

Supplementary Information for:

## Organophosphorus-B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> adducts: towards new solid-state emitting materials

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## 1. General section:

Reactions were carried out in dry glassware and under inert atmosphere of purified argon or nitrogen using Schlenk techniques. CH<sub>2</sub>Cl<sub>2</sub> was used directly from a solvent purification system MB SPS-800. Dried deuterated solvents were dried over molecular sieves. Compounds **1a** and **1b** were prepared according to our reported protocols.<sup>[S1]</sup>

**NMR:** <sup>1</sup>H, <sup>13</sup>C, <sup>31</sup>P, <sup>11</sup>B and <sup>19</sup>F NMR as well as COSY, ROESY, HSQC and HMBC spectra were recorded on a Bruker Avance III, Bruker Avance 400, Bruker Avance-III-300, Bruker Avance DRX-300, Bruker Avance 500 or Bruker Avance 600. Chemical shifts are expressed as parts per million (ppm, δ) and referenced to external 85% H<sub>3</sub>PO<sub>4</sub> (<sup>31</sup>P), or solvent signals (<sup>1</sup>H / <sup>13</sup>C): CDCl<sub>3</sub> (7.27 / 77.16 ppm) and CD<sub>2</sub>Cl<sub>2</sub> (5.33 / 53.80 ppm) as internal standards. Signal descriptions include: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet and br = broad. All coupling constants are absolute values and *J* values are expressed in Hertz (Hz).

**Mass spectrometry:** (MS and HRMS) were measured at the Institute of Organic Chemistry of the University Heidelberg. A Bruker ApexQe FT-ICR was used for ESI spectra and a JEOL JMS-700 MS for EI+ and LIFDI. GCMS was performed in a GC system 7890a from Agilent Technologies.

**X-Ray crystallography:** X-ray crystal structure analyses were measured on Bruker Smart CCD or Bruker Smart APEX instrument using Mo-K $\alpha$  radiation. Diffraction intensities were corrected for Lorentz and polarization effects. An empirical absorption correction was applied using SADABS<sup>[S2]</sup> based on the Laue symmetry of reciprocal space. Heavy atom diffractions were solved by direct methods and refined against F<sub>2</sub> with the full matrix least square algorithm. Hydrogen atoms were either isotropically refined or calculated. The structures were solved and refined using the SHELXTL<sup>[S3]</sup> software package. Crystal structure of **2a** (CCDC 1904487) was obtained by crystallization from DCM, crystals of **2b** (CCDC 1904488) were grown by slow diffusion of *n*-pentane into a saturated solution of DCM, crystal structures of **1a** and **1b** were obtained according to previously reported methods.<sup>[S1]</sup>

**Theoretical calculations:** Theoretical calculations have been carried out at the B3LYP/6-31G\* level using the GAUSSIAN 09 suite of programs.<sup>[S4]</sup>

**Steady-state spectroscopy:** Absorption and emission spectra were recorded from DCM solutions using a Jasco V660 and Jasco FP6500 spectrometer, respectively.

**Fluorescence quantum yields  $\Phi$ :** Quantum yields in solution were calculated relative to quinine sulfate in 0.1 M sulfuric acid as a reference ( $\Phi = 0.54$  according to the literature<sup>[S5]</sup>) from five dilutions and using the formula:

$$\Phi_x = \Phi_{st} (\text{Grad}_x / \text{Grad}_{st}) (n_x^2 / n_{st}^2)$$

$\Phi_x$ : quantum yield of sample X

$\Phi_{st}$ : quantum yield of the reference

Grad<sub>x</sub>: Gradient from the plot of integrated fluorescence intensity vs absorbance of the sample  
x

Grad<sub>st</sub>: Gradient from the plot of integrated fluorescence intensity vs absorbance of the reference

n<sub>x</sub>: refractive index from the solvent employed with the sample X

n<sub>st</sub>: refractive index from the solvent employed with the reference

Quantum yields in the solid state were measured with a calibrated Ulbricht sphere; values are an average from at least two independent measurements.

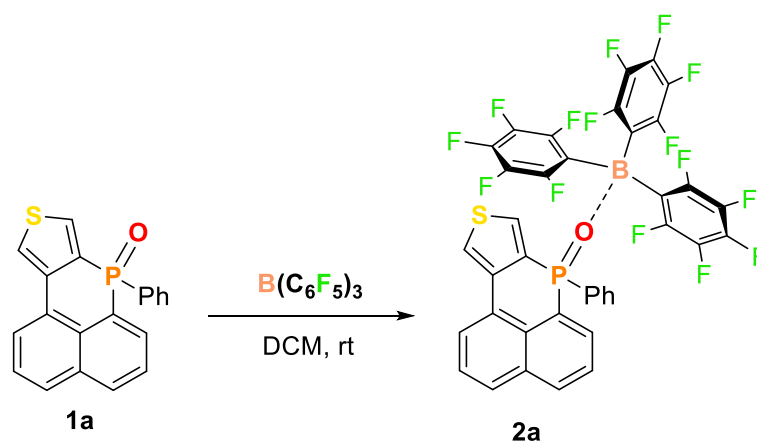
**Fluorescence lifetimes  $\tau$ :** The fluorescence decays were recorded with a HORIBA Scientific Fluorocube single photon counting system operated with HORIBA Scientific DataStation version 2.2. Fluorescence lifetimes were acquired by an exponential fit according to the least mean square with commercially available software HORIBA Scientific Decay Data Analyses 6 (DAS6) version 6.4.4.

**Deactivation pathways constants:** Radiative decay constant ( $k_r$ ) was calculated according to the following equation:  $k_r = \Phi / \tau$ ; while the non-radiative decay constant ( $k_{nr}$ ) was calculated using the following formula:  $k_{nr} = (1-\Phi) / \tau$ .

## 2. Experimental Details

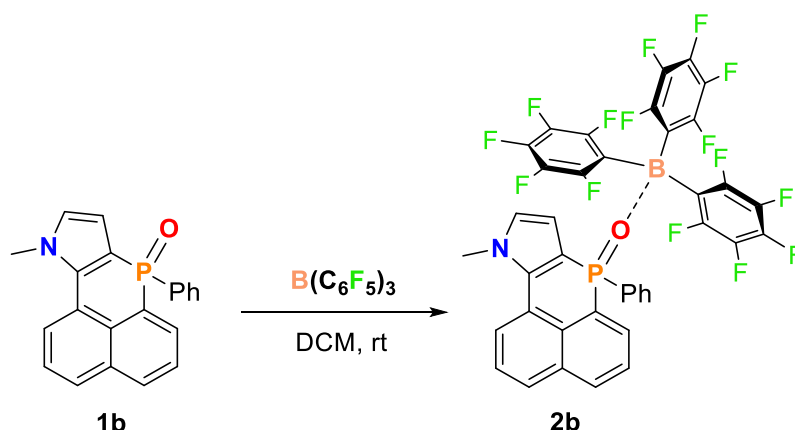
### 2.1. Synthetic procedures

#### (2a) 7-Phenylbenzo[4,5]phosphinolino[3,2-*b*]thiophene 7-oxide tris(pentafluorophenyl)borane adduct

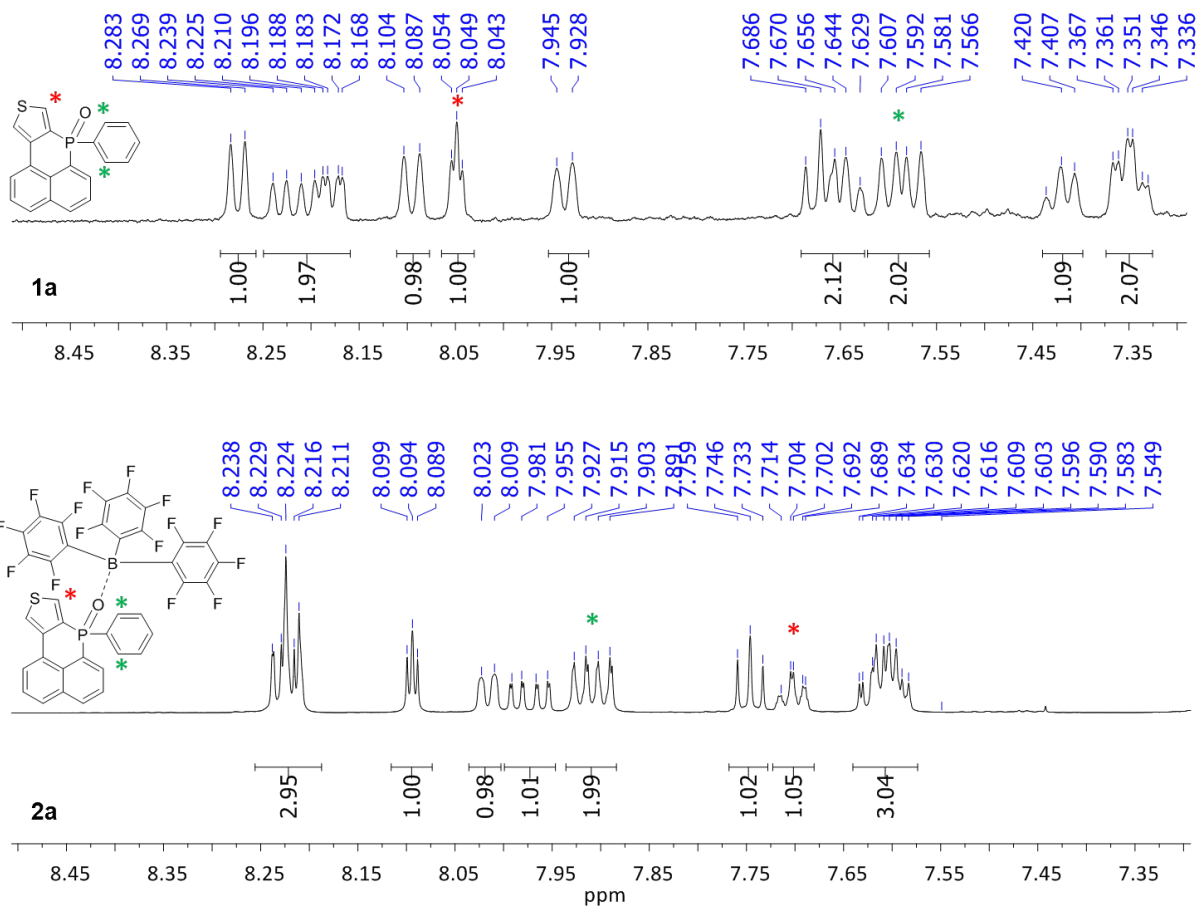


In a heated-out Schlenk flask 7-phenylbenzo[4,5]phosphinolino[3,2-*b*]thiophene 7-oxide (1.0 eq., 105  $\mu$ mol, 35 mg) was dissolved in 1 mL dry dichloromethane. Tris(pentafluorophenyl)-borane (1.0 eq., 105  $\mu$ mol, 54 mg) was added and the solution turned from yellow to dark orange. It was stirred at rt for 15 min and the solvent was removed under reduced pressure. Washing with pentane four times and drying under high vacuum at 40  $^{\circ}$ C yielded the pure product as the white solid (80 mg, 41  $\mu$ mol, 90 %).  $^1H$  NMR (600 MHz, in  $CDCl_3$ ):  $\delta$  8.22 (m,  $J = 3.6$  Hz, 3H), 8.09 (t,  $J = 3.0$  Hz, 1H), 7.97 (dq,  $J_1 = 7.7$  Hz,  $J_2 = 1.1$  Hz, 1H), 7.91 (m,  $J = 4.8$  Hz, 2H), 7.75 (t,  $J = 7.8$  Hz, 1H), 7.70 (dt,  $J_1 = 7.5$  Hz,  $J_2 = 1.7$  Hz, 1H), 7.61 (m,  $J = 3.8$  Hz, 3H).  $^{13}C\{^1H\}\{^31P\}$  and DEPT 135 $\{^31P\}$  NMR (151 MHz, in  $CDCl_3$ ):  $\delta$  147.1 (d,  $J = 240.0$  Hz, CF), 140.1 (s, C), 139.8 (s, CH), 139.7 (d,  $J = 249.7$  Hz, CF), 136.5 (d,  $J = 244.1$  Hz, CF), 134.2 (s, CH), 134.1 (s, C), 133.4 (s, CH), 132.7 (s, C), 130.7 (s, CH), 129.6 (s, CH), 128.0 (s, CH), 127.5 (s, C), 127.3 (s, C), 126.2 (s, CH), 125.5 (s, CH), 125.1 (s, CH), 122.1 (s, C), 122.0 (s, CH), 120.0 (s, C), 119.3 (s, C).  $^{31}P\{^1H\}$  NMR (400 MHz, in  $CDCl_3$ ):  $\delta$  19.17.  $^{11}B\{^1H\}$  NMR (128 MHz, in  $CDCl_3$ ):  $\delta$  -1.78.  $^{19}F\{^1H\}$  NMR (283 MHz, in  $CDCl_3$ ):  $\delta$  -132.37 (d,  $J = 23.4$  Hz, 6F, *o*-F), -158.49 (t,  $J = 20.8$  Hz, 3F, *p*-F), -164.62 (t,  $J = 18.21$  Hz, 6F, *m*-F).

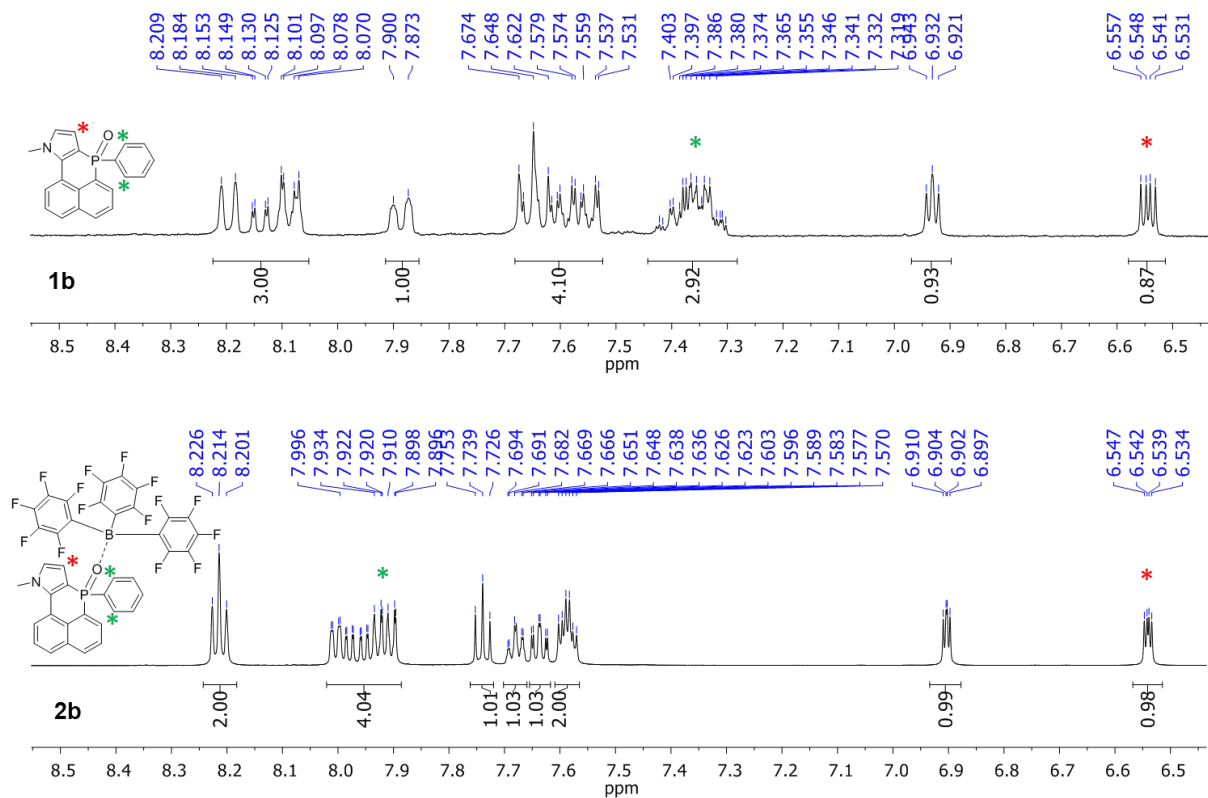
**(2b) 10-Methyl-7-phenyl-10H-benzo[4,5]phosphinolino[3,2-*b*]pyrrole 7-oxidetris(pentafluorophenyl)borane adduct**



In a heated-out Schlenk flask 10-methyl-7-phenyl-10H-benzo[4,5]phosphinolino[3,2-*b*]pyrrole 7-oxide (1.0 eq., 33  $\mu$ mol, 11 mg) was dissolved in 0.5 mL dry dichloromethane. Tris(pentafluorophenyl)borane (1.0 eq., 33  $\mu$ mol, 17 mg) was added and the solution turned from yellow to dark orange. It was stirred at rt for 15 min and the solvent was removed under reduced pressure. Washing with pentane three times yielded the pure product as bright yellow solid (27 mg, 32  $\mu$ mol, 96 %).  $^1H$  NMR (600 MHz, in  $CD_2Cl_2$ ):  $\delta$  8.21 (t,  $J$  = 9 Hz, 2H), 8.01 (dd,  $J_1$  = 1.5 Hz,  $J_2$  = 6.1 Hz, 1H), 7.97 (dq,  $J_1$  = 1.4 Hz,  $J_2$  = 7.6 Hz, 1H), 7.91 (dq,  $J_1$  = 1.2 Hz,  $J_2$  = 7.6 Hz, 2H), 7.74 (t,  $J$  = 7.8 Hz, 1H), 7.68 (dt,  $J_1$  = 1.6 Hz,  $J_2$  = 7.5 Hz, 1H), 7.64 (dt,  $J_1$  = 1.7 Hz,  $J_2$  = 7.7 Hz, 1H), 7.58 (dt,  $J_1$  = 3.9 Hz,  $J_2$  = 7.8 Hz, 2H), 6.90 (dd,  $J_1$  = 1.1 Hz,  $J_2$  = 7.4 Hz, 1H), 6.54 (dd,  $J_1$  = 1.9 Hz,  $J_2$  = 8.0 Hz, 1H), 4.13 (s, 3H).  $^{13}C\{^1H\}\{^{31}P\}$  and DEPT 135 $\{^{31}P\}$  NMR (151 MHz, in  $CD_2Cl_2$ ):  $\delta$  148.04 (d,  $J$  = 242 Hz, CF), 139.57 (dt,  $J_1$  = 247 Hz,  $J_2$  = 13.2 Hz, CF), 138.16 (s, C), 137.07 (s, CH), 136.96 (dq,  $J_1$  = 247 Hz,  $J_2$  = 10.6 Hz, CF), 136.47 (s, CH), 133.82 (s, CH), 133.39 (s, C), 133.10 (s, CH), 131.51 (s, CH), 130.82 (s, CH), 129.44 (s, CH), 128.99 (s, C), 127.79 (s, C), 126.94 (s, CH), 126.58 (s, CH), 125.25 (s, CH), 122.90 (s, C), 121.12 (s, C), 120.43 (s, C), 111.76 (s, CH), 102.55 (s, C), 40.25 (s,  $CH_3$ ).  $^{31}P\{^1H\}$  NMR (242 MHz, in  $CD_2Cl_2$ ):  $\delta$  21.82.  $^{11}B\{^1H\}$  NMR (96 MHz, in  $CD_2Cl_2$ ):  $\delta$  -2.22.  $^{19}F\{^1H\}$  NMR (470 MHz, in  $CD_2Cl_2$ ):  $\delta$  -132.53 (d,  $J$  = 24.7 Hz, 6F, *o*-F), -159.99 (t,  $J$  = 20.0 Hz, 3F, *p*-F), 165.93 (dt,  $J_1$  = 6.9 Hz,  $J_2$  = 22.4 Hz, 6F, *m*-F).

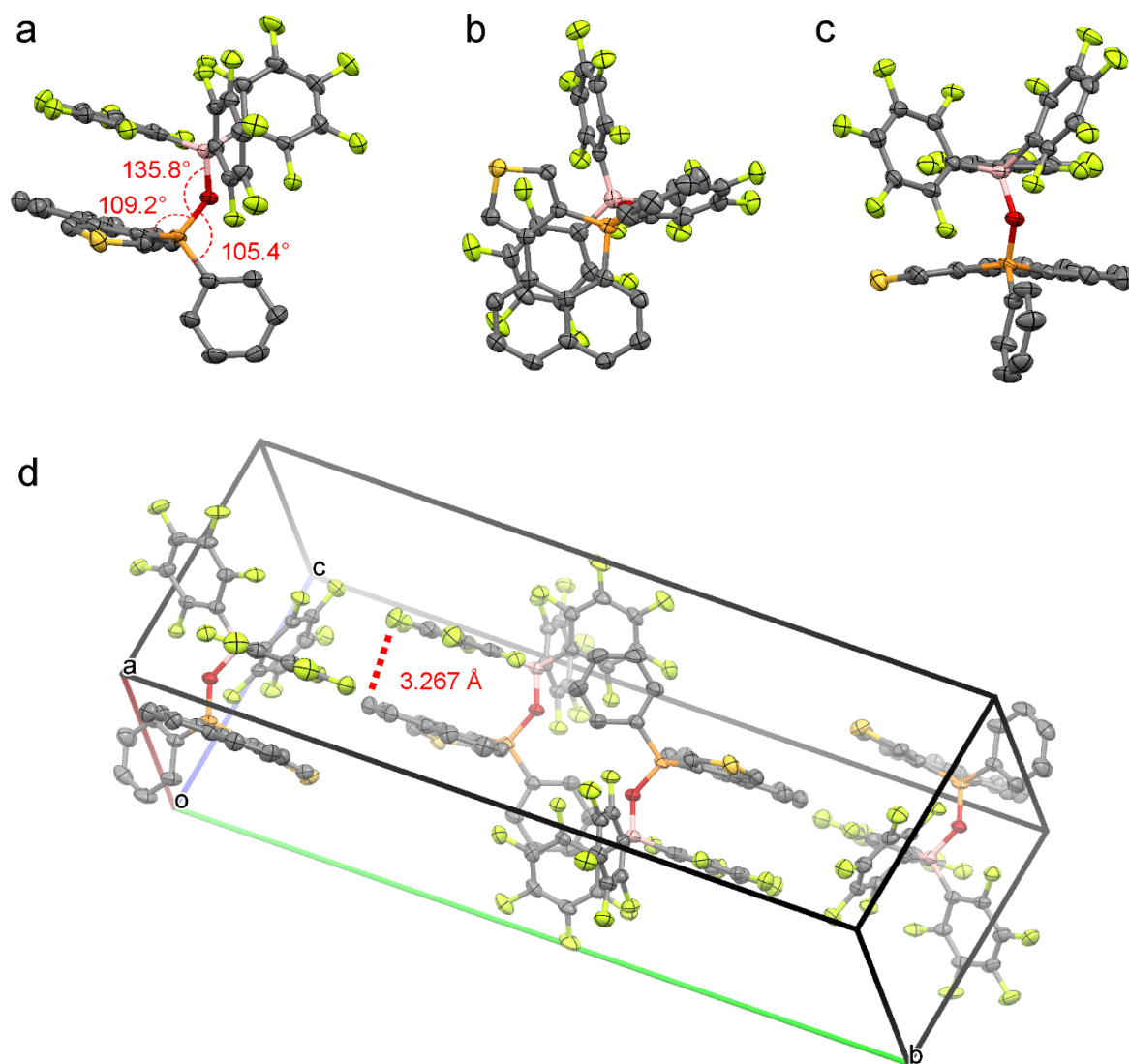


**Figure S1.**  $^1\text{H}$  NMR spectra of **1a** and **2a**.

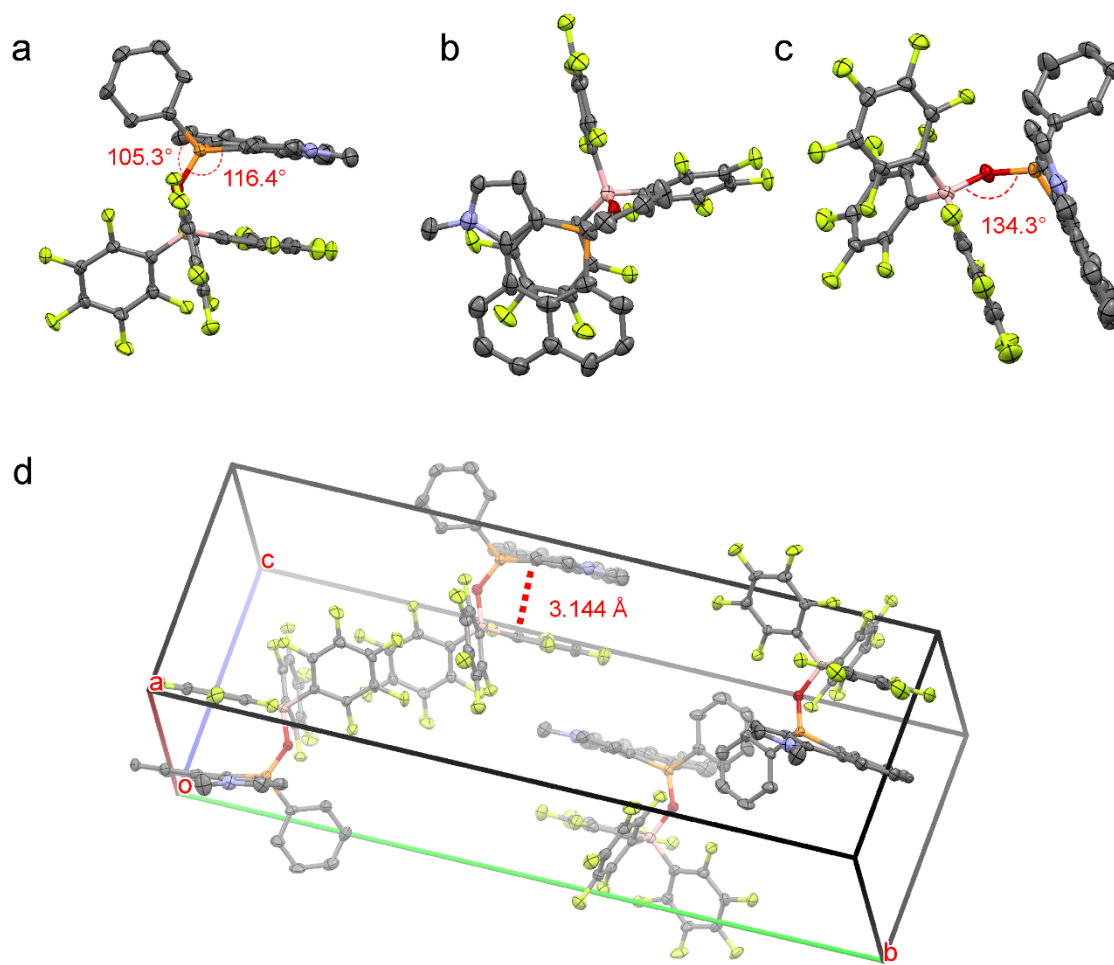


**Figure S2.**  $^1\text{H}$  NMR spectra of **1b** and **2b**.

### 2.3. Crystallographic data

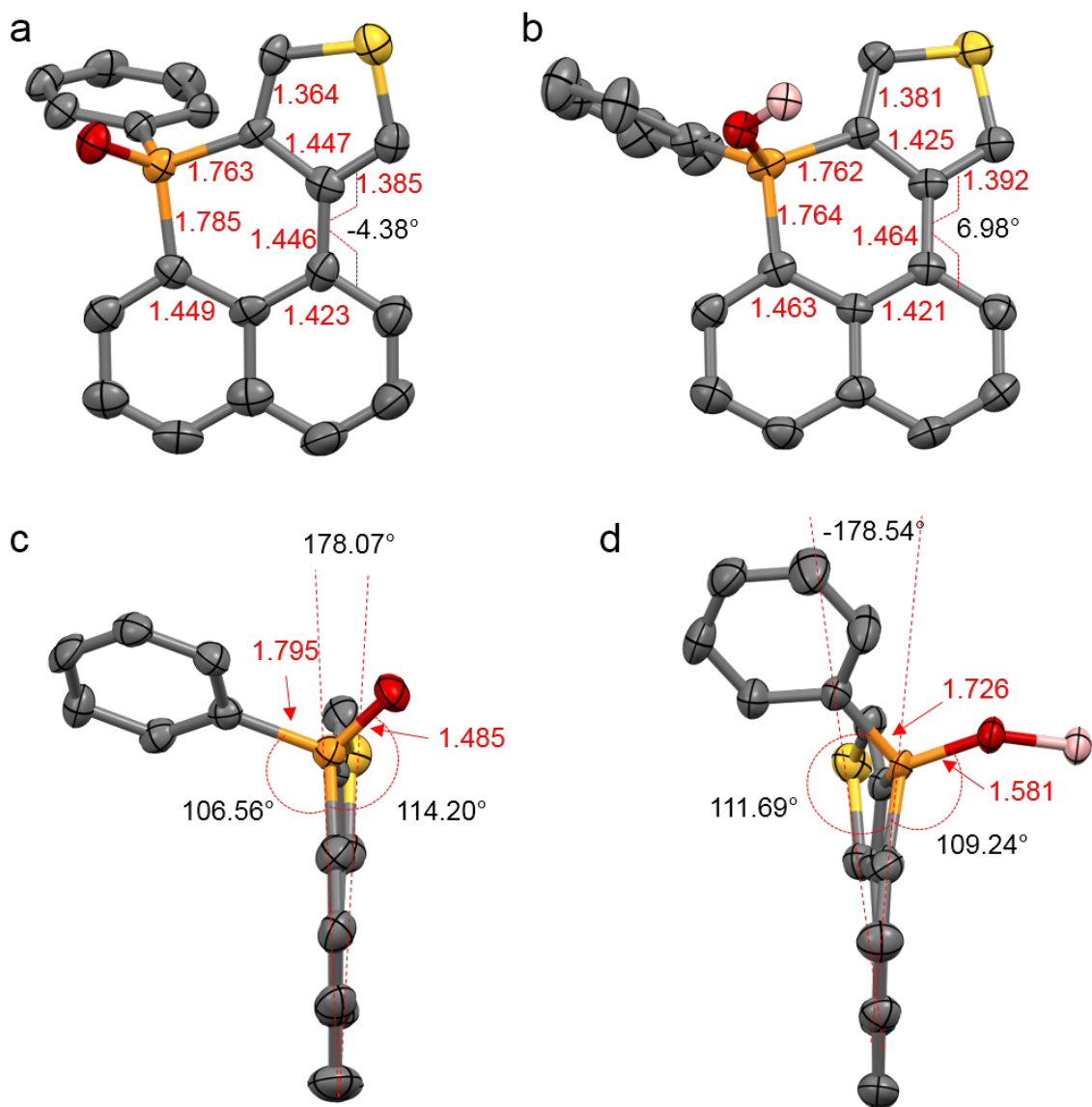


**Figure S3.** X-ray structures of **2a** (50% probability level ellipsoids). a) top view, b) front view, c) side view, and d) crystal packing. Hydrogens have been omitted for clarity.

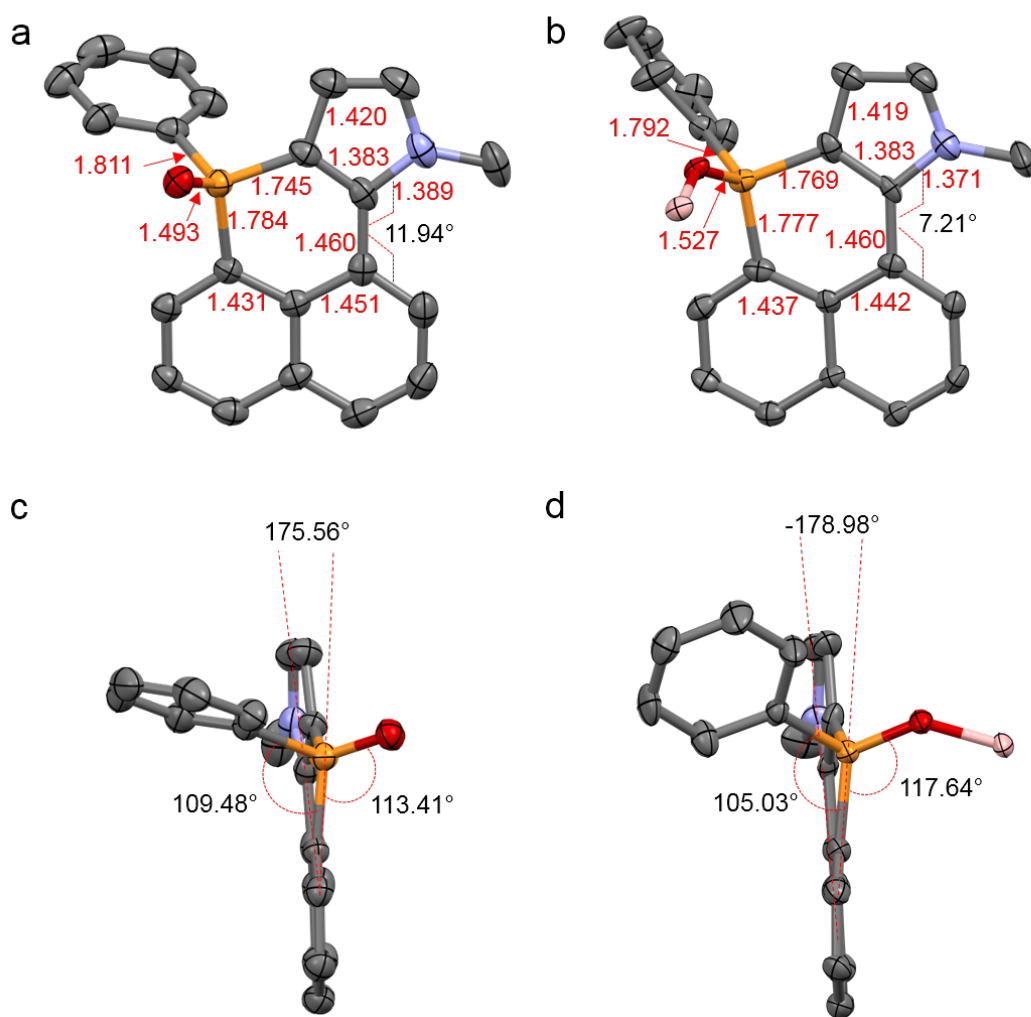


**Figure S4.** X-ray structures of **2b** (50% probability level ellipsoids). a) top view, b) front view, c) side view, and d) crystal packing. Hydrogens have been omitted for clarity.

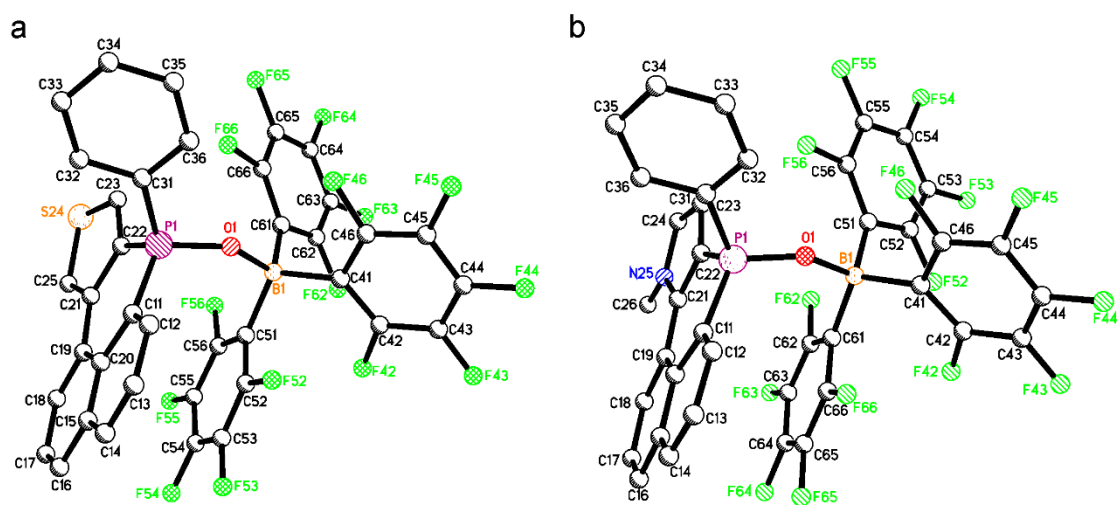




**Figure S5.** X-ray structure of **1a**<sup>[S1]</sup> (top (a) and front (c) views) compared with the simplified x-ray structure of **2a** (top (b) and front (d) views). Hydrogens and tris(pentafluorophenyl groups of **2a** have been omitted for clarity. Bond lengths are expressed in angstroms.



**Figure S6.** X-ray structure of **1b**<sup>[S1]</sup> (top (a) and front (c) views) compared with the simplified x-ray structure of **2b** (top (b) and front (d) views). Hydrogens and tris(pentafluorophenyl) groups of **2b** have been omitted for clarity. Bond lengths are expressed in angstroms.



**Figure S7.** X-ray structures of **2a** (a) and **2b** (b).

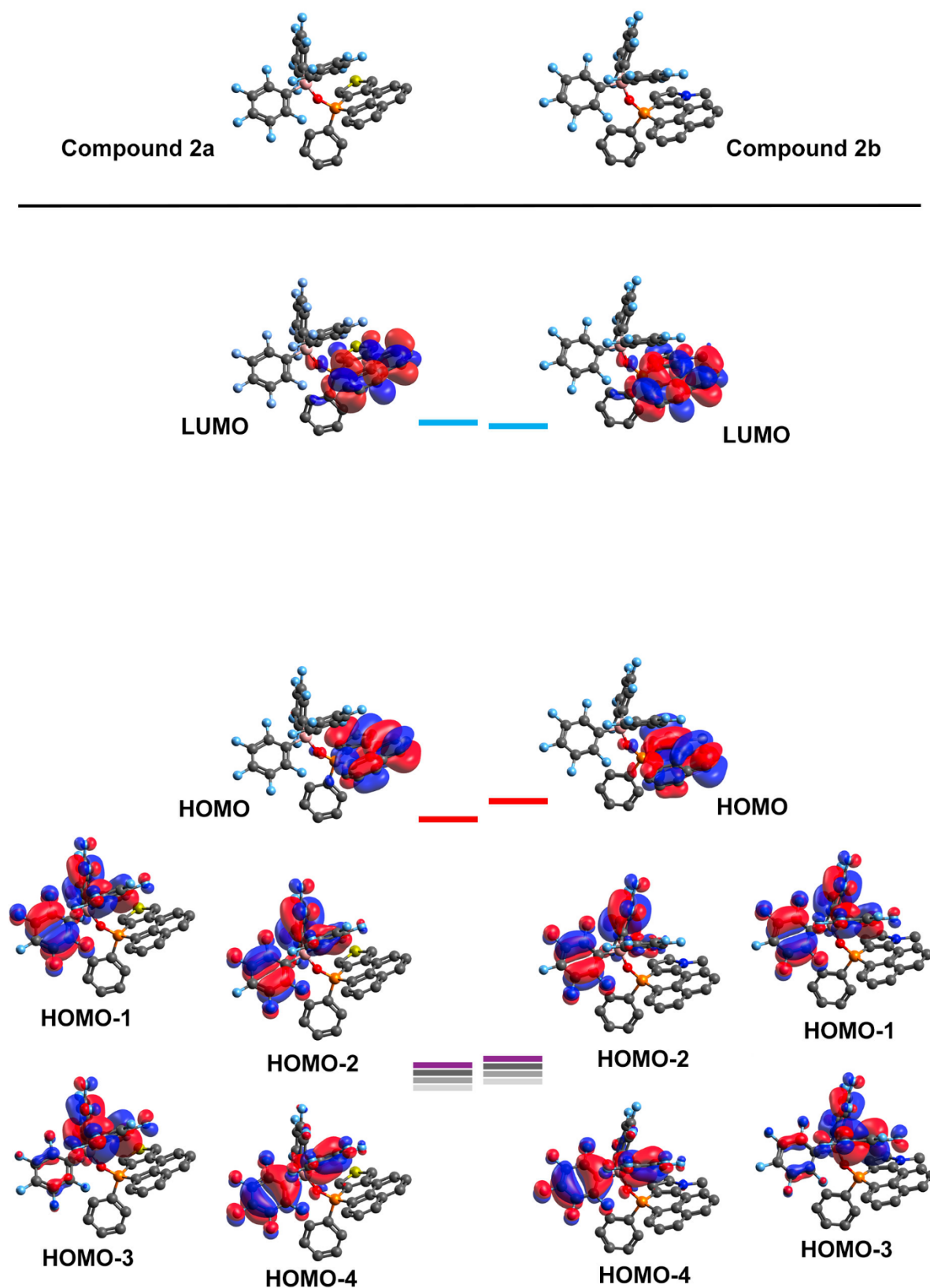
**Table S1.** Selected crystallographic data of adducts **2a** and **2b**.

	<b>Compound 2a</b>	<b>Compound 2b</b>
Empirical formula	C <sub>38</sub> H <sub>13</sub> BF <sub>15</sub> OPS	C <sub>39</sub> H <sub>16</sub> BF <sub>15</sub> NOP
Molecular weight	844.32	841.31
Temperature	100(2) K	100(2) K
Wavelength	1.54178 Å	1.54178 Å
Crystal system	monoclinic	monoclinic
Space group	P2 <sub>1</sub> /n	Pn
Z	4	4
a/Å	10.0001(3) Å; α = 90 °	9.9754(15) Å; α = 90 °
b/Å	29.9868(8) Å; β = 96.102(3) °	30.114(3) Å; β = 95.823(12) °
c/Å	10.9105(3) Å; γ = 90 °	10.9427(16) Å; γ = 90 °
Volume	3253.21(16) Å <sup>3</sup>	3270.2(8) Å <sup>3</sup>
Density (calculated)	1.72 g/cm <sup>3</sup>	1.709 g/cm <sup>3</sup>
Absorption coefficient	2.47 mm <sup>-1</sup>	1.882 mm <sup>-1</sup>
Crystal shape	irregular	rectangular
Crystal size	0.097 x 0.082 x 0.058 mm <sup>3</sup>	0.163 x 0.130 x 0.042 mm <sup>3</sup>
Crystal colour	colourless	light yellow/brown
Theta range for data collection	4.3 to 60.9 °	4.318 to 68.208 °
Index Ranges	-10 ≤ h ≤ 11, -33 ≤ k ≤ 28, -11 ≤ l ≤ 12	-11 ≤ h ≤ 10, -31 ≤ k ≤ 35, -6 ≤ l ≤ 13
Reflections collected	17238	22471
Independent reflections	4779 (R(int) = 0.0291)	7213 (R(int) = 0.0199)
Observed reflections	4000 (I > 2σ (I))	6688 (I > 2σ (I))
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	1.70 and 0.60	1.92 and 0.57
Refinement method	Full-matrix least-squares on F <sup>2</sup>	Full-matrix least-squares on F <sup>2</sup>
Data/restraints/parameters	4779 / 1259 / 659	7213 / 1618 / 1112
Goodness-of-fit on F <sup>2</sup>	1.21	1.04
Final R indices (I > 2σ (I))	R1 = 0.058, wR2 = 0.106	R1 = 0.036, wR2 = 0.091
Largest diff. peak and hole	0.43 and -0.32 eÅ <sup>-3</sup>	0.40 and -0.31 eÅ <sup>-3</sup>

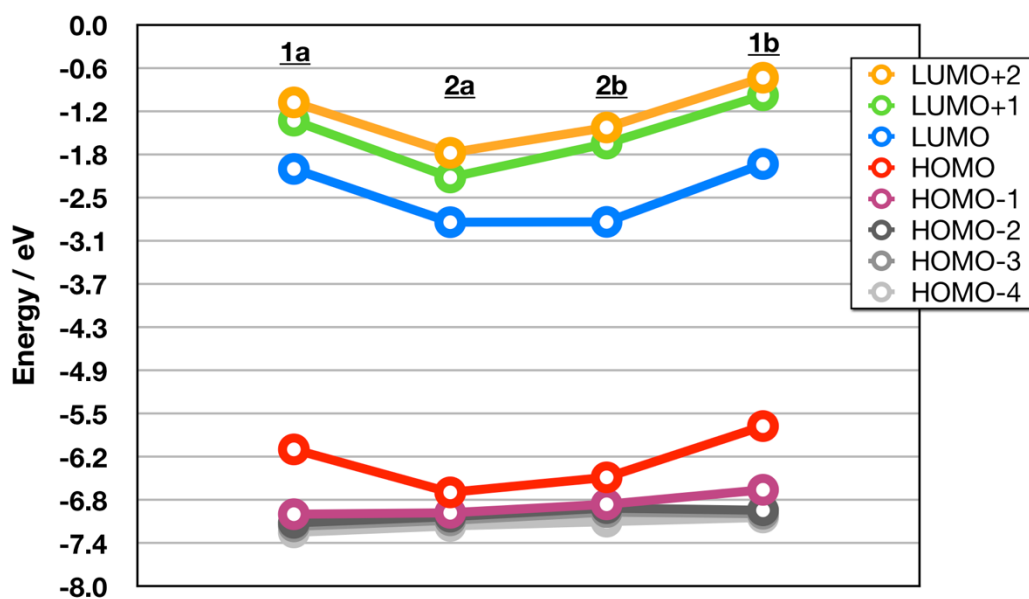
**Table S2.** Selected bond lengths (Å) and angles (°) for phosphaphenalene oxides (**1a** and **1b**)<sup>[S1]</sup> and their adducts with borane (**2a** and **2b**).

Selected bonds or angles	Compound			
	1a	1b	2a	2b
P1-O1	1.482(4)	1.493(2)	1.581(5)	1.540(4)
O1-B1	-	-	1.541(5)	1.526(7)
P1-C31	1.795(6)	1.811(3)	1.726(11)	1.792(6)
C31-C36	1.381(8)	1.392(4)	1.375(6)	1.382(8)
C31-C32	1.372(8)	1.383(4)	1.378(6)	1.361(9)
P1-O1-B1	-	-	135.8	134.3
C11-P1-O1	114.20	113.41	109.24	117.64
C11-P1-C22	106.56	109.48	111.69	105.03

### 2.3. DFT Calculations



**Figure S8.** Electronic density distribution of **2a** (left) and **2b** (right) at the B3LYP/6-31+G(d) level of theory. See Table S3 for values.



**Figure S9.** Energy levels' distribution of **1a**, **2a**, **1b** and **2b** the B3LYP/6-31+G(d) level of theory. See Table S3 for values.

**Table S3.** Orbitals' energy obtained by TD-DFT calculations at the B3LYP/6-31+G(d) level of theory.

	Compound			
	1a	2a	2b	1b
<b>LUMO+2</b>	-1.107	-1.826	-1.465	-0.755
<b>LUMO+1</b>	-1.367	-2.177	-1.694	-1.006
<b>LUMO</b>	-2.056	-2.815	-2.811	-1.985
<b>HOMO</b>	-6.054	-6.667	-6.453	-5.722
<b>HOMO-1</b>	-6.978	-6.958	-6.837	-6.63
<b>HOMO-2</b>	-7.101	-7.013	-6.891	-6.922
<b>HOMO-3</b>	-7.151	-7.065	-6.948	-6.971
<b>HOMO-4</b>	-7.237	-7.145	-7.084	-7.024
<b>Band GAP</b>	3.998	3.852	3.642	3.737

**Table S4.** Photo-induced transitions obtained by TD-DFT calculations at the B3LYP/6-31+G(d) level of theory.

Compound 2a	Calc. $\lambda_{\max}$ (nm)	$f^a$	Compound 2b	Calc. $\lambda_{\max}$ (nm)	$f^a$
HOMO-LUMO	447.7	0.0999	HOMO-LUMO	499.3	0.088
HOMO-5→LUMO	385.9	0.0009	HOMO-4→LUMO	390.66	0.001
HOMO-4→LUMO					
HOMO-3→LUMO					
HOMO-1→LUMO					
HOMO-5→LUMO	376.6	0.0004	HOMO-4→LUMO	383.02	0.0011
HOMO-4→LUMO					
HOMO-3→LUMO					
HOMO-1→LUMO					

<sup>a</sup> Oscillator strength

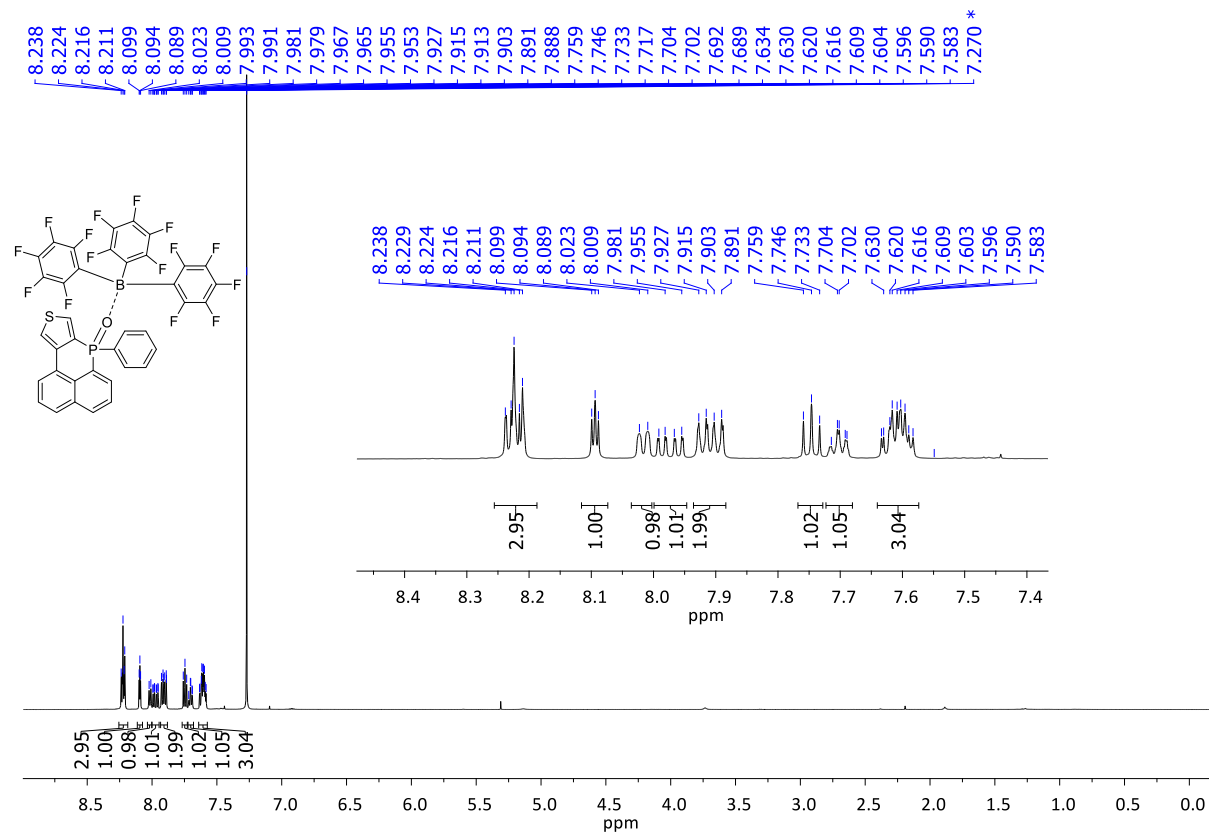
## 2.4. Device optimization

**Table S5.** Summary of the parameters investigated for the optimization of the device based on compound **2b** compared with those reported for the device based on compound **1b**.<sup>[S6]</sup>

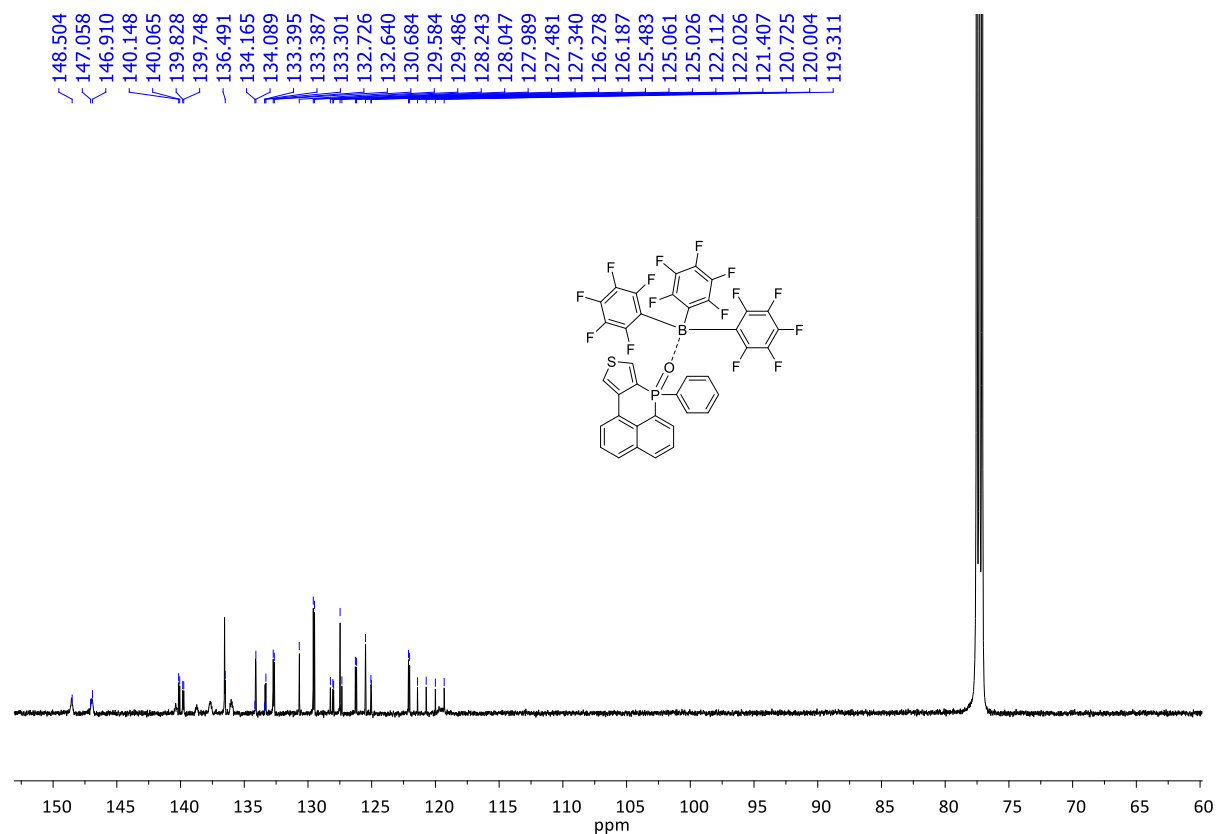
<b>Compound 2b</b>						
<b>Conditions</b>	<b>Stack</b>	<b>Thickness (nm)</b>	<b>Max. luminance (cd m<sup>-2</sup>)</b>	<b>V<sub>to</sub> (V)</b>	<b>Efficiency (cd A<sup>-1</sup>)</b>	<b>Efficacy (lm W<sup>-1</sup>)</b>
Toluene 10 g L <sup>-1</sup>	TPBi/LiF/Al	31±10	725±164	5.0±0.1	0.718±0.308	0.348±0.170
<i>o</i> -DCB 10 g L <sup>-1</sup>	TPBi/LiF/Al	31±9	723±174	4.1±0.1	0.316±0.098	0.165±0.045
DCM 10 g L <sup>-1</sup>	TPBi/LiF/Al	76±21	34±5	7.1±0.2	0.204±0.028	0.062±0.008
Toluene 10 g L <sup>-1</sup>	Ca/Al	32±6	5±1	7.8±1.0	0.003±0.001	0.001±0.001
<b>Compound 1b</b> <sup>[S6]</sup>						
<b>Conditions</b>	<b>Stack</b>	<b>Thickness (nm)</b>	<b>Max. luminance (cd m<sup>-2</sup>)</b>	<b>V<sub>to</sub> (V)</b>	<b>Efficiency (cd A<sup>-1</sup>)</b>	<b>Efficacy (lm W<sup>-1</sup>)</b>
Toluene 5 g L <sup>-1</sup>	TPBi/LiF/Al	48±7	694±13	5.3±0.1	0.350±0.018	0.133±0.01

## 2.5. NMR data

### $^1\text{H}$ NMR (600 MHz, $\text{CD}_2\text{Cl}_2$ ) of 2a

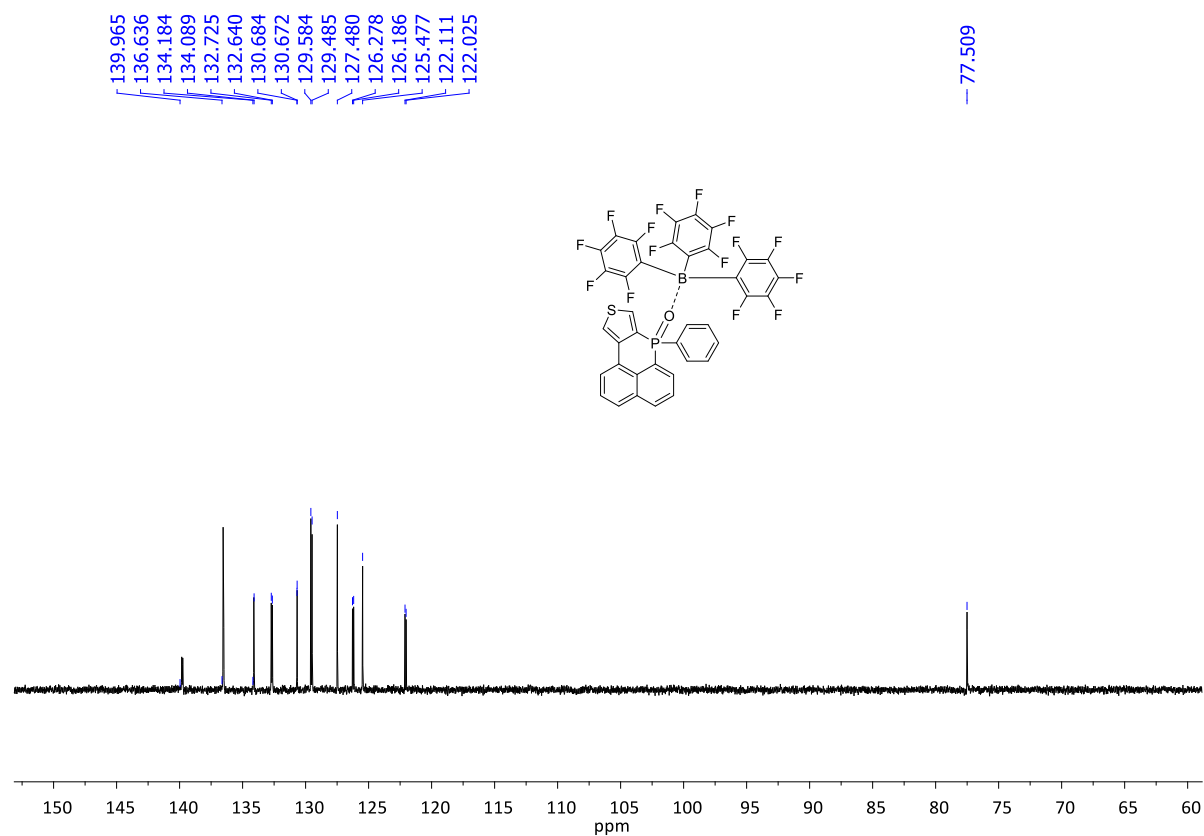


### $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, $\text{CD}_2\text{Cl}_2$ ) of 2a

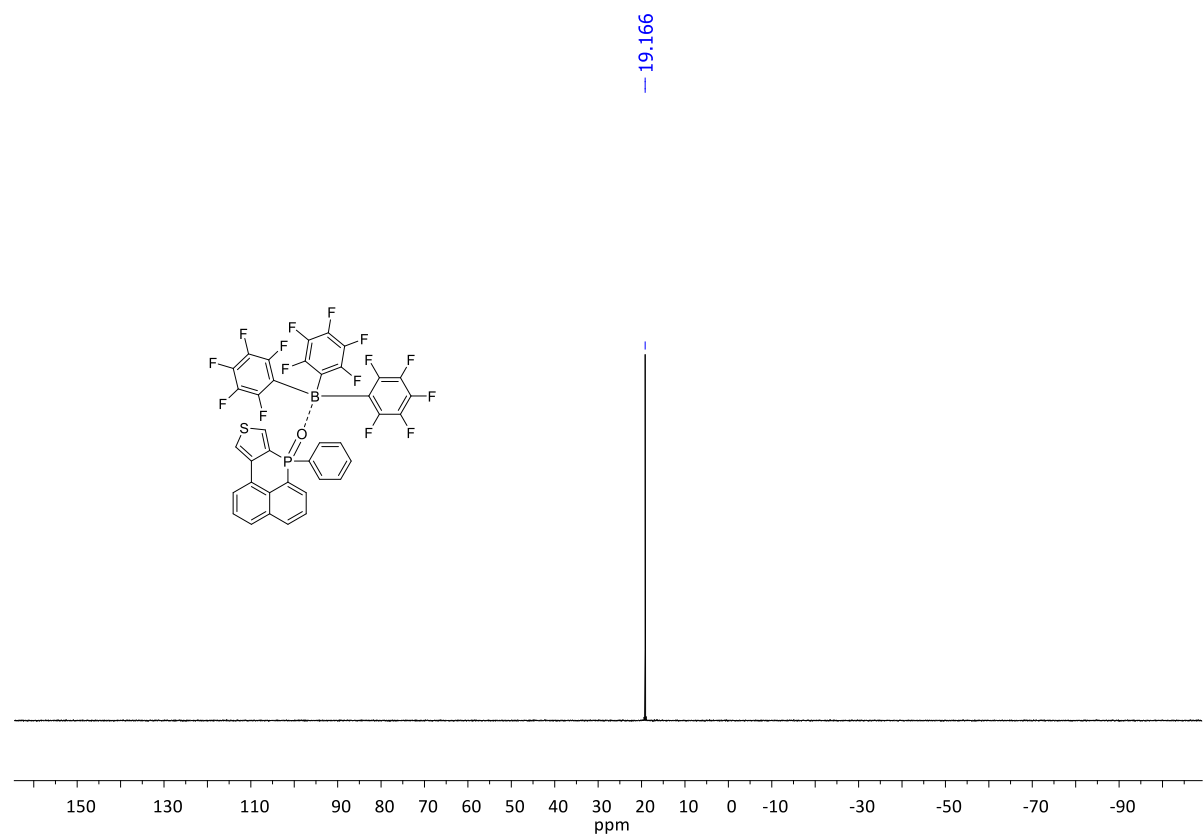




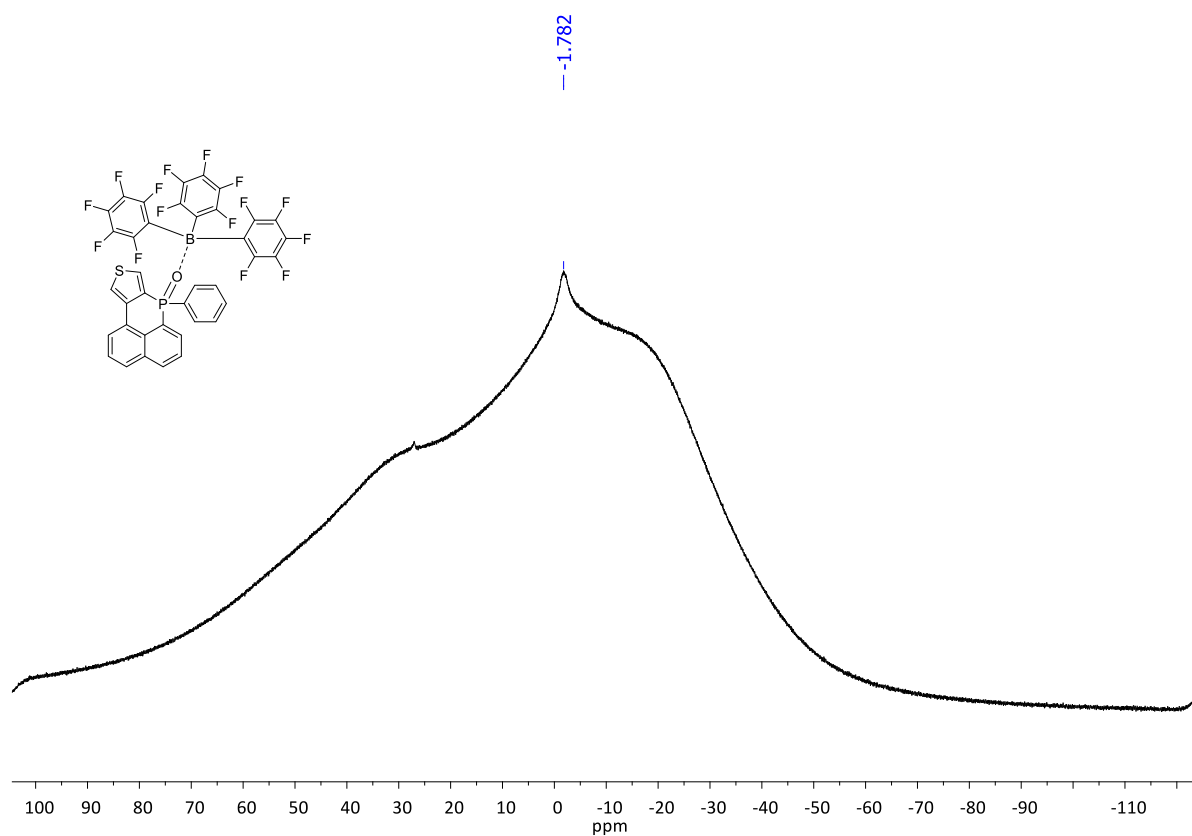
**$^{13}\text{C}$  DEPT 135 NMR (151 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2a**



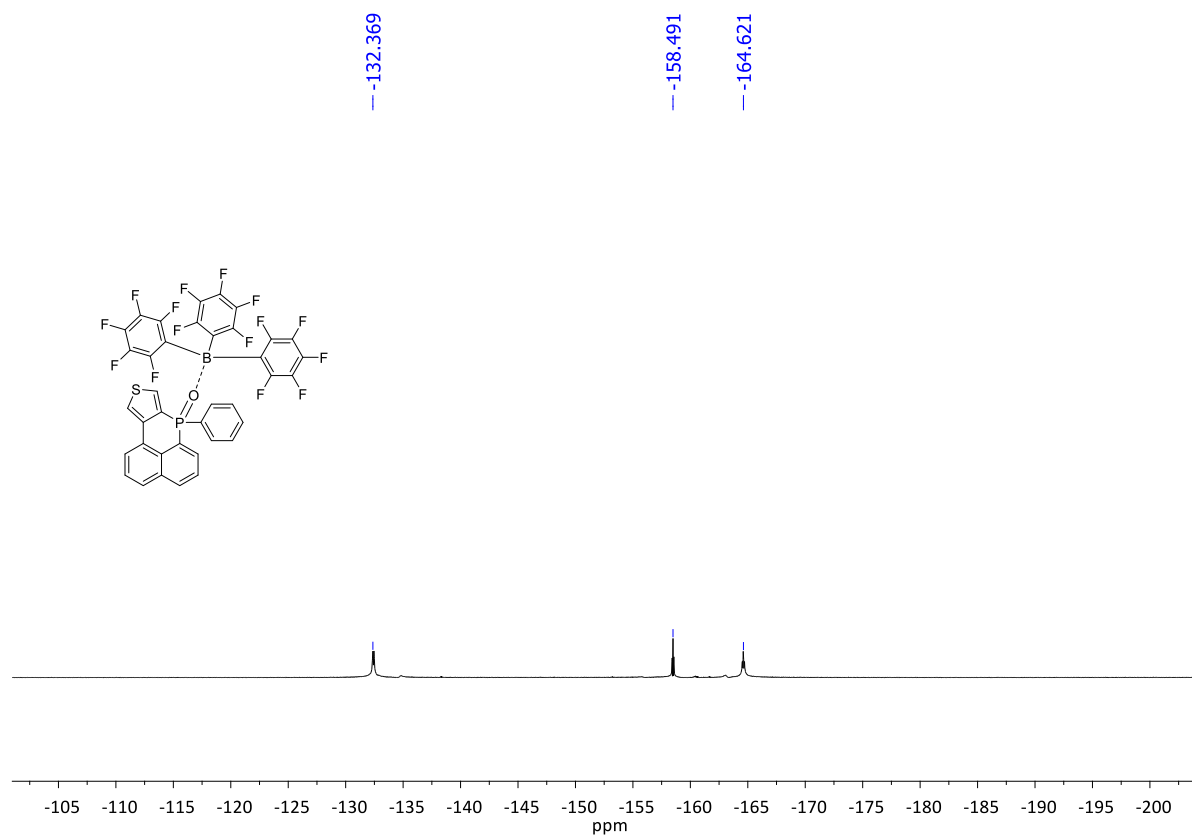
**$^{31}\text{P}\{^1\text{H}\}$  NMR (400 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2a**



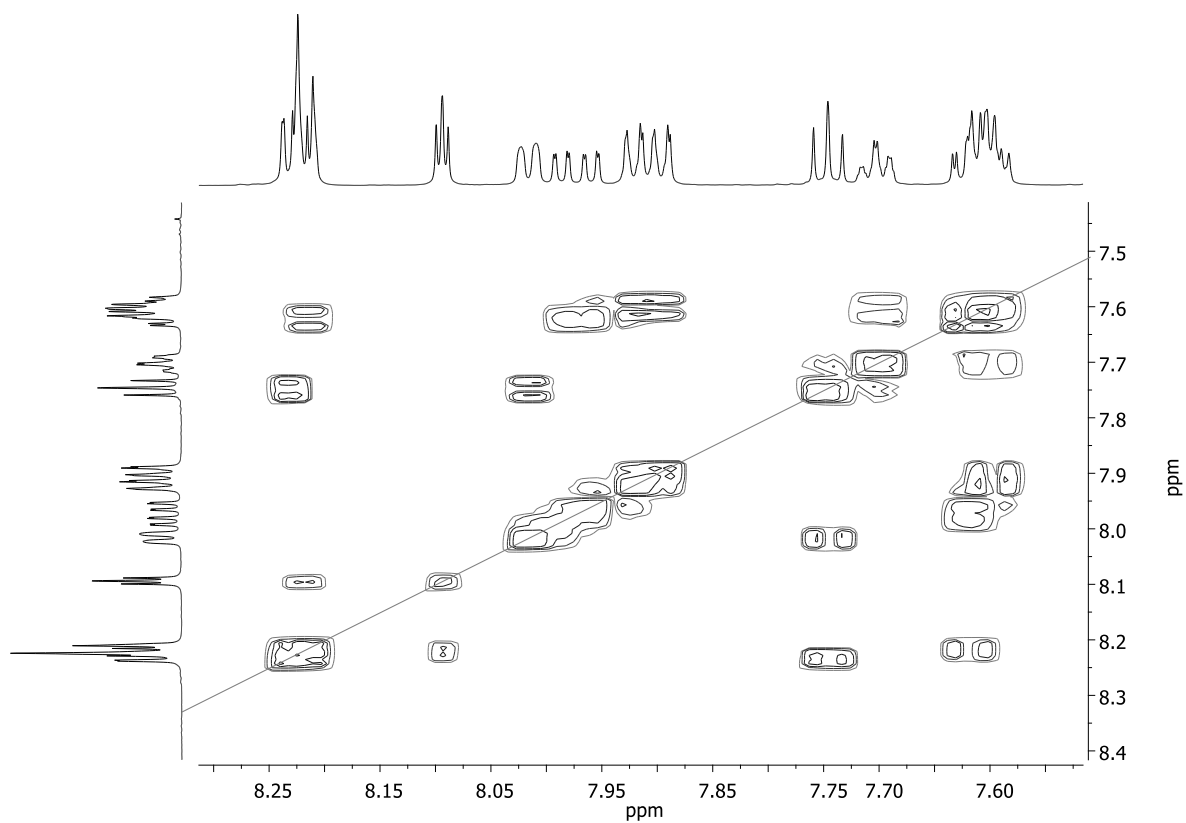
**$^{11}\text{B}\{1\text{H}\}$  NMR (128 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2a**



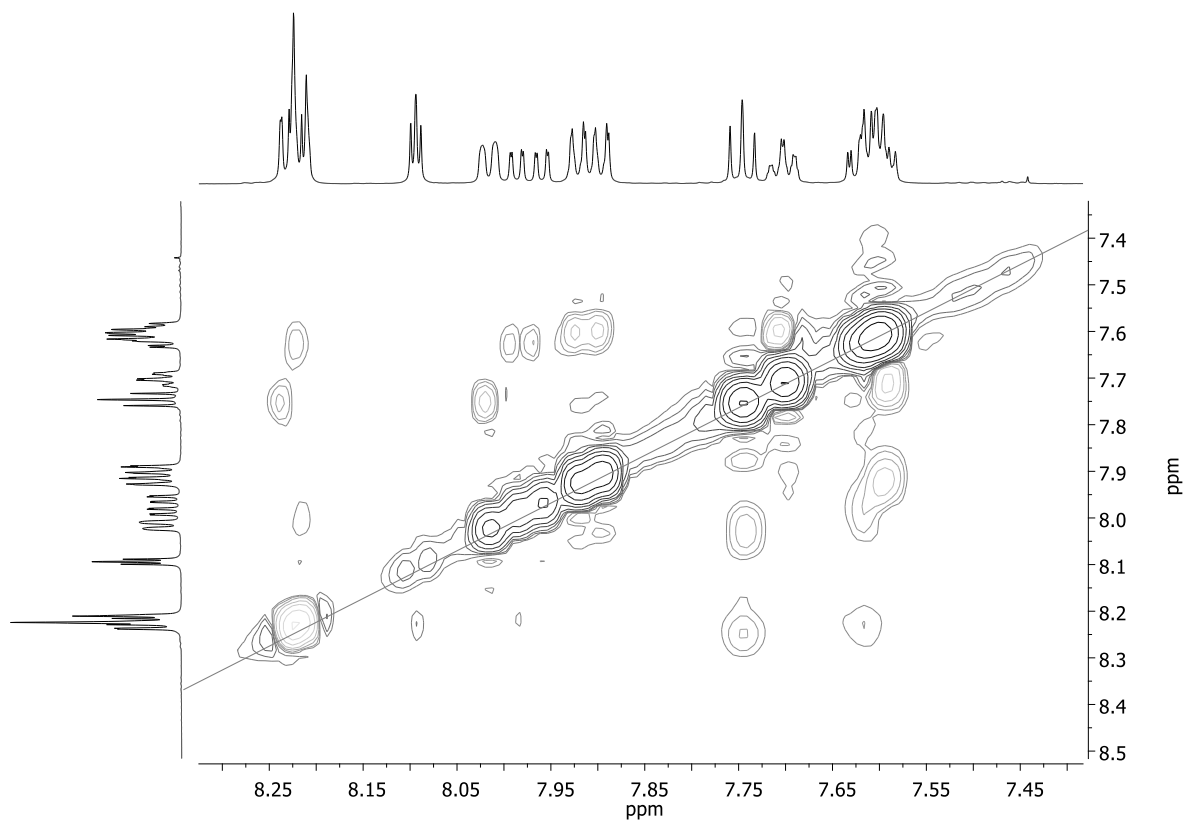
**$^{19}\text{F}\{1\text{H}\}$  NMR (283 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2a**



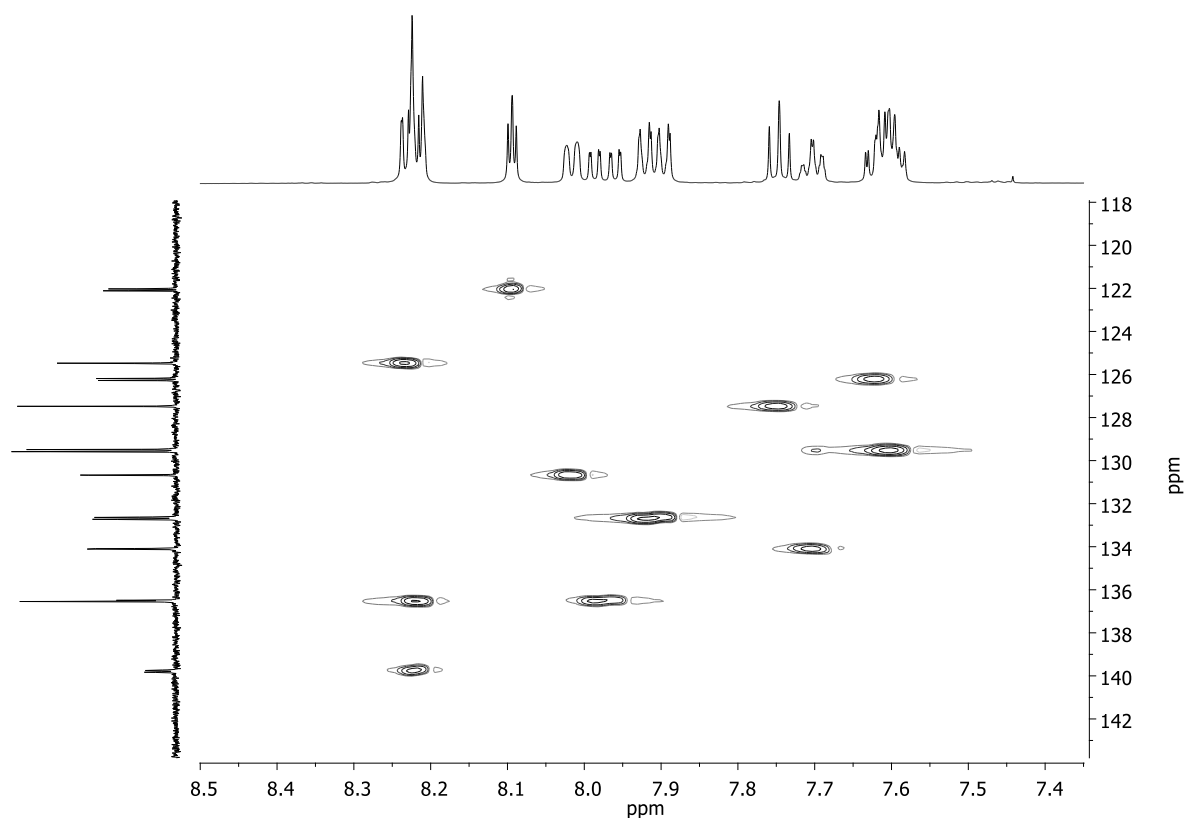
**$^1\text{H}$ - $^1\text{H}$  COSY NMR (600 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2a**



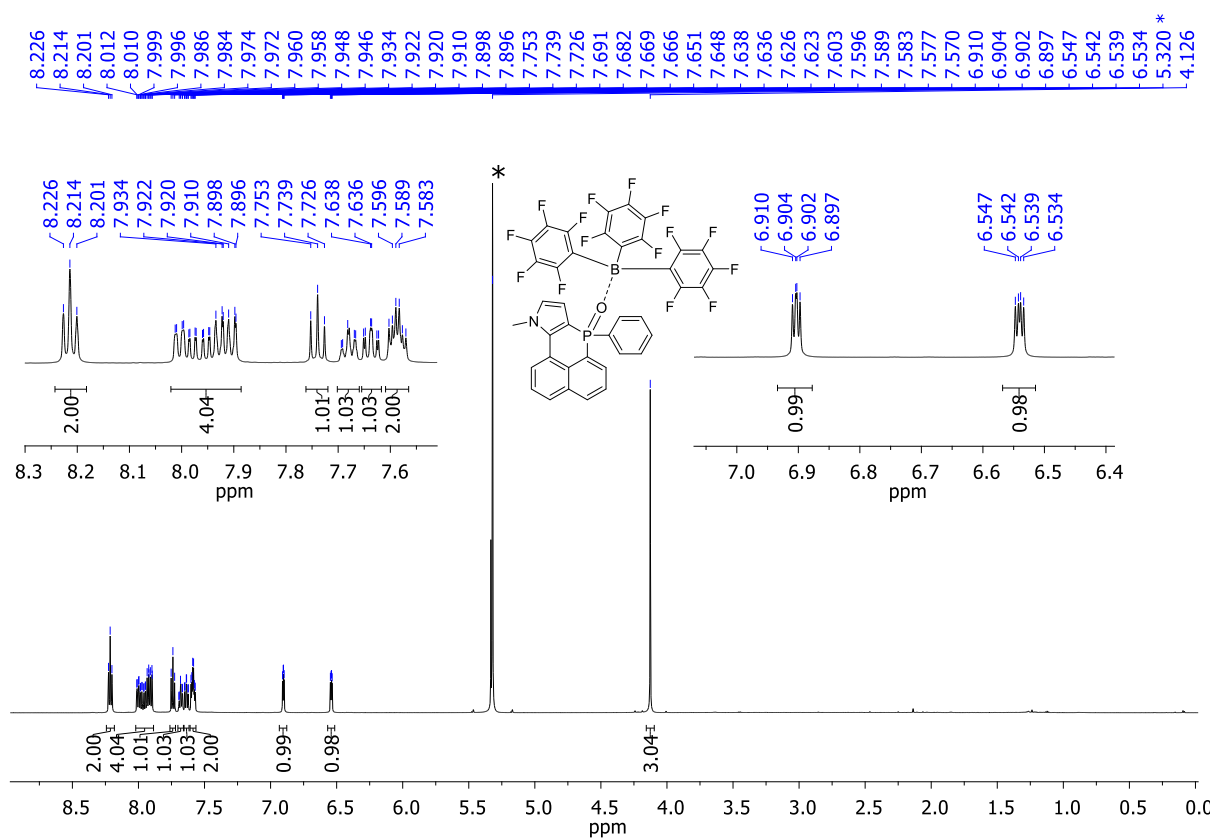
**$^1\text{H}$ - $^1\text{H}$  ROESY NMR (600 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2a**



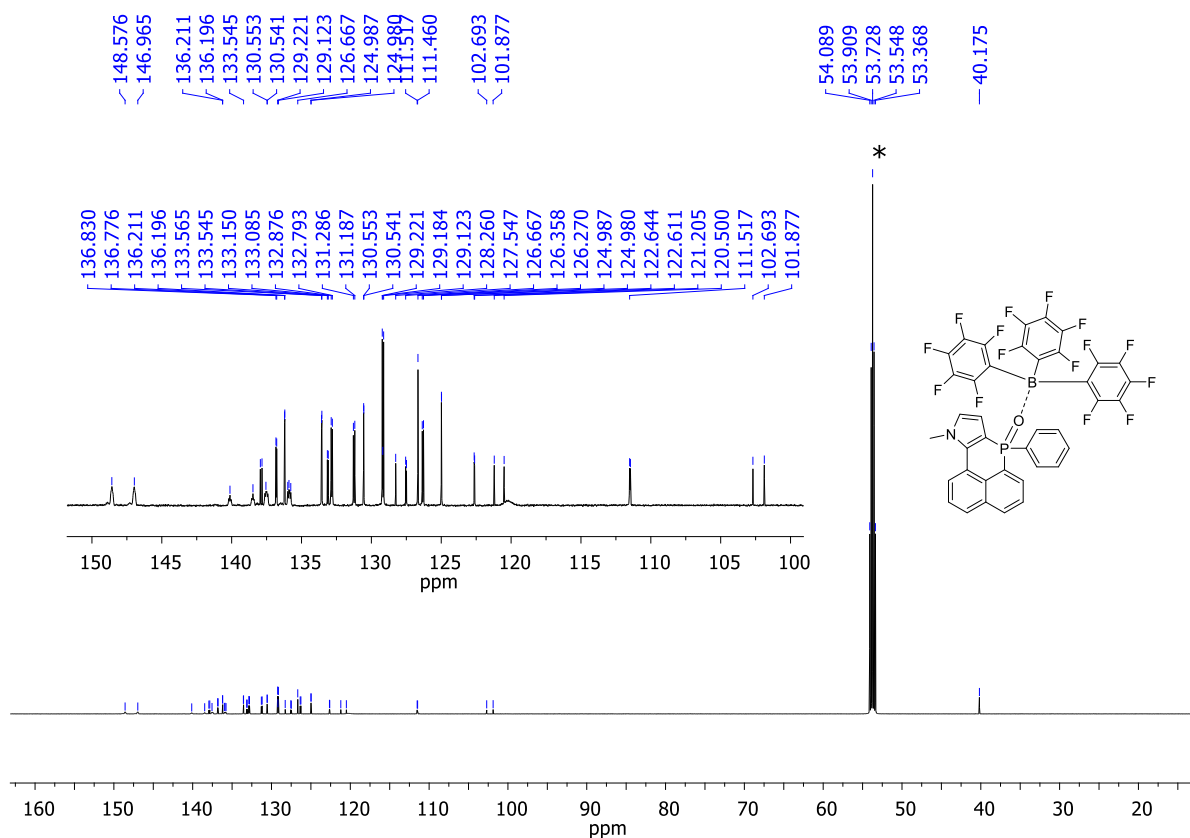
### HSQC-DEPT NMR (151 MHz, CD<sub>2</sub>Cl<sub>2</sub>) of 2a



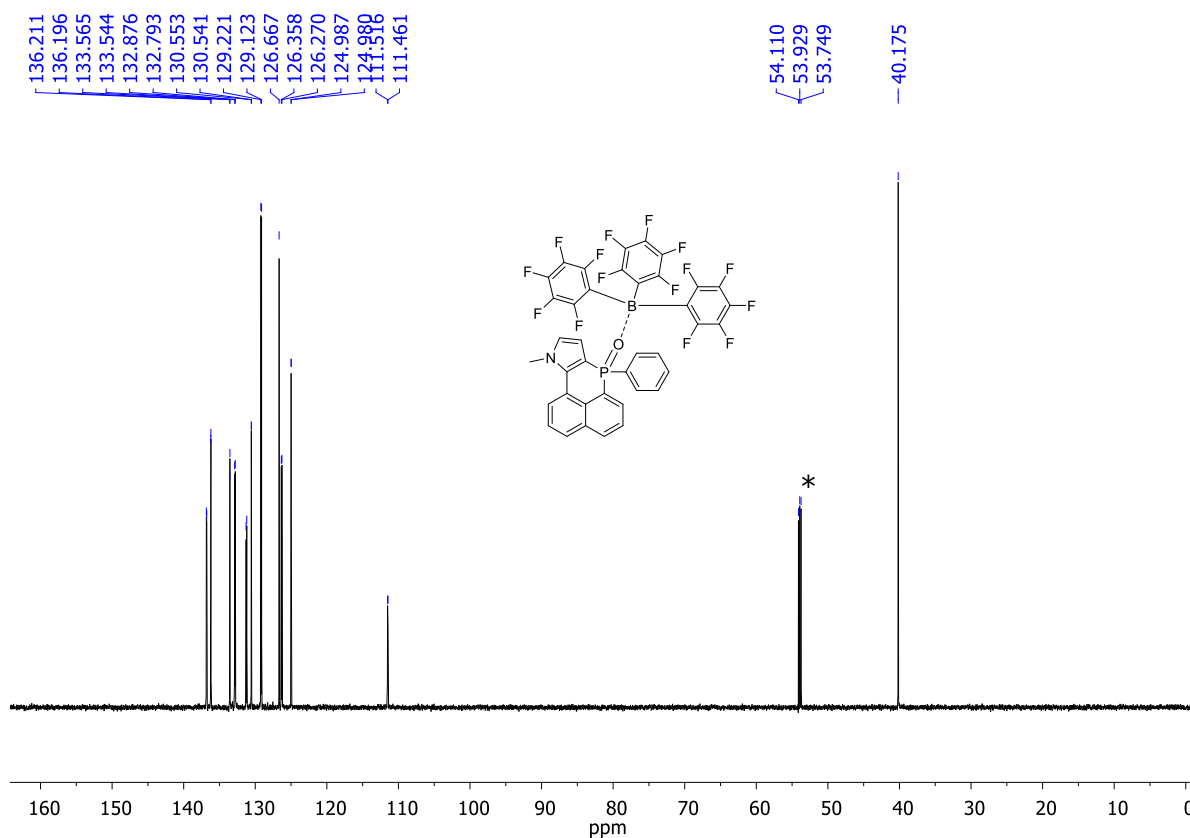
### <sup>1</sup>H NMR (600 MHz, CD<sub>2</sub>Cl<sub>2</sub>) of 2b



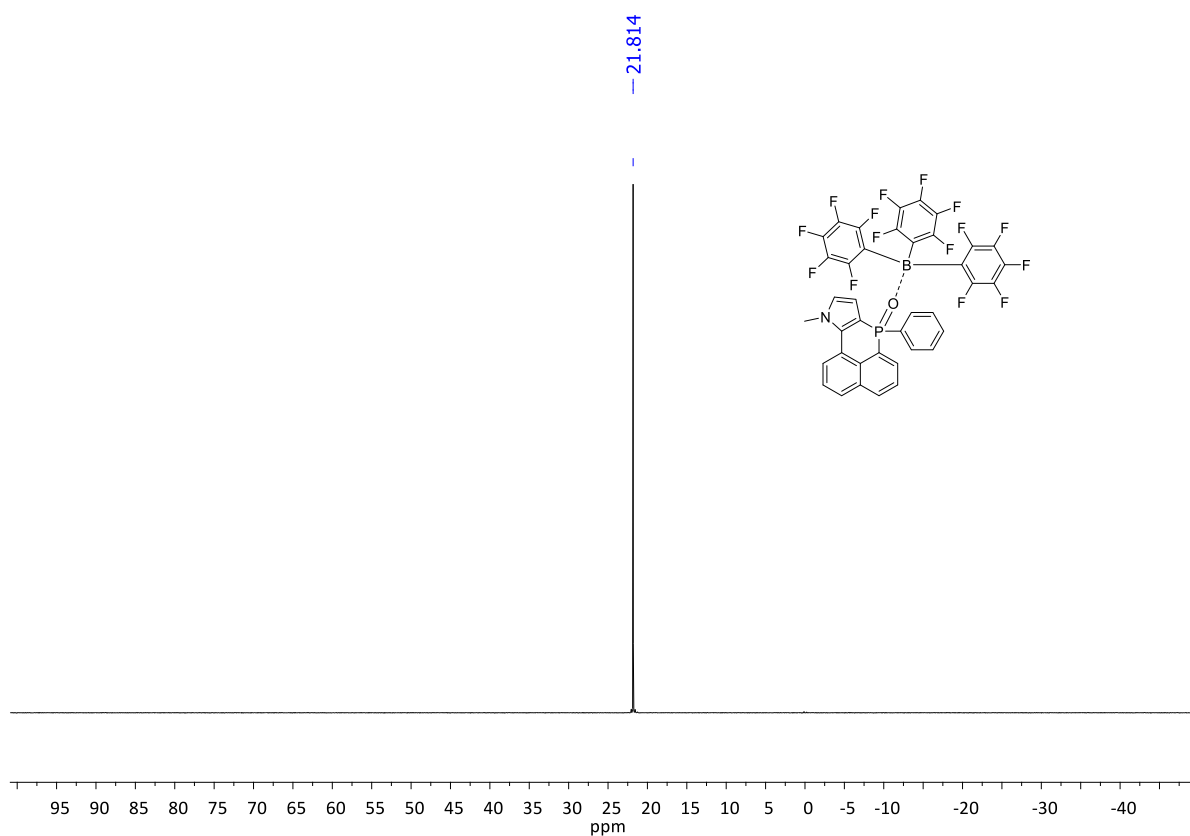
**$^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2b**



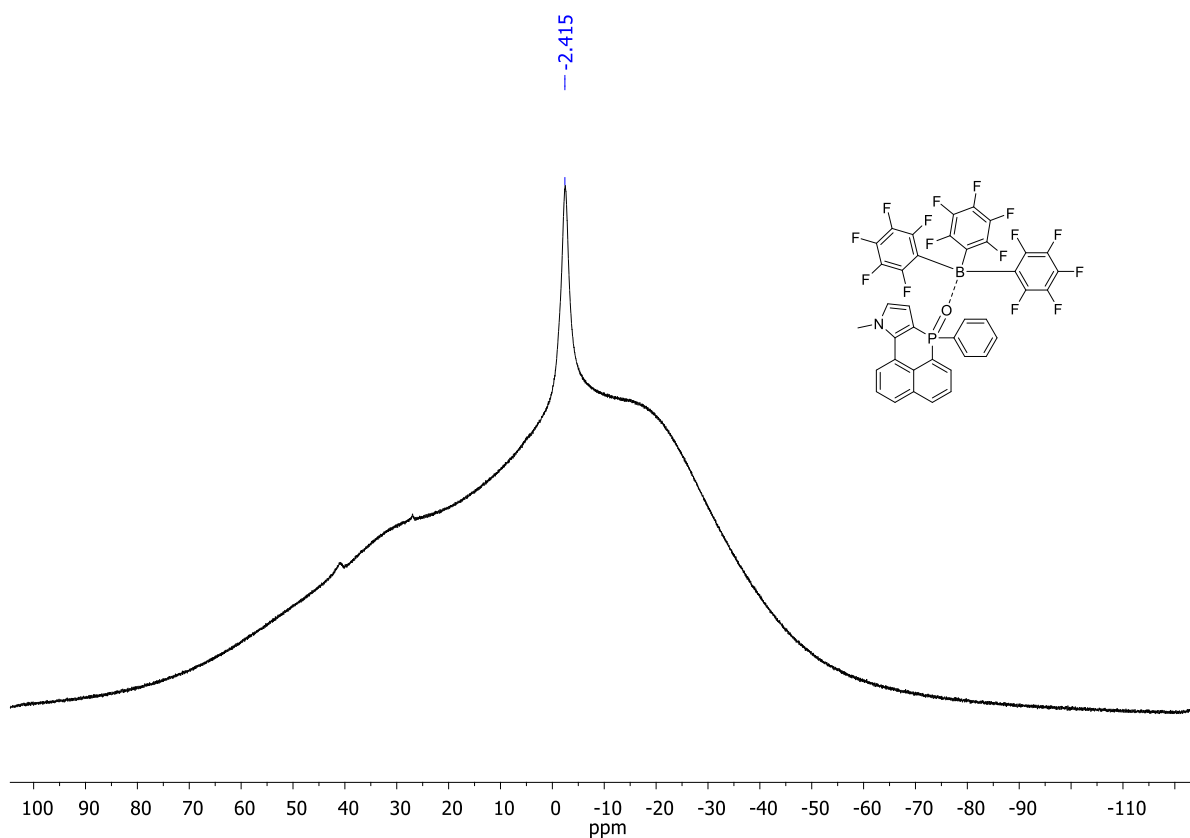
**$^{13}\text{C}$  DEPT 135 NMR (151 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2b**



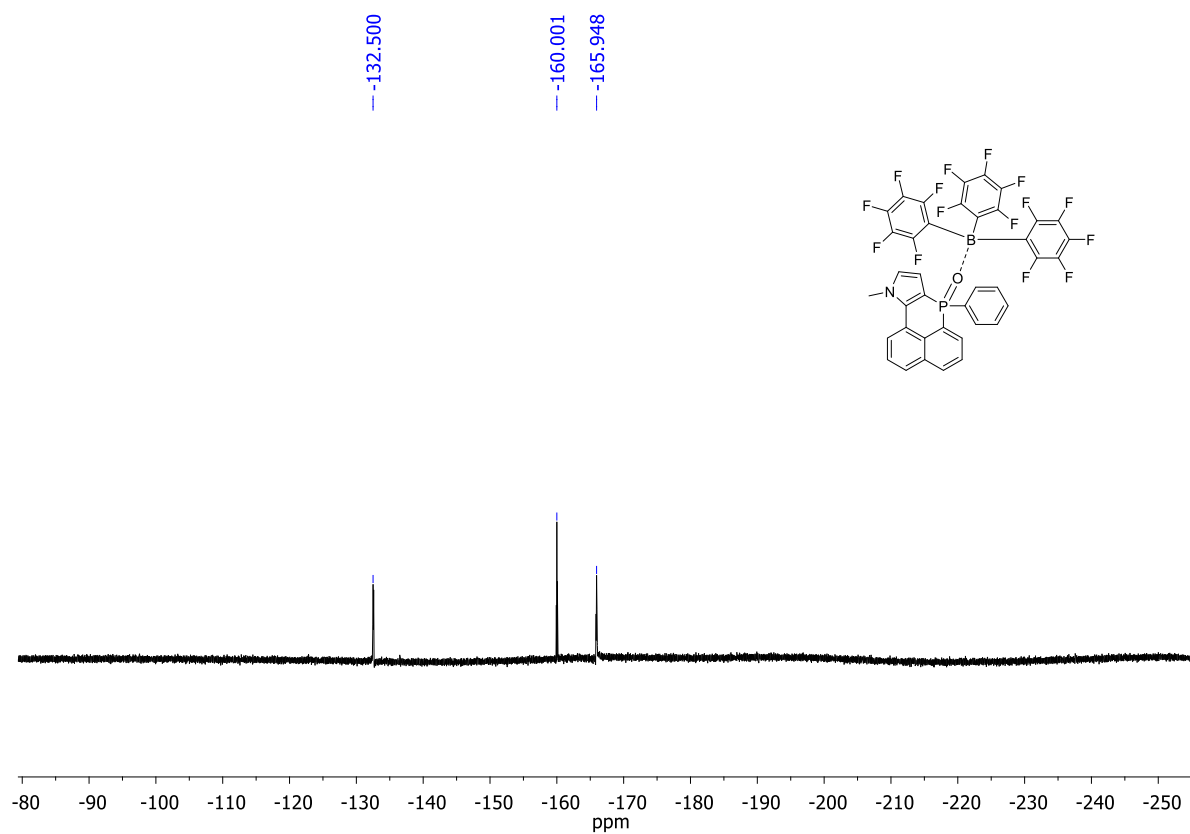
**$^{31}\text{P}\{^1\text{H}\}$  NMR (400 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2b**



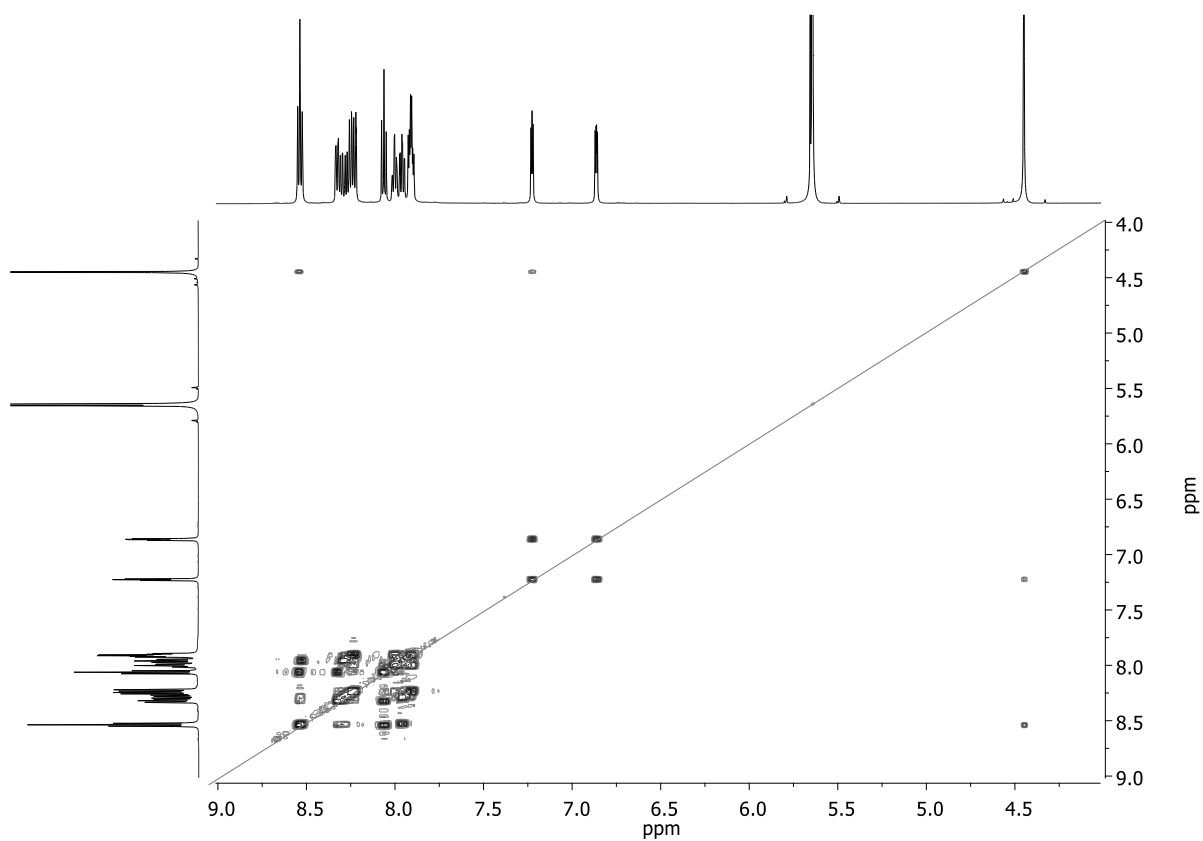
**$^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2b**



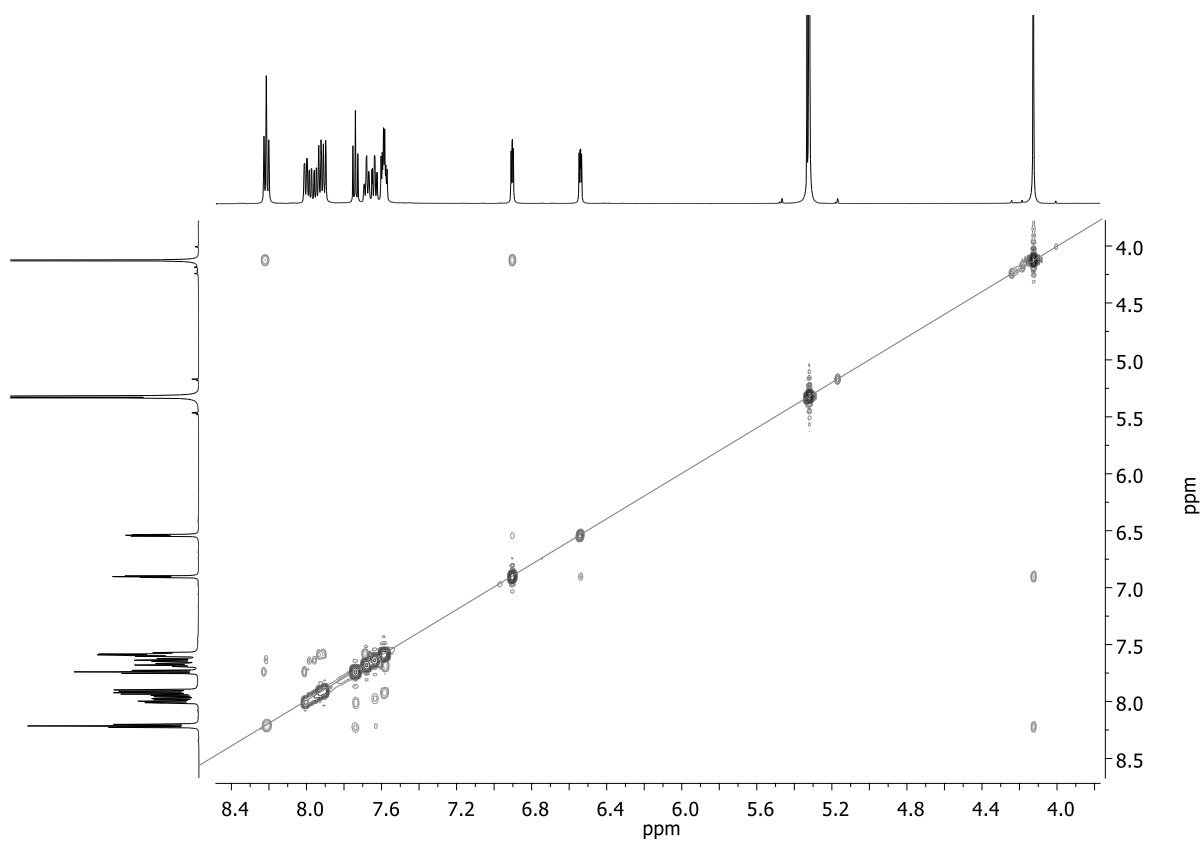
**$^{19}\text{F}\{^1\text{H}\}$  NMR (283 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2b**



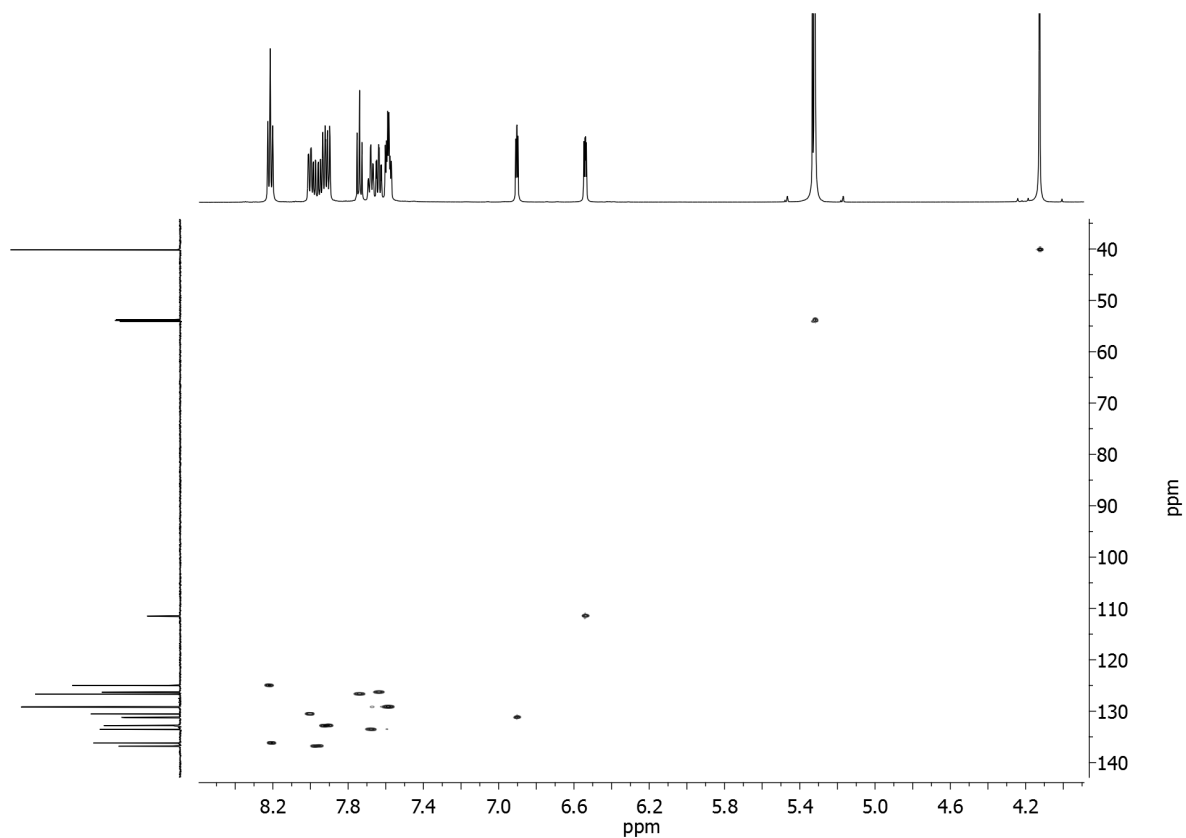
**$^1\text{H}\text{-}^1\text{H}$  COSY NMR (600 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2b**



**$^1\text{H}$ - $^1\text{H}$  ROESY NMR (600 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2b**



**HSQC-DEPT NMR (151 MHz,  $\text{CD}_2\text{Cl}_2$ ) of 2b**





### 3. Literature

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- S3.** Software package SHELXTL 2008/4 for structure solution and refinement; G.M. Sheldrick, *Acta Cryst.* 2008, **A64**, 112.
- S4.** Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford, CT, USA, 2009.
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- S6.** P. Hindenberg, J. Zimmermann, G. Hernandez-Sosa and C. Romero-Nieto, *Dalton Trans.*, 2019, **48**, 7503-7508.