-3.902321	-1.133385	-0.068629
5	-3.039618	0.007405	0.104430
6	-5.209969	0.738236	-0.098286
6	-5.214964	-0.672597	-0.197813
6	-6.405513	-1.363995	-0.402397
1	-6.419698	-2.443624	-0.490064
6	-7.593656	-0.634049	-0.485966
1	-8.529279	-1.158228	-0.642788
6	-7.591397	0.756107	-0.364253
1	-8.525613	1.302329	-0.424608
6	-6.399126	1.457877	-0.170845
1	-6.407582	2.537681	-0.085243
6	-3.552596	2.573768	0.269096
1	-2.558278	2.614287	0.716946
1	-4.244527	3.007831	0.999465
6	-3.576116	3.397701	-1.022695
1	-2.849458	3.014785	-1.743403
1	-3.326780	4.441013	-0.809214
1	-4.559310	3.373183	-1.496759
6	-3.562606	-2.548969	-0.161973
1	-2.492157	-2.618452	-0.363372
1	-4.075744	-2.978359	-1.029865
6	-3.906769	-3.352934	1.096315
1	-3.358390	-2.976009	1.962967
1	-3.640590	-4.404515	0.956473
1	-4.972373	-3.299660	1.327720
6	-1.483214	-0.011194	0.284709
6	-0.641706	0.787169	-0.507819
1	-1.070640	1.427992	-1.270639
6	0.742570	0.772442	-0.352747
1	1.356572	1.407857	-0.979875
6	1.333113	-0.046613	0.614882
6	0.513882	-0.838826	1.425833
1	0.959909	-1.451093	2.200963
6	-0.865722	-0.822348	1.253707
1	-1.476395	-1.438347	1.904825
6	3.809185	1.428953	0.115834
6	3.872431	2.568584	0.926305
1	3.571680	2.503343	1.965250
6	4.340402	3.770760	0.405835
1	4.387420	4.648250	1.040734
6	4.759457	3.844507	-0.921959
1	5.131518	4.780663	-1.322929
6	4.709197	2.711217	-1.729095
1	5.044772	2.760239	-2.758888
6	4.234736	1.505436	-1.214625

1	4.210599	0.626800	-1.847454
6	3.727595	-1.471846	-0.279389
6	2.966336	-1.894070	-1.374718
1	1.997224	-1.451254	-1.569542
6	3.444581	-2.899995	-2.212813
1	2.845535	-3.226841	-3.055352
6	4.682170	-3.487873	-1.964094
1	5.051405	-4.272136	-2.615378
6	5.440473	-3.073851	-0.869951
1	6.399753	-3.536111	-0.666572
6	4.965176	-2.074444	-0.026607
1	5.540648	-1.769281	0.839359
16	3.698746	-0.403314	2.732416

Compound 5

34	3.609334	-0.349411	2.522253
15	2.927558	-0.073804	0.514211
7	-4.164117	1.158845	0.134144
7	-4.157304	-1.130064	-0.147832
5	-3.299238	0.009543	0.053520
6	-5.483774	0.723183	-0.008649
6	-5.479065	-0.679440	-0.190611
6	-6.670556	-1.373115	-0.381219
1	-6.677619	-2.445995	-0.530808
6	-7.868649	-0.654810	-0.368493
1	-8.805113	-1.180921	-0.513372
6	-7.874908	0.725912	-0.165992
1	-8.816413	1.262701	-0.152124
6	-6.682239	1.430466	0.014602
1	-6.697612	2.503160	0.164373
6	-3.830422	2.555837	0.389520
1	-2.818816	2.583788	0.797921
1	-4.495812	2.939707	1.170845
6	-3.915814	3.450256	-0.851834
1	-3.215154	3.117687	-1.621562
1	-3.668938	4.483129	-0.590124
1	-4.917289	3.439652	-1.286582
6	-3.806826	-2.531860	-0.346820
1	-2.747374	-2.572546	-0.605830
1	-4.358406	-2.913496	-1.213410
6	-4.077084	-3.418007	0.873732
1	-3.487554	-3.089638	1.733061
1	-3.808849	-4.455233	0.653608
1	-5.129572	-3.392888	1.162942
6	-1.736027	0.000970	0.161843
6	-0.941425	0.852979	-0.622645
1	-1.412482	1.527203	-1.329808
6	0.448892	0.850744	-0.531692

1	1.025152	1.525761	-1.152845
6	1.092885	-0.008532	0.363989
6	0.321086	-0.855016	1.167084
1	0.810302	-1.495871	1.891749
6	-1.064632	-0.852030	1.056627
1	-1.636302	-1.511804	1.700287
6	3.533376	1.485780	-0.260366
6	3.642287	2.630919	0.536925
1	3.406423	2.569072	1.592913
6	4.077775	3.829748	-0.018497
1	4.160996	4.711533	0.606642
6	4.419288	3.894225	-1.368810
1	4.767110	4.827524	-1.797258
6	4.324079	2.754929	-2.163391
1	4.600094	2.796437	-3.211044
6	3.881375	1.552534	-1.614018
1	3.821113	0.669777	-2.238524
6	3.453360	-1.417038	-0.634485
6	2.626239	-1.868900	-1.668643
1	1.636483	-1.449022	-1.799577
6	3.067701	-2.873996	-2.527899
1	2.418360	-3.224149	-3.322446
6	4.333237	-3.430435	-2.361902
1	4.673478	-4.214163	-3.029425
6	5.157567	-2.985842	-1.328970
1	6.139487	-3.423586	-1.189485
6	4.719699	-1.987744	-0.464336
1	5.345164	-1.660279	0.358025

Compound 6

15	-2.138564	0.306978	0.340536
7	4.958915	0.844034	-0.768705
7	4.927478	-0.988786	0.631578
5	4.083978	-0.023045	-0.023119
6	6.272845	0.411333	-0.570221
6	6.254322	-0.706287	0.295878
6	7.440480	-1.324798	0.680270
1	7.438338	-2.175758	1.350443
6	8.644060	-0.828267	0.174644
1	9.576214	-1.300516	0.462197
6	8.660569	0.260054	-0.698778
1	9.605223	0.624009	-1.085850
6	7.475239	0.893141	-1.079531
1	7.500074	1.741463	-1.752577
6	4.631389	1.953667	-1.657681
1	3.571305	1.875712	-1.905165
1	5.183111	1.827888	-2.595852
6	4.926822	3.334170	-1.061983

1	4.341220	3.502614	-0.154819
1	4.672246	4.117375	-1.781665
1	5.981490	3.442097	-0.801414
6	4.568453	-2.070052	1.542838
1	3.554284	-1.877915	1.897690
1	5.222992	-2.024110	2.420489
6	4.642083	-3.463795	0.910655
1	3.952535	-3.547806	0.067220
1	4.373279	-4.226444	1.646988
1	5.645735	-3.685589	0.542804
6	2.521387	0.071629	0.065829
6	1.879464	1.276537	0.398556
1	2.472391	2.159825	0.609548
6	0.492901	1.372381	0.480708
1	0.037235	2.322009	0.734887
6	-0.306105	0.253087	0.224056
6	0.311869	-0.954719	-0.121919
1	-0.293278	-1.824876	-0.351971
6	1.698454	-1.039303	-0.190607
1	2.145530	-1.985318	-0.475278
6	-2.581969	2.083781	0.171528
6	-2.712236	2.615697	-1.118221
1	-2.583080	1.974465	-1.983077
6	-3.022001	3.960570	-1.293168
1	-3.123810	4.361754	-2.294881
6	-3.216310	4.783737	-0.184889
1	-3.467316	5.829255	-0.322926
6	-3.099302	4.258233	1.099225
1	-3.259318	4.892369	1.963787
6	-2.782009	2.913133	1.280295
1	-2.702243	2.511356	2.283037
6	-2.538603	-0.131547	2.080983
6	-1.584917	-0.077944	3.103404
1	-0.563951	0.208137	2.882123
6	-1.941249	-0.406226	4.410119
1	-1.194574	-0.367922	5.195129
6	-3.247731	-0.787067	4.705525
1	-3.521230	-1.045934	5.722070
6	-4.200828	-0.846201	3.689952
1	-5.216202	-1.153340	3.912136
6	-3.848751	-0.526403	2.382512
1	-4.587901	-0.594987	1.592144
79	-3.189223	-1.037305	-1.187156
17	-4.258105	-2.398834	-2.726135

Compound 7

15	3.185196	-0.068215	0.813489
7	-3.831764	1.157192	0.105170
7	-3.831027	-1.141621	-0.116195
5	-2.981725	-0.000920	0.088969
6	-5.149635	0.723638	-0.078671
6	-5.147808	-0.680194	-0.227846
6	-6.334800	-1.372595	-0.454524
1	-6.344767	-2.448015	-0.581970
6	-7.524267	-0.646298	-0.506429
1	-8.458072	-1.167905	-0.678628
6	-7.528952	0.740155	-0.333488
1	-8.466607	1.281562	-0.370819
6	-6.342581	1.441257	-0.118966
1	-6.357976	2.516916	0.005611
6	-3.510123	2.562339	0.340522
1	-2.519724	2.606201	0.798123
1	-4.210729	2.961883	1.081000
6	-3.542417	3.425192	-0.924988
1	-2.813299	3.075948	-1.660948
1	-3.308170	4.464399	-0.678818
1	-4.524700	3.403406	-1.399847
6	-3.495666	-2.554412	-0.271942
1	-2.429661	-2.621413	-0.499136
1	-4.023826	-2.944525	-1.148118
6	-3.825159	-3.408332	0.956666
1	-3.269200	-3.069851	1.835074
1	-3.565157	-4.453791	0.770095
1	-4.887291	-3.362870	1.202742
6	-1.420376	-0.016318	0.267289
6	-0.590621	0.883048	-0.425503
1	-1.028862	1.593432	-1.116202
6	0.791117	0.883946	-0.265910
1	1.393905	1.595033	-0.817764
6	1.392226	-0.031694	0.607676
6	0.588519	-0.945376	1.307783
1	1.026238	-1.668728	1.986586
6	-0.789032	-0.929284	1.134531
1	-1.388143	-1.631877	1.701243
6	3.923430	1.459789	0.177897
6	3.740231	2.660737	0.881078
1	3.165279	2.687225	1.799527
6	4.295013	3.837962	0.392981
1	4.155865	4.763407	0.938466
6	5.028297	3.826397	-0.793690
1	5.460264	4.746233	-1.169540
6	5.206626	2.637232	-1.495802
1	5.775579	2.628668	-2.417517
6	4.657689	1.451250	-1.014591

1	4.805849	0.529063	-1.562459
6	3.896041	-1.501850	-0.036838
6	3.137897	-2.212322	-0.975768
1	2.116145	-1.922643	-1.187267
6	3.701040	-3.301984	-1.635362
1	3.113197	-3.851583	-2.360443
6	5.011618	-3.684711	-1.361522
1	5.445061	-4.534892	-1.874665
6	5.769151	-2.977998	-0.427319
1	6.788408	-3.276615	-0.214435
6	5.218129	-1.887306	0.235117
1	5.822036	-1.343085	0.952055
6	3.570443	-0.205130	2.589654
1	4.650489	-0.182853	2.736688
1	3.117331	0.626585	3.129687
1	3.174596	-1.143306	2.979462

Compound 8

16	-0.061273	0.507931	-1.021232
15	3.003808	0.186657	-1.152114
7	-3.635266	-1.255489	0.128273
7	-3.390613	1.033615	-0.035828
5	-2.653437	-0.202552	0.045235
6	-4.903120	-0.672529	0.098020
6	-4.753022	0.730222	-0.002577
6	-5.869157	1.560821	-0.042992
1	-5.765158	2.636516	-0.117732
6	-7.136849	0.975983	0.006899
1	-8.015736	1.609513	-0.024920
6	-7.284993	-0.409052	0.091286
1	-8.277970	-0.842404	0.122887
6	-6.169497	-1.248604	0.139363
1	-6.295191	-2.322205	0.210578
6	-3.446403	-2.700205	0.177314
1	-2.437386	-2.912060	-0.180023
1	-4.137991	-3.169478	-0.531157
6	-3.644720	-3.300799	1.573213
1	-2.928522	-2.881367	2.284225
1	-3.501501	-4.384797	1.543042
1	-4.647817	-3.100495	1.955484
6	-2.908883	2.410100	-0.089975
1	-1.882570	2.418178	0.280031
1	-3.499604	3.013747	0.607657
6	-2.960795	3.027084	-1.491137
1	-2.325377	2.470832	-2.184008
1	-2.606125	4.061318	-1.460806
1	-3.977143	3.026791	-1.890963
6	-1.111085	-0.393155	0.046772
6	-0.343719	-1.254619	0.802682

1	-0.769600	-1.916607	1.546127
6	1.051056	-1.179666	0.549467
1	1.788485	-1.787521	1.056894
6	1.384412	-0.255778	-0.412853
6	4.034210	-1.243289	-0.573747
6	4.056604	-2.381112	-1.392810
1	3.480551	-2.390637	-2.312392
6	4.810888	-3.496327	-1.040767
1	4.813562	-4.369720	-1.683518
6	5.571870	-3.484274	0.127289
1	6.167843	-4.348639	0.398079
6	5.570214	-2.353063	0.939406
1	6.165252	-2.334160	1.846021
6	4.805586	-1.239322	0.593753
1	4.815870	-0.364770	1.233024
6	3.580940	1.572118	-0.062942
6	4.645653	2.349781	-0.539466
1	5.088373	2.119854	-1.503354
6	5.138012	3.416238	0.207743
1	5.965134	4.004945	-0.173280
6	4.558581	3.734896	1.434727
1	4.933926	4.571784	2.012976
6	3.489552	2.978838	1.910335
1	3.030477	3.225670	2.861500
6	3.004370	1.902989	1.168660
1	2.171579	1.321170	1.545770

Compound 9

16	0.221246	0.500576	0.816181
16	-2.976346	0.392621	2.751170
15	-2.850928	0.090494	0.803995
7	3.843851	-1.284578	-0.051868
7	3.566181	1.005306	-0.138191
5	2.850233	-0.243635	-0.113668
6	5.103100	-0.681762	-0.038597
6	4.932843	0.721002	-0.092743
6	6.036793	1.568905	-0.103109
1	5.917645	2.644677	-0.146721
6	7.311726	1.001739	-0.046299
1	8.181428	1.648513	-0.051452
6	7.479284	-0.382246	0.023225
1	8.477905	-0.800558	0.072930
6	6.376900	-1.239598	0.026019
1	6.517963	-2.312599	0.073909
6	3.672789	-2.729730	0.042683
1	2.652887	-2.919048	0.381330
1	4.340440	-3.112295	0.822308
6	3.933285	-3.467159	-1.274981

1	3.241450	-3.133715	-2.052687
1	3.800926	-4.544286	-1.138750
1	4.948470	-3.291993	-1.636936
6	3.066197	2.373160	-0.240757
1	2.052330	2.328076	-0.641644
1	3.671916	2.910134	-0.978732
6	3.066493	3.131326	1.090207
1	2.413193	2.643433	1.816963
1	2.705043	4.152824	0.941734
1	4.069312	3.183371	1.519367
6	1.308986	-0.459120	-0.153304
6	0.586448	-1.394167	-0.865093
1	1.048519	-2.104363	-1.538693
6	-0.814395	-1.333379	-0.652245
1	-1.525809	-1.995461	-1.127008
6	-1.181910	-0.348119	0.234243
6	-3.894950	-1.297931	0.189941
6	-4.128776	-2.382376	1.042462
1	-3.723406	-2.368178	2.047258
6	-4.894539	-3.459467	0.606646
1	-5.072890	-4.295570	1.273235
6	-5.439842	-3.458486	-0.676199
1	-6.042435	-4.295448	-1.010805
6	-5.218999	-2.375736	-1.524080
1	-5.651692	-2.364965	-2.518106
6	-4.448352	-1.296686	-1.095220
1	-4.294397	-0.452979	-1.756671
6	-3.335262	1.552430	-0.206087
6	-4.356137	2.384878	0.265178
1	-4.813295	2.179354	1.225832
6	-4.764138	3.481807	-0.487616
1	-5.554821	4.123424	-0.115672
6	-4.151797	3.762053	-1.708201
1	-4.466778	4.621836	-2.288828
6	-3.128245	2.941721	-2.176355
1	-2.641613	3.161983	-3.119851
6	-2.719744	1.838261	-1.429474
1	-1.914687	1.210429	-1.792549

Compound 10

16	-0.399934	-0.494660	0.632119
15	2.669011	-0.064718	0.491394
7	-4.060700	1.280392	-0.052687
7	-3.781645	-1.004157	-0.227700
5	-3.068247	0.245594	-0.188390
6	-5.317237	0.673269	-0.011860
6	-5.146347	-0.726278	-0.121046
6	-6.248297	-1.576846	-0.119968

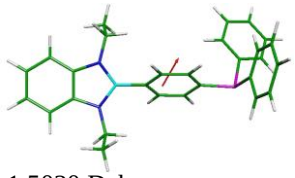
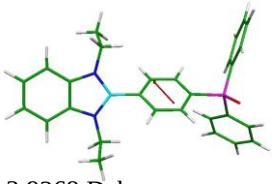
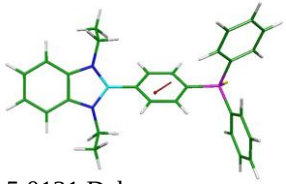
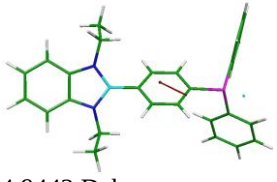
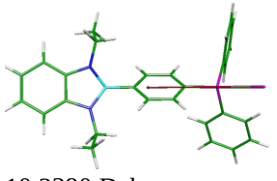
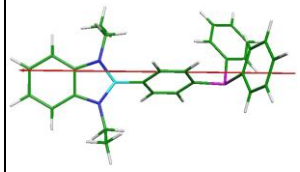
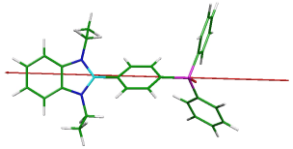
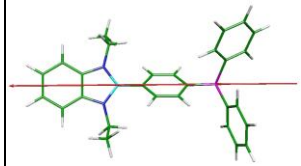
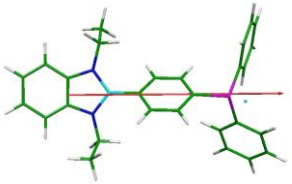
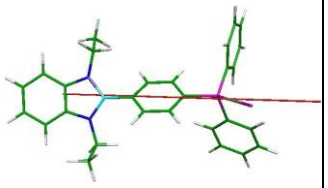
1	-6.128726	-2.650002	-0.206155
6	-7.521326	-1.016237	0.004470
1	-8.389356	-1.665236	0.008973
6	-7.688779	0.363895	0.129261
1	-8.685577	0.777009	0.231437
6	-6.588756	1.224220	0.120667
1	-6.729965	2.294369	0.211842
6	-3.887862	2.721609	0.088100
1	-2.854639	2.900773	0.389926
1	-4.522330	3.072856	0.909109
6	-4.204218	3.507627	-1.188530
1	-3.543919	3.207049	-2.005943
1	-4.068670	4.579212	-1.016436
1	-5.232940	3.342836	-1.515454
6	-3.281229	-2.365501	-0.393897
1	-2.281362	-2.302026	-0.826273
1	-3.909419	-2.879787	-1.129291
6	-3.234018	-3.168640	0.909504
1	-2.559225	-2.701944	1.630555
1	-2.872748	-4.182243	0.714029
1	-4.221747	-3.241393	1.369534
6	-1.530260	0.468760	-0.283519
6	-0.842739	1.417008	-1.012357
1	-1.335465	2.132732	-1.657877
6	0.565548	1.362235	-0.856674
1	1.253943	2.033676	-1.351650
6	0.973643	0.368048	0.002085
6	3.666549	1.369065	-0.100029
6	3.917362	2.422482	0.785303
1	3.556231	2.356836	1.805185
6	4.646262	3.529915	0.362500
1	4.838623	4.341585	1.054884
6	5.137404	3.590148	-0.940690
1	5.711885	4.450424	-1.265455
6	4.899279	2.538223	-1.821988
1	5.289751	2.575043	-2.832737
6	4.165379	1.428768	-1.406188
1	3.996739	0.610139	-2.095148
6	3.149274	-1.470602	-0.599173
6	4.240806	-2.263713	-0.229136
1	4.751096	-2.066032	0.706366
6	4.647537	-3.314064	-1.045772
1	5.493546	-3.925034	-0.752247
6	3.963074	-3.588569	-2.229107
1	4.277287	-4.412866	-2.859461
6	2.868996	-2.808768	-2.595133
1	2.326900	-3.024760	-3.508911
6	2.461663	-1.750156	-1.784875
1	1.604705	-1.152155	-2.070945
34	2.881369	-0.481257	2.573833

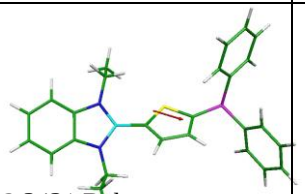
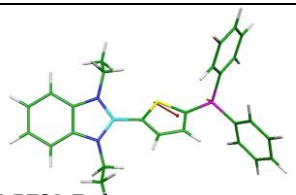
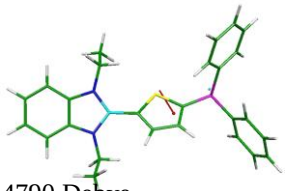
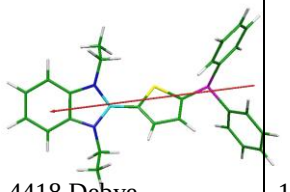
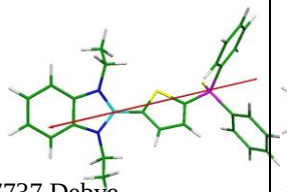
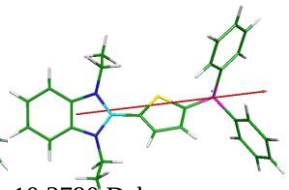
Compound 11

16	0.174288	0.506820	0.820231
15	-2.889276	0.074472	0.715533
7	3.787808	-1.268170	-0.129982
7	3.514390	1.025093	-0.029771
5	2.806202	-0.221621	-0.109185
6	5.049086	-0.667976	-0.063329
6	4.882700	0.732781	-0.006860
6	5.988053	1.578857	0.051207
1	5.873980	2.655081	0.090399
6	7.258115	1.004750	0.066960
1	8.130130	1.645775	0.114443
6	7.422311	-0.383004	0.028012
1	8.420049	-0.804631	0.046458
6	6.321402	-1.235190	-0.038720
1	6.461101	-2.308434	-0.075334
6	3.624506	-2.719663	-0.163084
1	2.611668	-2.948602	0.173811
1	4.303618	-3.162291	0.572178
6	3.874587	-3.334631	-1.543259
1	3.178182	-2.936241	-2.286009
1	3.747158	-4.419619	-1.502006
1	4.886191	-3.125840	-1.895829
6	3.025994	2.402047	-0.032532
1	2.017479	2.400828	-0.451198
1	3.644040	2.986783	-0.720655
6	3.019124	3.056528	1.352022
1	2.360663	2.518239	2.038662
1	2.666063	4.088751	1.279205
1	4.017940	3.070447	1.791823
6	1.259200	-0.434416	-0.166100
6	0.533722	-1.348154	-0.908216
1	0.998599	-2.034682	-1.602254
6	-0.862400	-1.297355	-0.701716
1	-1.570194	-1.941812	-1.206413
6	-1.232852	-0.334986	0.216658
6	-3.977041	-1.325421	0.344051
6	-3.797932	-2.535517	1.032675
1	-3.010944	-2.645313	1.770044
6	-4.631963	-3.613082	0.760052
1	-4.495364	-4.545988	1.293359
6	-5.640726	-3.492790	-0.196439
1	-6.288985	-4.335552	-0.404964
6	-5.816475	-2.294680	-0.883367
1	-6.598627	-2.202351	-1.627010
6	-4.988178	-1.206947	-0.617090
1	-5.132281	-0.277001	-1.152639
6	-3.478636	1.568788	-0.123910
6	-4.601440	2.253700	0.365815

1	-5.123787	1.910844	1.251358
6	-5.060291	3.387489	-0.295289
1	-5.925193	3.917283	0.084997
6	-4.408034	3.840833	-1.441793
1	-4.767991	4.726162	-1.952286
6	-3.295549	3.160583	-1.931062
1	-2.788661	3.513925	-2.820758
6	-2.826466	2.025024	-1.276164
1	-1.956914	1.502416	-1.655721
6	-2.899588	0.380892	2.510755
1	-3.913377	0.605134	2.843259
1	-2.539520	-0.505866	3.032932
1	-2.248267	1.225242	2.741984

B3LYP/6-311G(d,p) ground and excited state dipole moments (Debye), ΔSCF Ionization Energy (eV), HOMO, LUMO energies, Δ(HOMO-LUMO) (eV-nm), Electron Affinity (calculated with 6-311+G(d,p)) and first HOMO→LUMO UV transition for compounds **2**-**6**, **8**-**10**.

	2	**3**	**4**	**5**	**6**
Ground state dipole moment	 1.5020 Debye	 3.9268 Debye	 5.0121 Debye	 4.9442 Debye	 10.2380 Debye
First excited state dipole moment	 15.2555 Debye	 19.2097 Debye	 18.6145 Debye	 11.0900 Debye	 25.2700 Debye
Energy (eV)	-1559.979712	-1635.252850	-1958.220149	-3961.557618	-2156.080655
ΔSCF (Ionization Energy IE) (eV)	6.829	7.182	6.991	6.821	7.257
HOMO (eV)	-5.536	-5.635	-5.670	-5.553	-5.802
LUMO (eV)	-0.978	-1.241	-1.344	-1.346	-1.664
Δ(HOMO-LUMO) (eV-nm)	4.558 - 272.32	4.394 - 282.49	4.325 - 286.99	4.207 - 295.04	4.138 - 299.96
Electron Affinity (EA) (eV)	-0.081	0.166	0.246	0.270	0.581
First HOMO→LUMO UV transition (eV - nm)	4.0207- 308.37	3.8857 - 319.08	3.8136 - 325.11	3.5137 – 352.86	3.6476 – 339.91

	8	**9**	**10**
Ground state dipole moment	 2.3431 Debye	 5.5792 Debye	 5.4790 Debye
First excited state dipole moment	 11.4418 Debye	 13.7737 Debye	 10.3790 Debye
Energy (eV)	-1880.751312	-2278.990166	-4282.327461
ΔSCF (Ionization Energy IE) (eV)	6.781	6.966	6.820
HOMO (eV)	-5.490	-5.646	-5.565
LUMO (eV)	-1.185	-1.460	-1.472
Δ(HOMO-LUMO) (eV-nm)	4.305 - 288.33	4.186 - 296.52	4.093 - 303.26
Electron Affinity (EA) (eV)	0.074	0.312	0.339
First HOMO→LUMO UV transition (eV - nm)	3.7901 - 327.12	3.6728 - 337.57	3.4033 - 364.31

B3LYP/6-311G(d,p) ground and excited state dipole moments (Debye), HOMO, LUMO energies, Δ(HOMO-LUMO) (eV) and first HOMO→LUMO UV transition for compounds **7** and **11**.

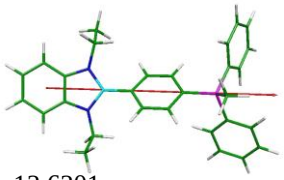
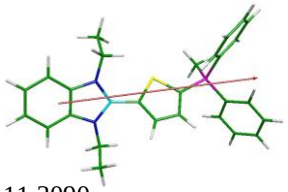
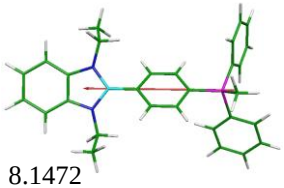
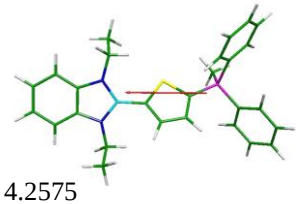
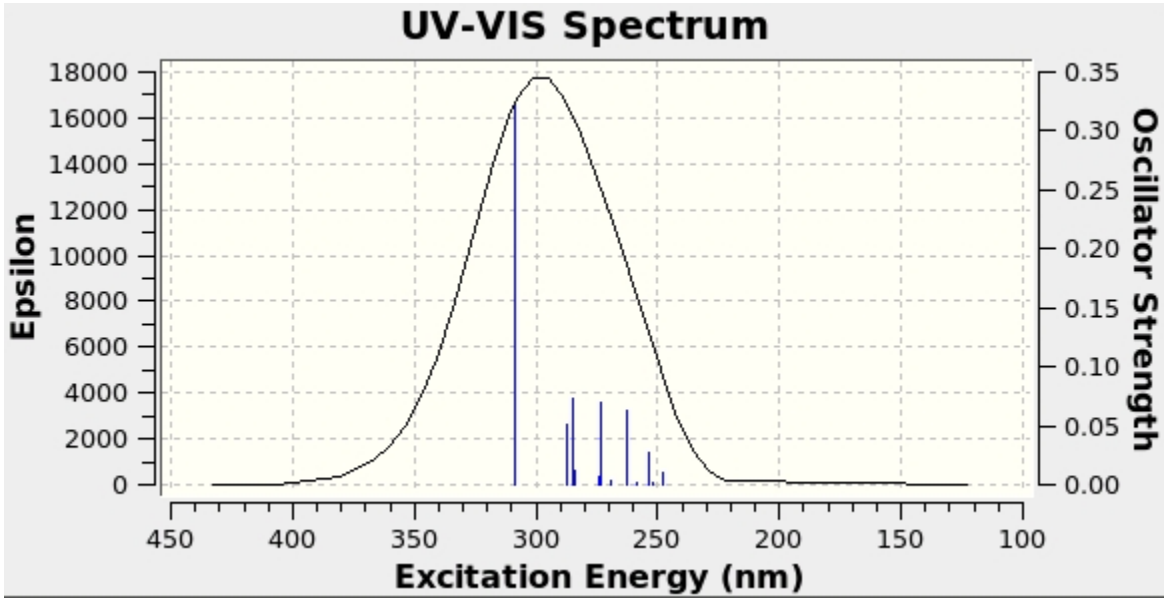
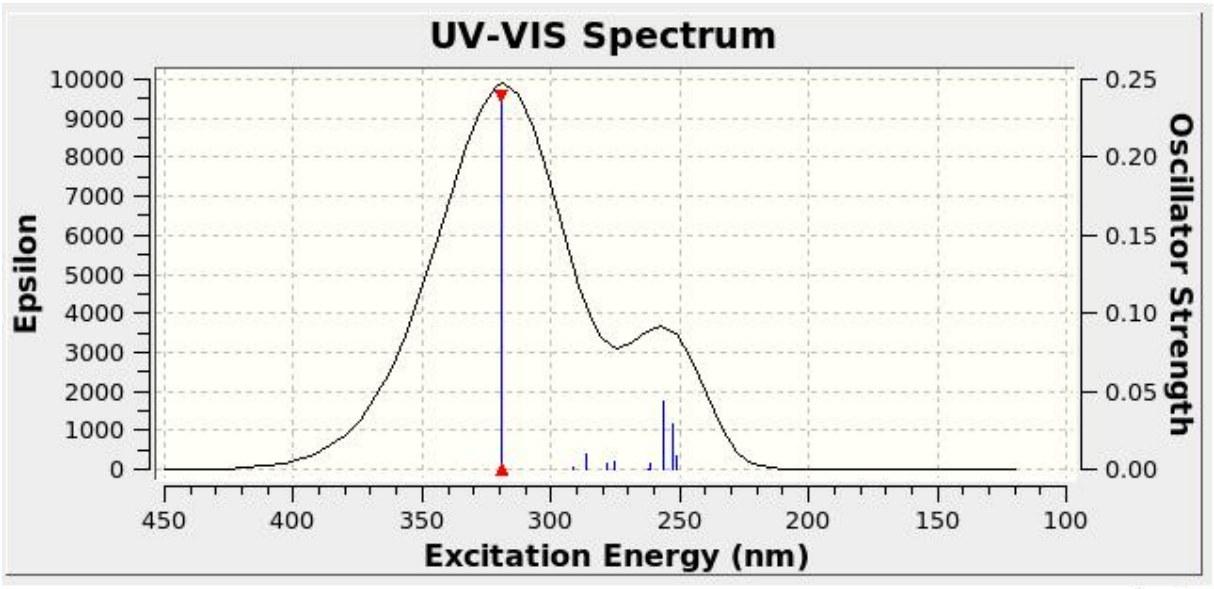
	7	**11**
Ground state dipole moment	 12.6201	 11.3090
First excited state dipole moment	 8.1472	 4.2575
Energy (eV)	-1599.707459	-1920.477396
HOMO (eV)	-7.576	-7.723
LUMO (eV)	-4.501	-4.624
Δ(HOMO-LUMO) (eV- nm)	3.075 - 403.65	3.099 - 400.53
First HOMO→LUMO UV transition (eV - nm)	2.6802 - 462.59	2.6760 - 463.31

Figure 1. B3LYP/6-311G+(d,p) calculated UV-VIS spectrum of **2**.



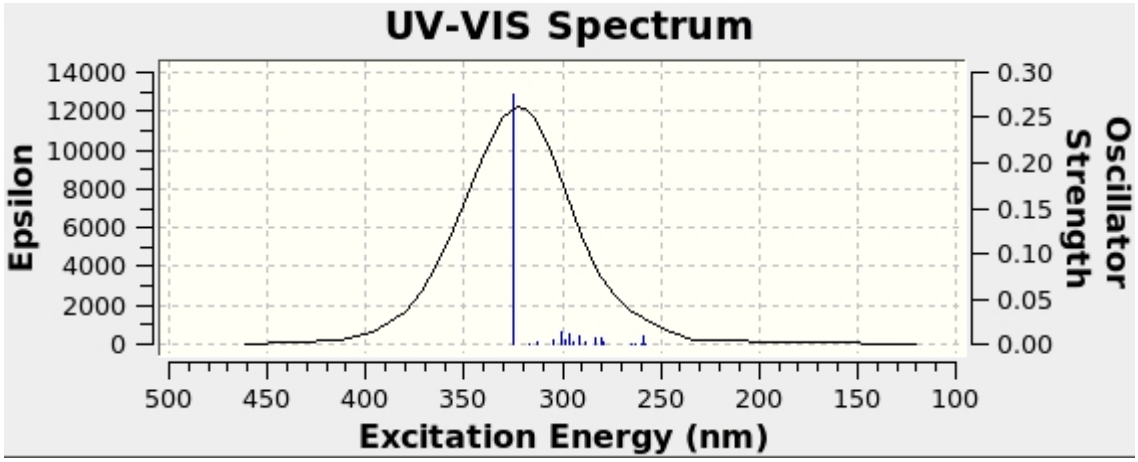
Excited State	1:	Singlet-A	4.0207 eV	308.37 nm	f=0.3217
Excited State	2:	Singlet-A	4.3098 eV	287.68 nm	f=0.0511
Excited State	3:	Singlet-A	4.3525 eV	284.86 nm	f=0.0724
Excited State	4:	Singlet-A	4.3702 eV	283.71 nm	f=0.0123
Excited State	5:	Singlet-A	4.5161 eV	274.54 nm	f=0.0072
Excited State	6:	Singlet-A	4.5321 eV	273.57 nm	f=0.0700
Excited State	7:	Singlet-A	4.5996 eV	269.56 nm	f=0.0039
Excited State	8:	Singlet-A	4.7161 eV	262.90 nm	f=0.0632
Excited State	9:	Singlet-A	4.8005 eV	258.27 nm	f=0.0010
Excited State	10:	Singlet-A	4.8808 eV	254.03 nm	f=0.0068
Excited State	11:	Singlet-A	4.8828 eV	253.92 nm	f=0.0009
Excited State	12:	Singlet-A	4.8931 eV	253.39 nm	f=0.0277
Excited State	13:	Singlet-A	4.9236 eV	251.81 nm	f=0.0010
Excited State	14:	Singlet-A	5.0020 eV	247.87 nm	f=0.0097
Excited State	15:	Singlet-A	5.0088 eV	247.53 nm	f=0.0012

Figure 2. B3LYP/6-311G+(d,p) calculated UV-VIS spectrum of **3**.



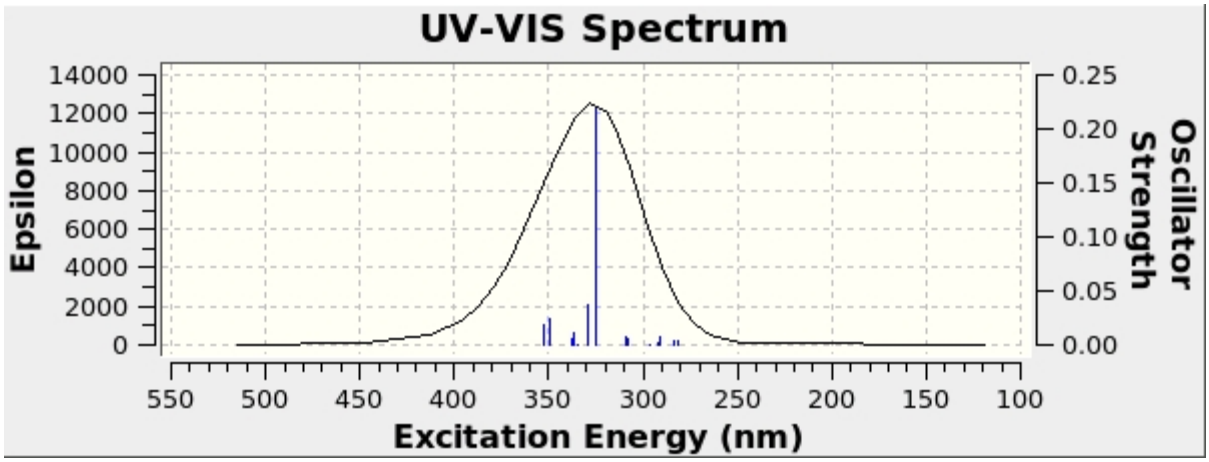
Excited State	1:	Singlet-A	3.8857 eV	319.08 nm	f=0.2395
Excited State	2:	Singlet-A	4.2506 eV	291.69 nm	f=0.0012
Excited State	3:	Singlet-A	4.3291 eV	286.40 nm	f=0.0091
Excited State	4:	Singlet-A	4.4582 eV	278.11 nm	f=0.0040
Excited State	5:	Singlet-A	4.4987 eV	275.60 nm	f=0.0047
Excited State	6:	Singlet-A	4.7313 eV	262.05 nm	f=0.0001
Excited State	7:	Singlet-A	4.7463 eV	261.22 nm	f=0.0035
Excited State	8:	Singlet-A	4.8335 eV	256.51 nm	f=0.0435
Excited State	9:	Singlet-A	4.9065 eV	252.69 nm	f=0.0295
Excited State	10:	Singlet-A	4.9403 eV	250.96 nm	f=0.0087

Figure 3. B3LYP/6-311G+(d,p) calculated UV-VIS spectrum of **4**.



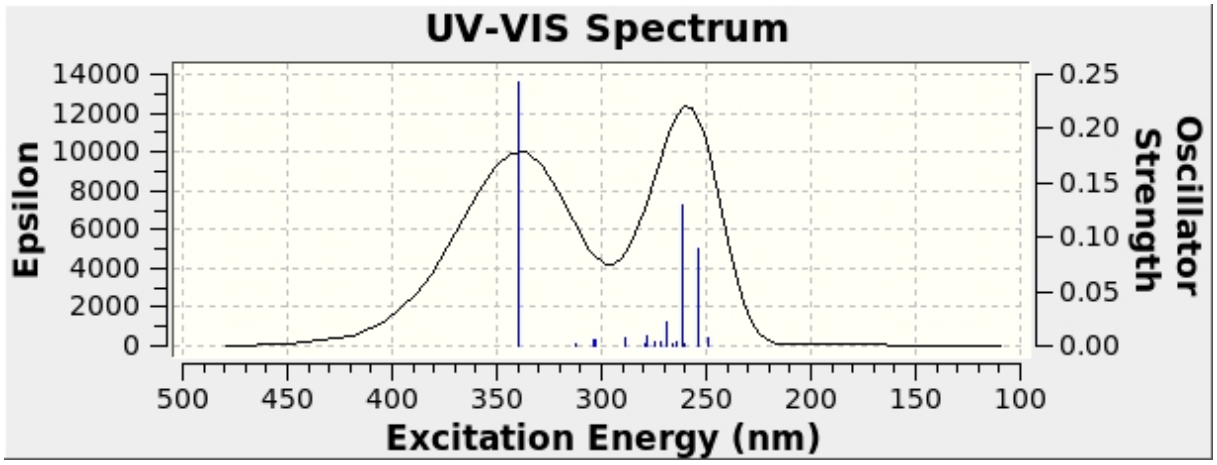
Excited State 1:	Singlet-A	3.8136 eV	325.11 nm	f=0.2757
Excited State 2:	Singlet-A	3.9181 eV	316.44 nm	f=0.0005
Excited State 3:	Singlet-A	3.9690 eV	312.38 nm	f=0.0027
Excited State 4:	Singlet-A	4.0706 eV	304.59 nm	f=0.0036
Excited State 5:	Singlet-A	4.1313 eV	300.11 nm	f=0.0132
Excited State 6:	Singlet-A	4.1603 eV	298.02 nm	f=0.0053
Excited State 7:	Singlet-A	4.1766 eV	296.86 nm	f=0.0117
Excited State 8:	Singlet-A	4.2042 eV	294.90 nm	f=0.0020
Excited State 9:	Singlet-A	4.2610 eV	290.97 nm	f=0.0091
Excited State 10:	Singlet-A	4.3060 eV	287.93 nm	f=0.0014
Excited State 11:	Singlet-A	4.3777 eV	283.22 nm	f=0.0063
Excited State 12:	Singlet-A	4.4213 eV	280.42 nm	f=0.0066
Excited State 13:	Singlet-A	4.4486 eV	278.70 nm	f=0.0033
Excited State 14:	Singlet-A	4.6727 eV	265.34 nm	f=0.0002
Excited State 15:	Singlet-A	4.7127 eV	263.09 nm	f=0.0003
Excited State 16:	Singlet-A	4.7770 eV	259.54 nm	f=0.0006
Excited State 17:	Singlet-A	4.7831 eV	259.21 nm	f=0.0079
Excited State 18:	Singlet-A	4.7932 eV	258.67 nm	f=0.0039
Excited State 19:	Singlet-A	4.7943 eV	258.61 nm	f=0.0076
Excited State 20:	Singlet-A	4.8167 eV	257.41 nm	f=0.0010

Figure 4. B3LYP/6-311G+(d,p) calculated UV-VIS spectrum of **5**.



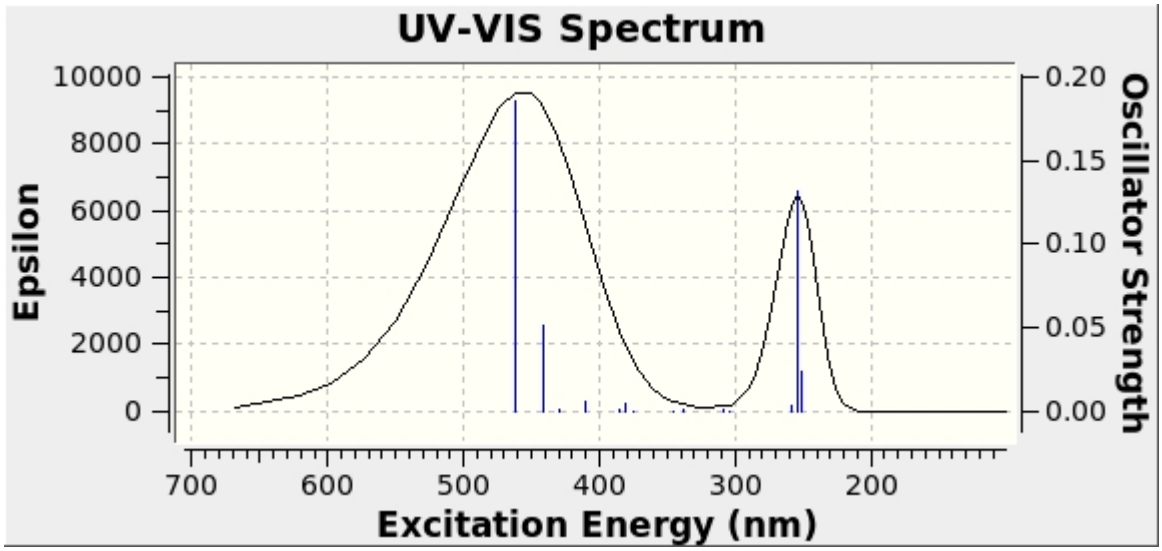
Excited State	1:	Singlet-A	3.5137 eV	352.86 nm	f=0.0182
Excited State	2:	Singlet-A	3.5534 eV	348.91 nm	f=0.0234
Excited State	3:	Singlet-A	3.6710 eV	337.74 nm	f=0.0063
Excited State	4:	Singlet-A	3.6813 eV	336.79 nm	f=0.0102
Excited State	5:	Singlet-A	3.7008 eV	335.02 nm	f=0.0001
Excited State	6:	Singlet-A	3.7636 eV	329.43 nm	f=0.0362
Excited State	7:	Singlet-A	3.8209 eV	324.49 nm	f=0.2187
Excited State	8:	Singlet-A	4.0170 eV	308.65 nm	f=0.0076
Excited State	9:	Singlet-A	4.0230 eV	308.19 nm	f=0.0062
Excited State	10:	Singlet-A	4.1859 eV	296.19 nm	f=0.0005
Excited State	11:	Singlet-A	4.2497 eV	291.75 nm	f=0.0022
Excited State	12:	Singlet-A	4.2577 eV	291.20 nm	f=0.0072
Excited State	13:	Singlet-A	4.3778 eV	283.21 nm	f=0.0029
Excited State	14:	Singlet-A	4.4017 eV	281.68 nm	f=0.0034
Excited State	15:	Singlet-A	4.4050 eV	281.47 nm	f=0.0041

Figure 5. B3LYP/6-311G+(d,p) calculated UV-VIS spectrum of **6**.



Excited State	1:	Singlet-A	3.6476 eV	339.91 nm	f=0.2431
Excited State	2:	Singlet-A	3.9762 eV	311.82 nm	f=0.0012
Excited State	3:	Singlet-A	4.0815 eV	303.77 nm	f=0.0060
Excited State	4:	Singlet-A	4.0952 eV	302.75 nm	f=0.0046
Excited State	5:	Singlet-A	4.2990 eV	288.40 nm	f=0.0080
Excited State	6:	Singlet-A	4.4333 eV	279.67 nm	f=0.0016
Excited State	7:	Singlet-A	4.4446 eV	278.96 nm	f=0.0001
Excited State	8:	Singlet-A	4.4559 eV	278.25 nm	f=0.0099
Excited State	9:	Singlet-A	4.5130 eV	274.73 nm	f=0.0040
Excited State	10:	Singlet-A	4.5637 eV	271.68 nm	f=0.0034
Excited State	11:	Singlet-A	4.5644 eV	271.63 nm	f=0.0004
Excited State	12:	Singlet-A	4.6054 eV	269.21 nm	f=0.0222
Excited State	13:	Singlet-A	4.6541 eV	266.40 nm	f=0.0024
Excited State	14:	Singlet-A	4.6977 eV	263.92 nm	f=0.0028
Excited State	15:	Singlet-A	4.7006 eV	263.76 nm	f=0.0031
Excited State	16:	Singlet-A	4.7475 eV	261.16 nm	f=0.1289
Excited State	17:	Singlet-A	4.7683 eV	260.02 nm	f=0.0019
Excited State	18:	Singlet-A	4.8768 eV	254.23 nm	f=0.0899
Excited State	19:	Singlet-A	4.8864 eV	253.73 nm	f=0.0486
Excited State	20:	Singlet-A	4.9859 eV	248.67 nm	f=0.0073

Figure 6. B3LYP/6-311G+(d,p) calculated UV-VIS spectrum of **7**.



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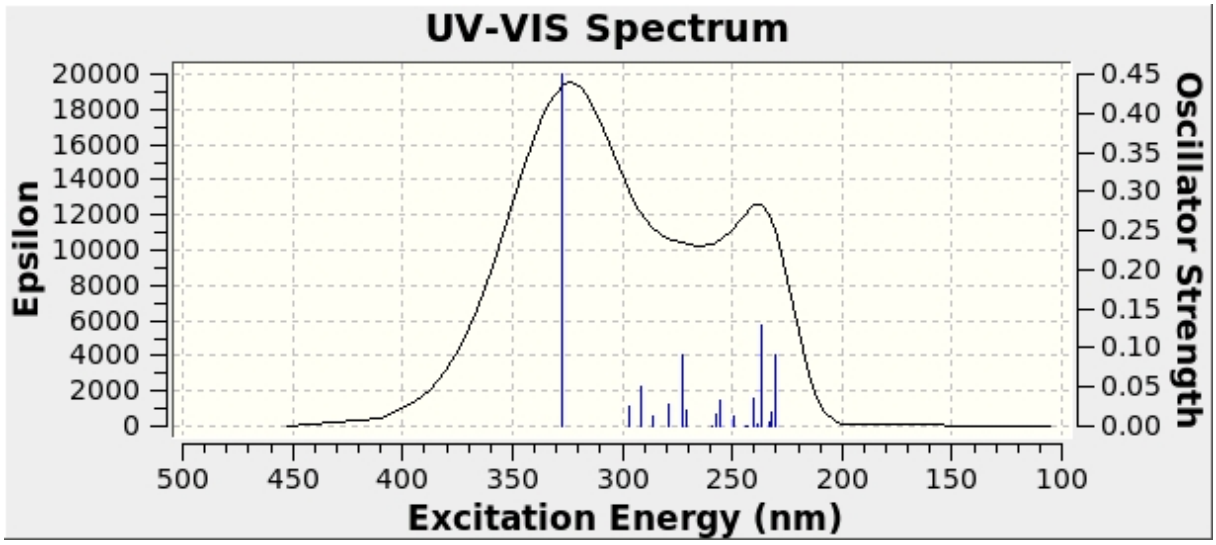
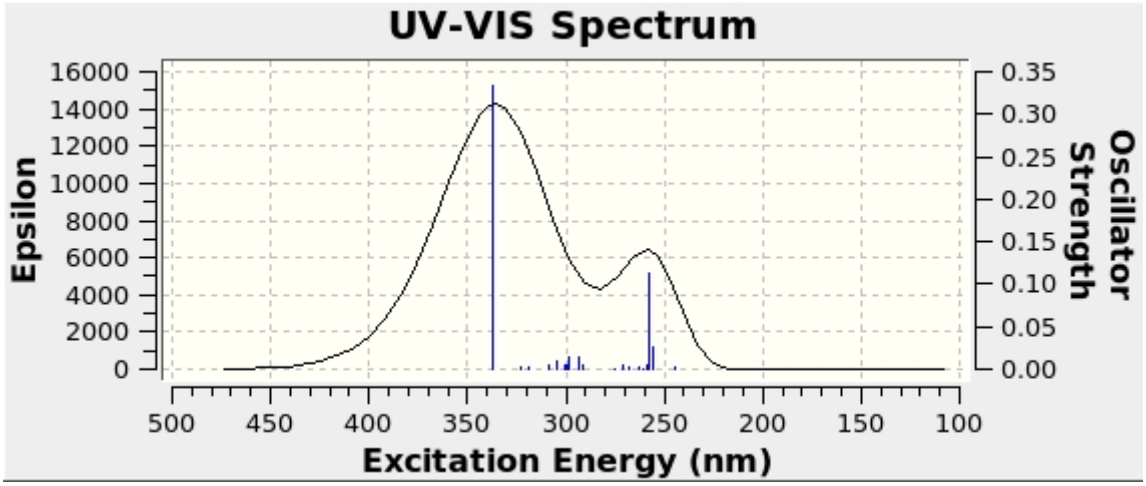
Excited State	1:	Singlet-A	2.6802 eV	462.59 nm	f=0.1857
Excited State	2:	Singlet-A	2.8122 eV	440.89 nm	f=0.0508
Excited State	3:	Singlet-A	2.8849 eV	429.76 nm	f=0.0006
Excited State	4:	Singlet-A	3.0262 eV	409.70 nm	f=0.0054
Excited State	5:	Singlet-A	3.2181 eV	385.27 nm	f=0.0009
Excited State	6:	Singlet-A	3.2526 eV	381.18 nm	f=0.0042
Excited State	7:	Singlet-A	3.3006 eV	375.64 nm	f=0.0001
Excited State	8:	Singlet-A	3.5969 eV	344.70 nm	f=0.0002
Excited State	9:	Singlet-A	3.6654 eV	338.25 nm	f=0.0002
Excited State	10:	Singlet-A	3.6754 eV	337.33 nm	f=0.0006
Excited State	11:	Singlet-A	4.0251 eV	308.02 nm	f=0.0009
Excited State	12:	Singlet-A	4.0787 eV	303.98 nm	f=0.0000
Excited State	13:	Singlet-A	4.7996 eV	258.32 nm	f=0.0029
Excited State	14:	Singlet-A	4.8743 eV	254.36 nm	f=0.1319
Excited State	15:	Singlet-A	4.9320 eV	251.39 nm	f=0.0240

Figure .7 B3LYP/6-311G+(d,p) calculated UV-VIS spectrum of **8**.



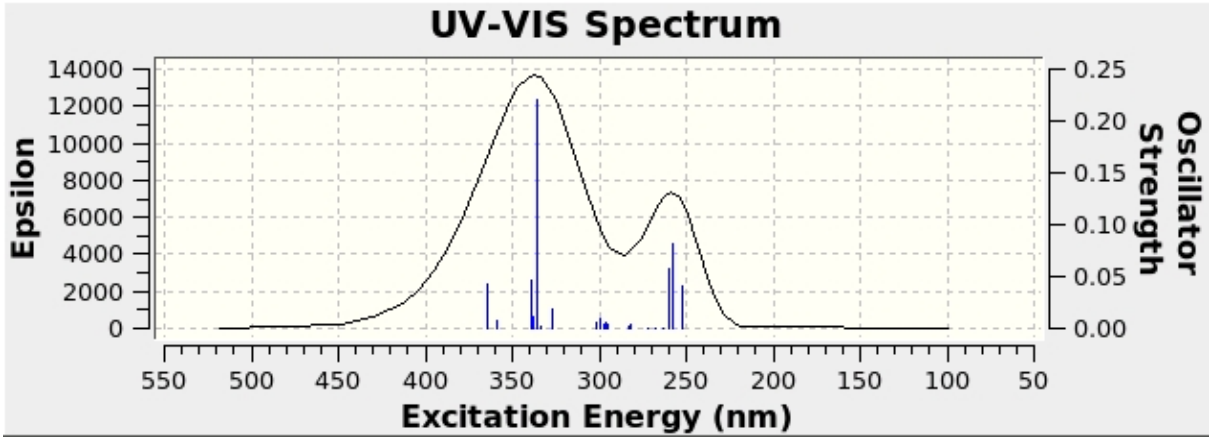
Excited State 1:	Singlet-A	3.7901 eV	327.12 nm	f=0.4491
Excited State 2:	Singlet-A	4.1709 eV	297.26 nm	f=0.0253
Excited State 3:	Singlet-A	4.2545 eV	291.42 nm	f=0.0498
Excited State 4:	Singlet-A	4.3279 eV	286.48 nm	f=0.0134
Excited State 5:	Singlet-A	4.4528 eV	278.44 nm	f=0.0278
Excited State 6:	Singlet-A	4.5530 eV	272.31 nm	f=0.0904
Excited State 7:	Singlet-A	4.5848 eV	270.43 nm	f=0.0212
Excited State 8:	Singlet-A	4.7898 eV	258.85 nm	f=0.0008
Excited State 9:	Singlet-A	4.8244 eV	257.00 nm	f=0.0146
Excited State 10:	Singlet-A	4.8456 eV	255.87 nm	f=0.0230
Excited State 11:	Singlet-A	4.8515 eV	255.56 nm	f=0.0336
Excited State 12:	Singlet-A	4.9827 eV	248.83 nm	f=0.0134
Excited State 13:	Singlet-A	5.0835 eV	243.90 nm	f=0.0004
Excited State 14:	Singlet-A	5.0974 eV	243.23 nm	f=0.0009
Excited State 15:	Singlet-A	5.1701 eV	239.81 nm	f=0.0366
Excited State 16:	Singlet-A	5.2085 eV	238.04 nm	f=0.0015
Excited State 17:	Singlet-A	5.2467 eV	236.31 nm	f=0.1279
Excited State 18:	Singlet-A	5.3154 eV	233.25 nm	f=0.0060
Excited State 19:	Singlet-A	5.3321 eV	232.53 nm	f=0.0165
Excited State 20:	Singlet-A	5.3776 eV	230.56 nm	f=0.0905

Figure 8. B3LYP/6-311G+(d,p) calculated UV-VIS spectrum of **9**.



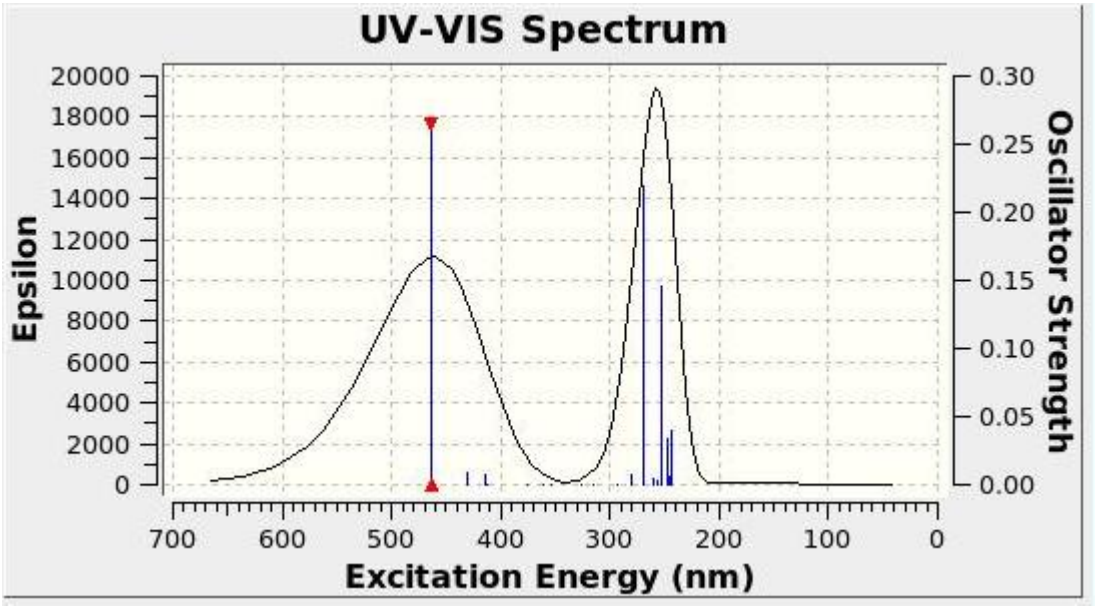
Excited State	1:	Singlet-A	3.6728 eV	337.57 nm	f=0.3338
Excited State	2:	Singlet-A	3.8434 eV	322.59 nm	f=0.0017
Excited State	3:	Singlet-A	3.8862 eV	319.04 nm	f=0.0025
Excited State	4:	Singlet-A	4.0192 eV	308.48 nm	f=0.0039
Excited State	5:	Singlet-A	4.0683 eV	304.76 nm	f=0.0083
Excited State	6:	Singlet-A	4.1190 eV	301.00 nm	f=0.0048
Excited State	7:	Singlet-A	4.1406 eV	299.44 nm	f=0.0058
Excited State	8:	Singlet-A	4.1469 eV	298.98 nm	f=0.0133
Excited State	9:	Singlet-A	4.2209 eV	293.74 nm	f=0.0142
Excited State	10:	Singlet-A	4.2608 eV	290.99 nm	f=0.0050
Excited State	11:	Singlet-A	4.5039 eV	275.28 nm	f=0.0009
Excited State	12:	Singlet-A	4.5817 eV	270.61 nm	f=0.0051
Excited State	13:	Singlet-A	4.6248 eV	268.08 nm	f=0.0003
Excited State	14:	Singlet-A	4.6296 eV	267.81 nm	f=0.0022
Excited State	15:	Singlet-A	4.7099 eV	263.24 nm	f=0.0033
Excited State	16:	Singlet-A	4.7508 eV	260.98 nm	f=0.0005
Excited State	17:	Singlet-A	4.7917 eV	258.75 nm	f=0.0044
Excited State	18:	Singlet-A	4.8143 eV	257.53 nm	f=0.1127
Excited State	19:	Singlet-A	4.8396 eV	256.19 nm	f=0.0265
Excited State	20:	Singlet-A	5.0785 eV	244.14 nm	f=0.0014

Figure 9. B3LYP/6-311G+(d,p) calculated UV-VIS spectrum of **10**.



Excited State	1:	Singlet-A	3.4033 eV	364.31 nm	f=0.0432
Excited State	2:	Singlet-A	3.4555 eV	358.80 nm	f=0.0080
Excited State	3:	Singlet-A	3.6521 eV	339.48 nm	f=0.0467
Excited State	4:	Singlet-A	3.6657 eV	338.23 nm	f=0.0111
Excited State	5:	Singlet-A	3.6917 eV	335.85 nm	f=0.2207
Excited State	6:	Singlet-A	3.7126 eV	333.96 nm	f=0.0021
Excited State	7:	Singlet-A	3.7968 eV	326.55 nm	f=0.0193
Excited State	8:	Singlet-A	4.1040 eV	302.10 nm	f=0.0060
Excited State	9:	Singlet-A	4.1355 eV	299.80 nm	f=0.0098
Excited State	10:	Singlet-A	4.1718 eV	297.19 nm	f=0.0035
Excited State	11:	Singlet-A	4.1875 eV	296.08 nm	f=0.0057
Excited State	12:	Singlet-A	4.1976 eV	295.37 nm	f=0.0037
Excited State	13:	Singlet-A	4.3804 eV	283.04 nm	f=0.0027
Excited State	14:	Singlet-A	4.4071 eV	281.33 nm	f=0.0044
Excited State	15:	Singlet-A	4.5606 eV	271.86 nm	f=0.0003
Excited State	16:	Singlet-A	4.6257 eV	268.03 nm	f=0.0002
Excited State	17:	Singlet-A	4.7184 eV	262.77 nm	f=0.0003
Excited State	18:	Singlet-A	4.7666 eV	260.11 nm	f=0.0565
Excited State	19:	Singlet-A	4.8063 eV	257.96 nm	f=0.0824
Excited State	20:	Singlet-A	4.9081 eV	252.61 nm	f=0.0403

Figure 10. B3LYP/6-311G+(d,p) calculated UV-VIS spectrum of **11**.



Excited State	1:	Singlet-A	2.6760 eV	463.31 nm	f=0.2653
Excited State	2:	Singlet-A	2.8760 eV	431.10 nm	f=0.0093
Excited State	3:	Singlet-A	2.9959 eV	413.84 nm	f=0.0067
Excited State	4:	Singlet-A	3.0042 eV	412.71 nm	f=0.0002
Excited State	5:	Singlet-A	3.3072 eV	374.89 nm	f=0.0003
Excited State	6:	Singlet-A	3.4336 eV	361.09 nm	f=0.0002
Excited State	7:	Singlet-A	3.5135 eV	352.88 nm	f=0.0003
Excited State	8:	Singlet-A	3.8006 eV	326.22 nm	f=0.0001
Excited State	9:	Singlet-A	3.9378 eV	314.86 nm	f=0.0001
Excited State	10:	Singlet-A	4.2248 eV	293.47 nm	f=0.0000
Excited State	11:	Singlet-A	4.4317 eV	279.77 nm	f=0.0073
Excited State	12:	Singlet-A	4.6110 eV	268.89 nm	f=0.2194
Excited State	13:	Singlet-A	4.7735 eV	259.74 nm	f=0.0037
Excited State	14:	Singlet-A	4.8307 eV	256.66 nm	f=0.0034
Excited State	15:	Singlet-A	4.9018 eV	252.94 nm	f=0.1070
Excited State	16:	Singlet-A	4.9148 eV	252.27 nm	f=0.1462
Excited State	17:	Singlet-A	4.9973 eV	248.10 nm	f=0.0341
Excited State	18:	Singlet-A	5.0055 eV	247.70 nm	f=0.0043
Excited State	19:	Singlet-A	5.0386 eV	246.07 nm	f=0.0060
Excited State	20:	Singlet-A	5.0890 eV	243.63 nm	f=0.0402