# Supplementary Information

## Boron-containing D-A-A type TADF materials with tiny singlet-triplet energy splittings and high photoluminescence quantum yields for highly efficient OLEDs with low efficiency roll-offs

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## 1. Supplementary figures

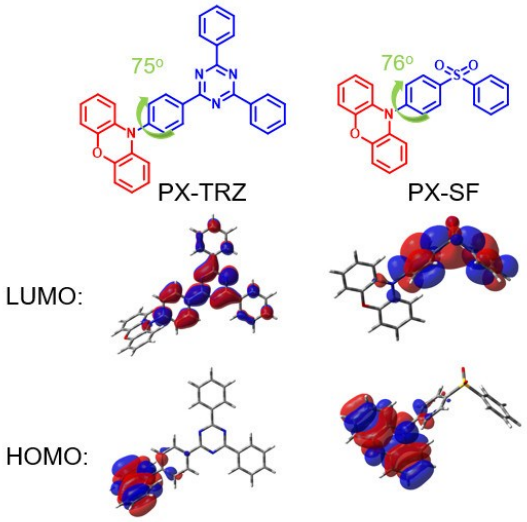


**Fig. S1** Molecular structures and frontier molecular orbital distributions of the boryl-acceptor-free PX-TRZ and PX-SF calculated by DFT (B3LYP/6-31G(d,p)). The angles show the case in the optimized geometries.

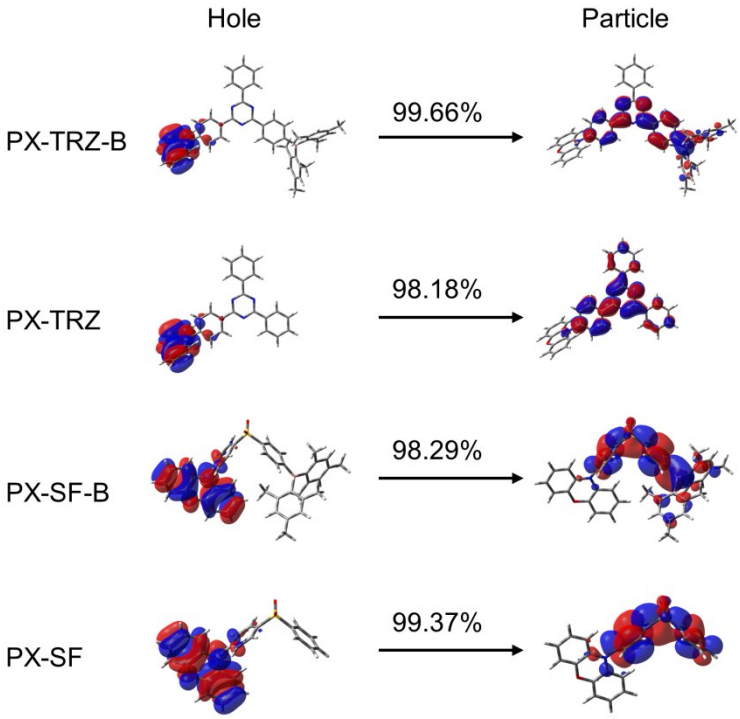


**Fig. S2** Natural transition orbital analyses for the $S_1$-state excitations of PX-TRZ-B, PX-TRZ, PX-SF-B and PX-SF.

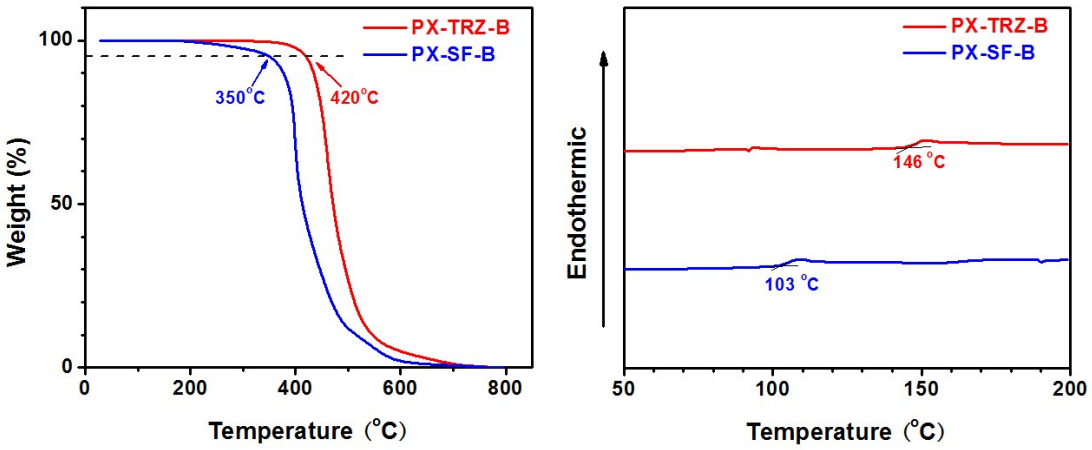


**Fig. S3** TGA (left) and DSC (right) curves of PX-TRZ-B and PX-SF-B measured at a heating rate of 10 °C/min under nitrogen atmosphere.

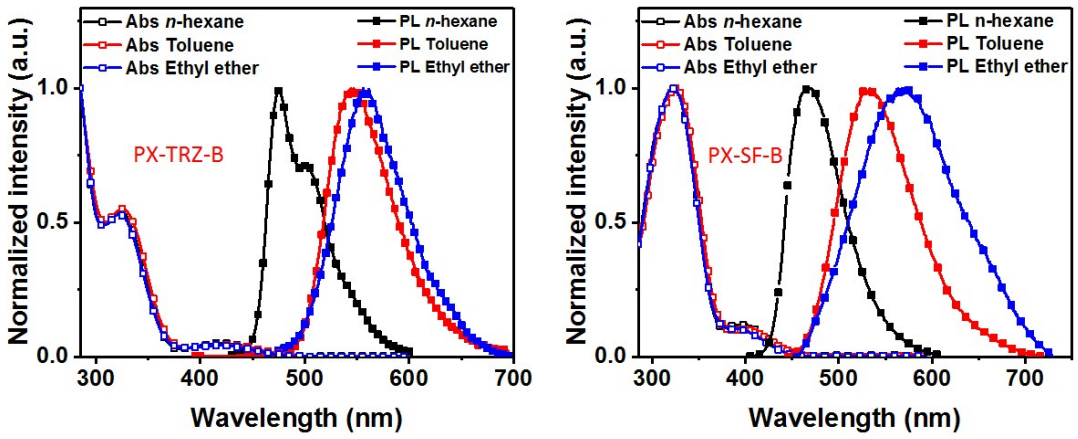


**Fig. S4** Absorption and photoluminescence spectra of PX-TRZ-B (left) and PX-SF-B (right) measured at room temperature with various solvents.

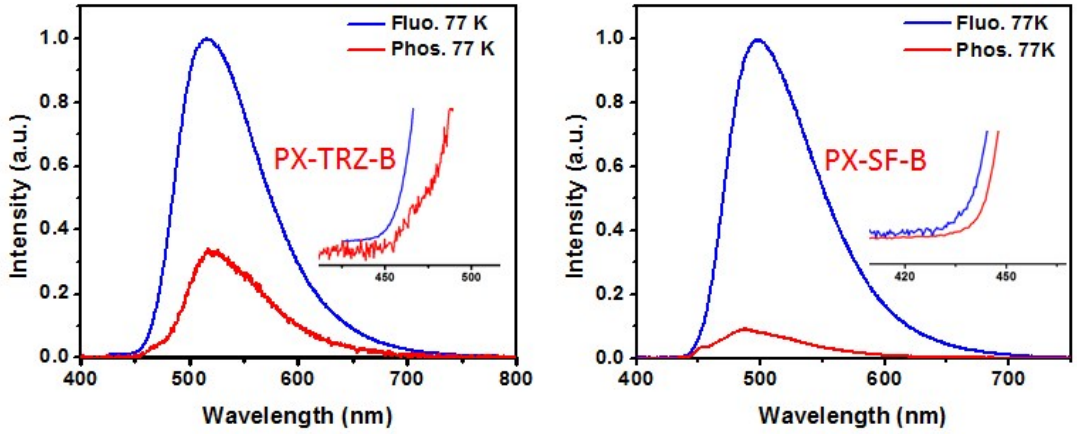


**Fig. S5** Fluorescence and phosphorescence spectra of PX-TRZ-B (left) and PX-SF-B (right) measured at 77 K in toluene. Insets show the case at the onsets of the spectra.

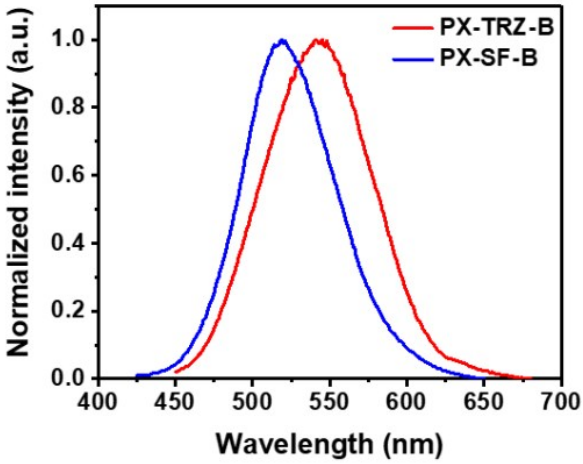


**Fig. S6** Fluorescence spectra of the doped films of PX-TRZ-B and PX-SF-B in CBP host (5 wt% doping concentration).

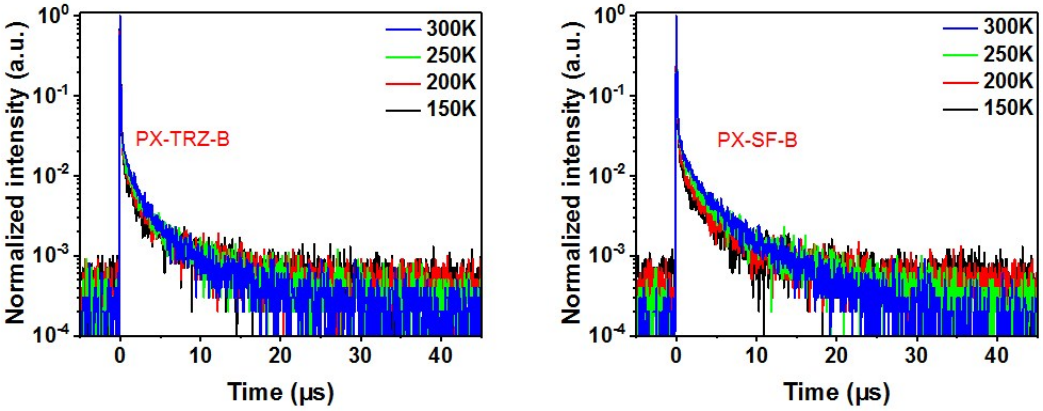


**Fig. S7** Temperature-dependent transient PL decay curves of PX-TRZ-B and PX-SF-B in CBP (5 wt% doping concentration) at the temperatures ranging from 150 K to 300 K.

## 2. Supplementary tables

**Table S1.** Contributions of molecular fragments to HOMO and LUMO.[a]

| | PX-TRZ-B | | PX-TRZ | | PX-SF-B | | PX-SF | |
|---|---|---|---|---|---|---|---|---|
| | HOMO | LUMO | HOMO | LUMO | HOMO | LUMO | HOMO | LUMO |
| phenoxazine | 94.0% | 0.6% | 93.97% | 5.82% | 93.9% | 1.2% | 94.1% | 5.4% |
| Triphenyltriazine /sulfonyldibenzene | 5.8% | 73.3% | 3.81% | 96.06% | 5.7% | 53.9% | 5.7% | 94.2% |
| boron | -- | 11.8% | | | -- | 19.2% | | |
| mesityl | -- | 11.3% | | | -- | 19.4% | | |

[a]Contributions over 0.5% are shown, and contributions from the hydrogen atoms are not included.

**Table S2.** TD-DFT calculation results and the HOMO-LUMO overlap integrals for PX-TRZ-B, PX-TRZ, PX-SF-B and PX-SF.

| | PX-TRZ-B | PX-TRZ | PX-SF-B | PX-SF |
|---|---|---|---|---|
| $E_{S1}$ / eV[a] | 2.040 | 2.155 | 2.263 | 2.578 |
| $E_{T1}$ / eV[a] | 2.010 | 2.099 | 2.244 | 2.522 |
| $\Delta E_{ST}$ / eV[b] | 0.030 | 0.056 | 0.019 | 0.056 |
| $f_{S1\leftarrow S0}$[c] | 0.024 | 0.046 | 0.010 | 0.024 |
| $C_{S1\leftarrow S0}$[d] | HOMO→LUMO (98.29%) | HOMO→LUMO (98.18%) | HOMO→LUMO (99.66%) | HOMO→LUMO (99.37%) |
| $O_{HOMO-LUMO}$[e] | 0.085 | 0.182 | 0.098 | 0.195 |

[a]Singlet ($E_{S1}$) and triplet ($E_{T1}$) energy levels. [b]Energy splitting between $S_1$ and $T_1$ states. [c]Oscillator strength for S1←S0 transition. [d]Orbital contributions for S1←S0 transition (contributions over 5% are given). [e]Overlap integral of HOMO and LUMO.

**Table S3.** Rate constants of PX-TRZ-B and PX-SF-B determined by the photoluminescence quantum yields and lifetimes of the doped films of these compounds.

| Compounds | $\Phi_{PF}$[a] (%) | $\Phi_{DF}$[b] (%) | $k_{P(total)}$[c] ($10^6$ $s^{-1}$) | $k_{P(r)}$[d] ($10^6$ $s^{-1}$) | $k_{IC}$[e] ($10^6$ $s^{-1}$) | $k_{D(r)}$[f] ($10^6$ $s^{-1}$) | $k_{ISC}$[g] ($10^6$ $s^{-1}$) | $k_{RISC}$[h] ($10^6$ $s^{-1}$) |
|---|---|---|---|---|---|---|---|---|
| PX-TRZ-B | 18.0 | 47.0 | 21.9 | 3.95 | 2.13 | 0.16 | 15.9 | 0.57 |
| PX-SF-B | 23.0 | 61.0 | 18.3 | 4.21 | 0.80 | 0.16 | 13.3 | 0.58 |

[a]Prompt fluorescence component of $\Phi_{PL}$. [b]Delayed fluorescence component of $\Phi_{PL}$. [c]Total decay rate constant of the prompt component. [d]Radiative decay rate constant of the prompt component. [e]Internal conversion rate constant of the prompt component. [f]Radiative decay rate constant of the delayed component. [g]Rate constant for intersystem crossing. [h]Rate constant for reverse intersystem crossing.

The rate constants were determined by using the following formula:[1]

$k_{P(r)} = \Phi_{PF}/\tau_{PF}$

$k_{D(r)} = \Phi_{DF}/\tau_{DF}$

$k_{P(total)} = k_{P(r)} + k_{IC} + k_{ISC} = k_{P(r)}/\Phi_{PF}$

$k_{ISC} = \Phi_{DF}k_{P(total)}/\Phi_{PL}$

$k_{RISC} = k_{D(r)}k_{P(total)}\Phi_{DF}/(k_{ISC}\Phi_{PF})$

## 3. NMR spectra

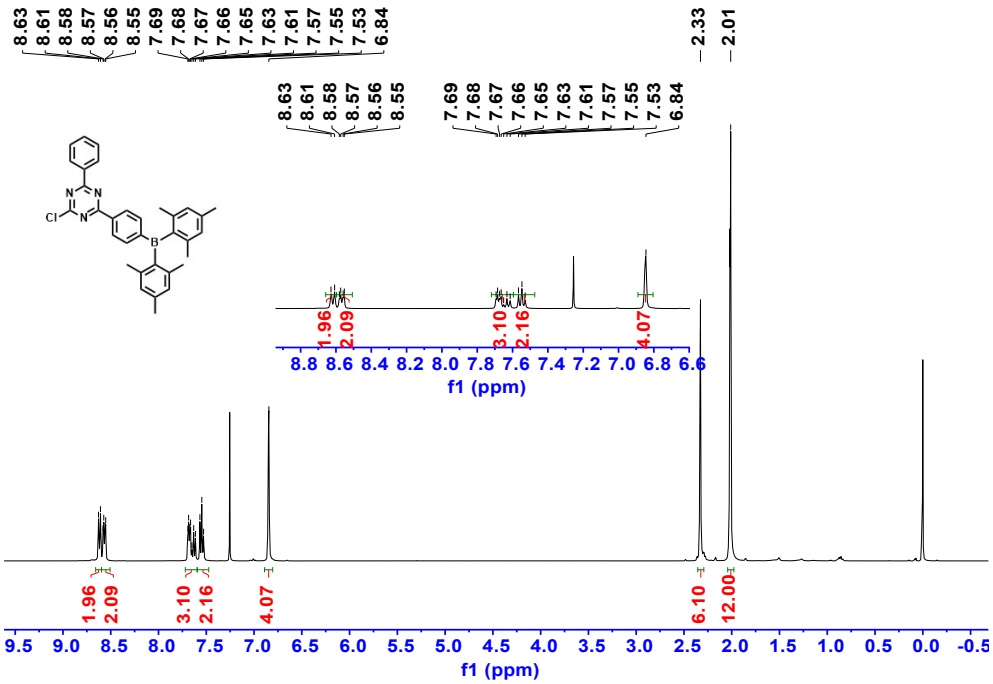


**Fig. S8** $^{1}$H NMR spectrum of 2-chloro-4-(4-(dimesitylboraneyl)phenyl)-6-phenyl -1,3,5-triazine in $CDCl_3$ (400 MHz).

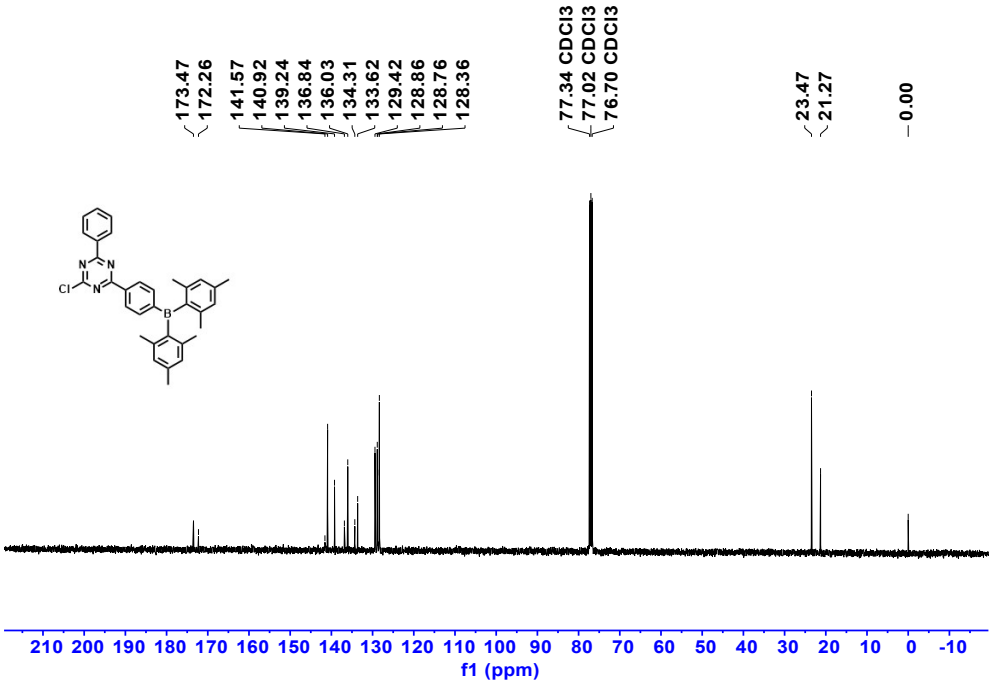


**Fig. S9** $^{13}$C{$^{1}$H} NMR spectrum of 2-chloro-4-(4-(dimesitylboraneyl)phenyl)-6-phenyl-1,3,5-triazine in $CDCl_3$ (100 MHz).

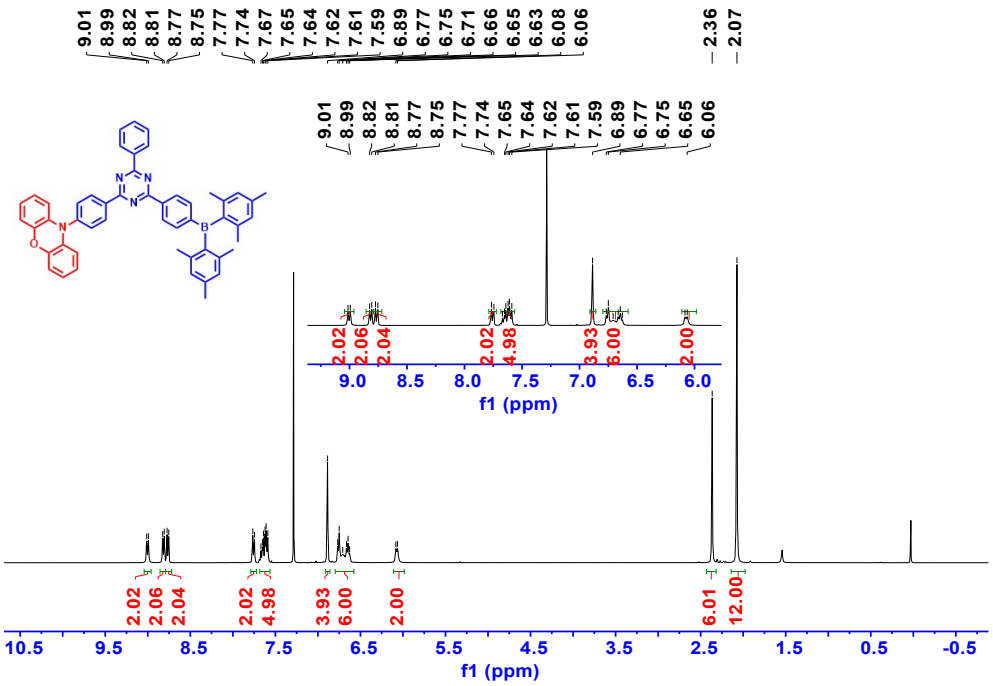


**Fig. S10** $^{1}H$ NMR spectrum of PX-TRZ-B in $CDCl_3$ (400 MHz).

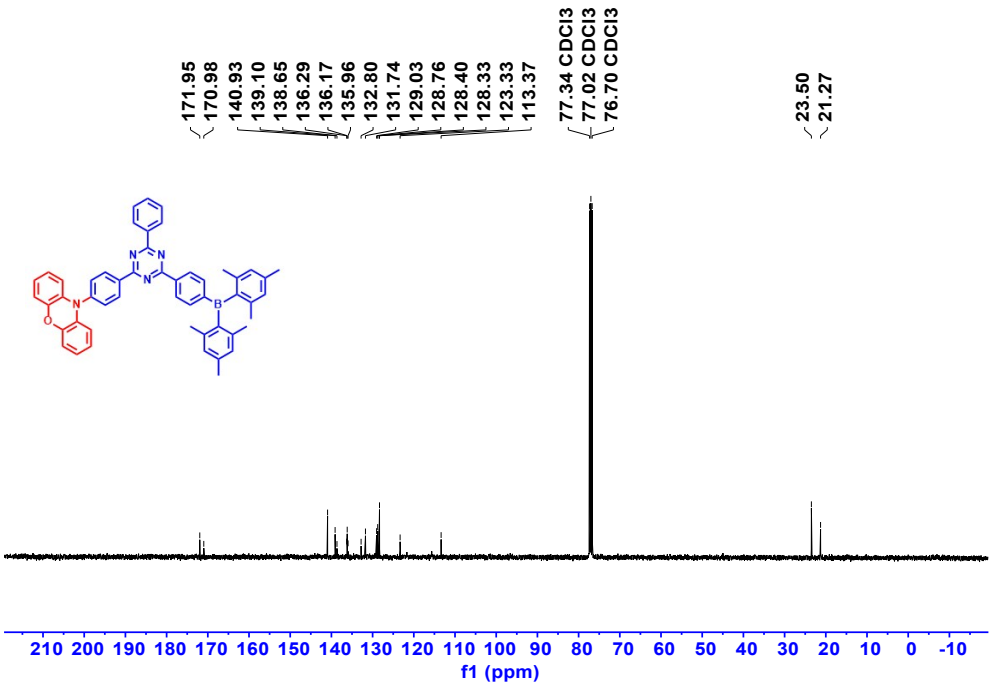


**Fig. S11** $^{13}C\{^{1}H\}$ NMR spectrum of PX-TRZ-B in $CDCl_3$ (100 MHz).

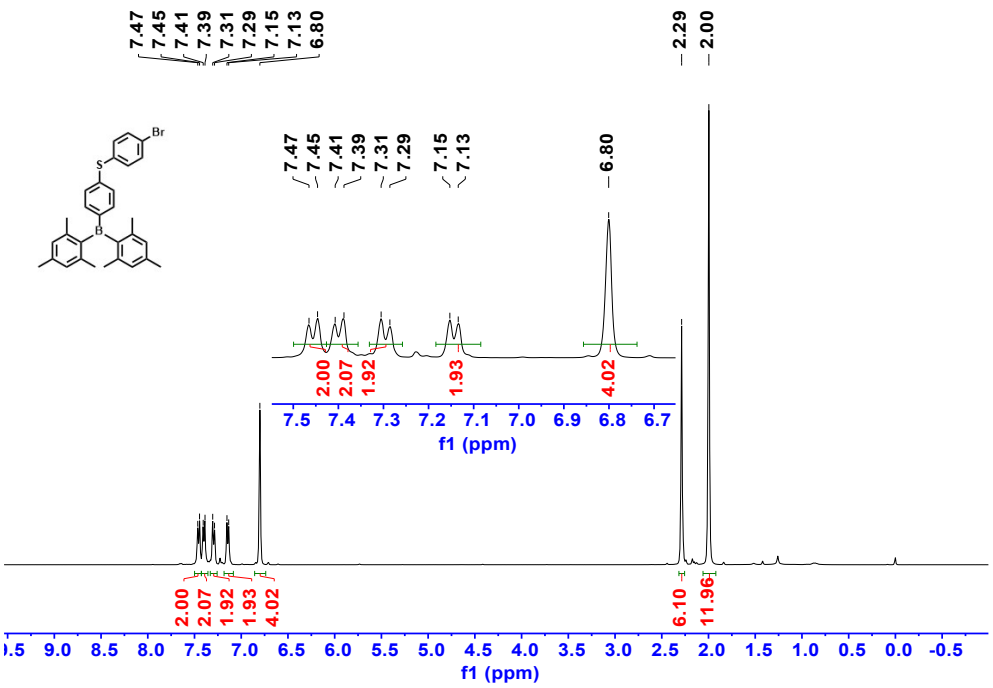


**Fig. S12** $^{1}$H NMR spectrum of (4-((4-bromophenyl)thio)phenyl)dimesitylborane in $CDCl_3$ (400 MHz).

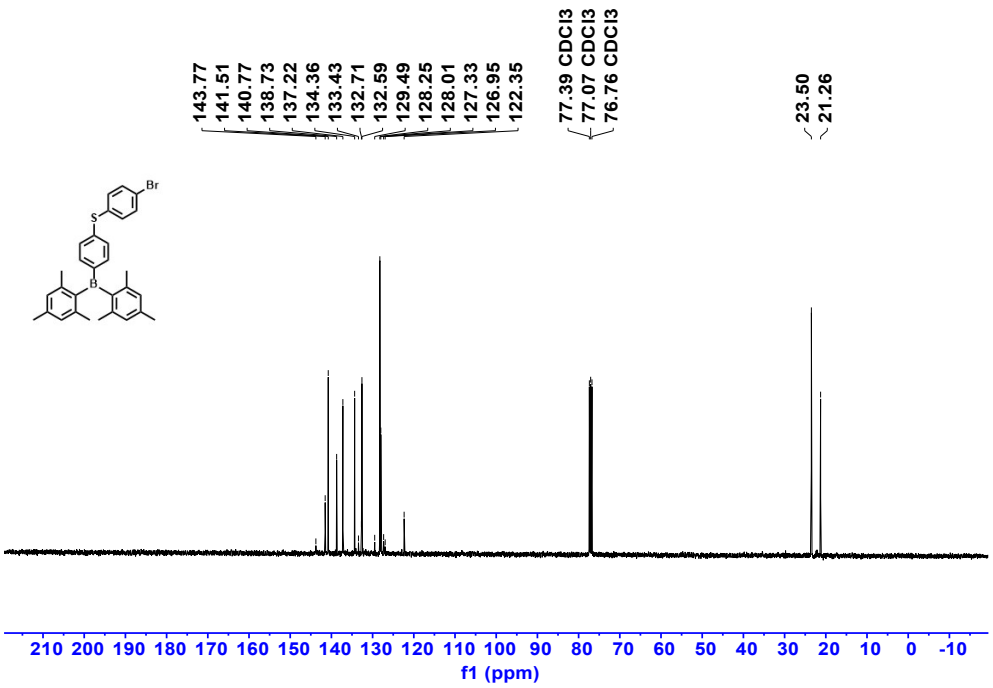


**Fig. S13** $^{13}$C{$^{1}$H} NMR spectrum of (4-((4-bromophenyl)thio)phenyl)dimesitylborane in $CDCl_3$ (100 MHz).

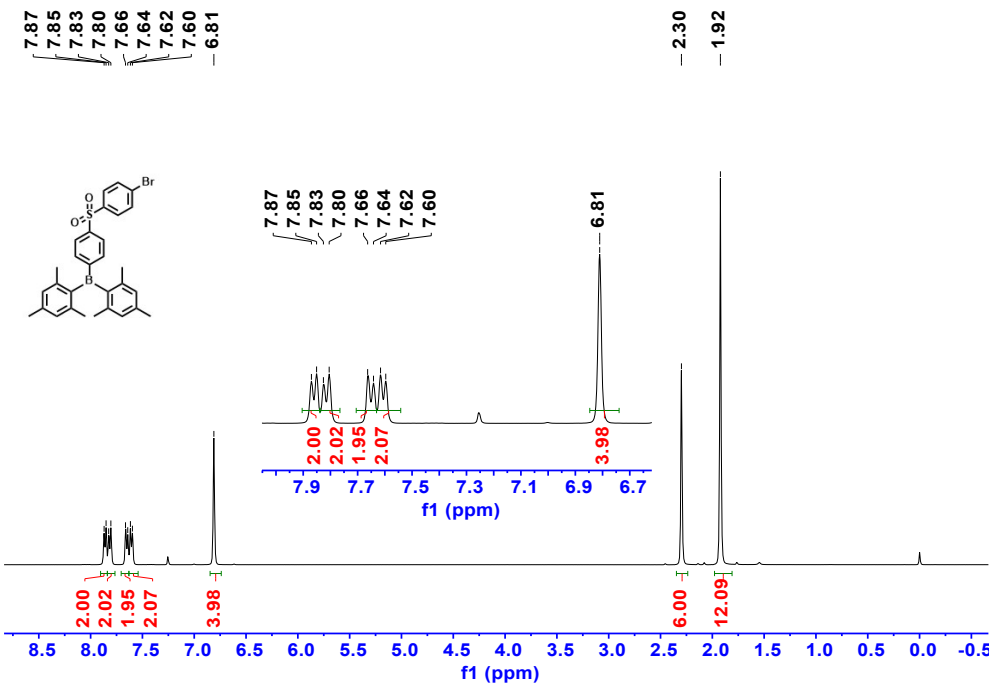


**Fig. S14** $^{1}$H NMR spectrum of (4-((4-bromophenyl)sulfonyl)phenyl)dimesitylborane in $CDCl_3$ (400 MHz).

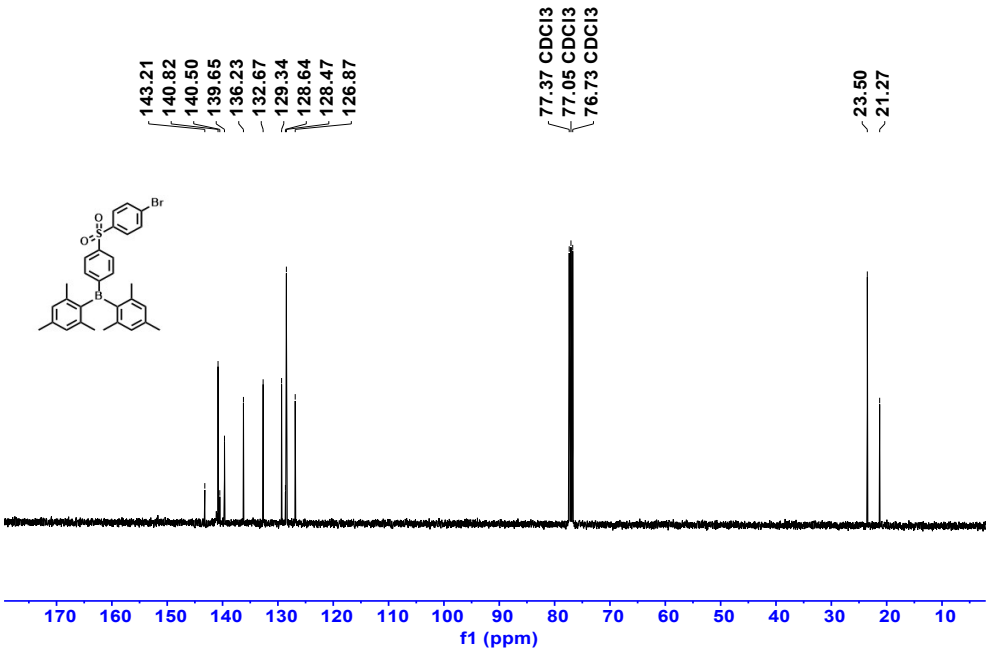


**Fig. S15** $^{13}C\{^{1}H\}$ NMR spectrum of (4-((4-bromophenyl)sulfonyl)phenyl)dimesitylborane in $CDCl_3$ (100 MHz).

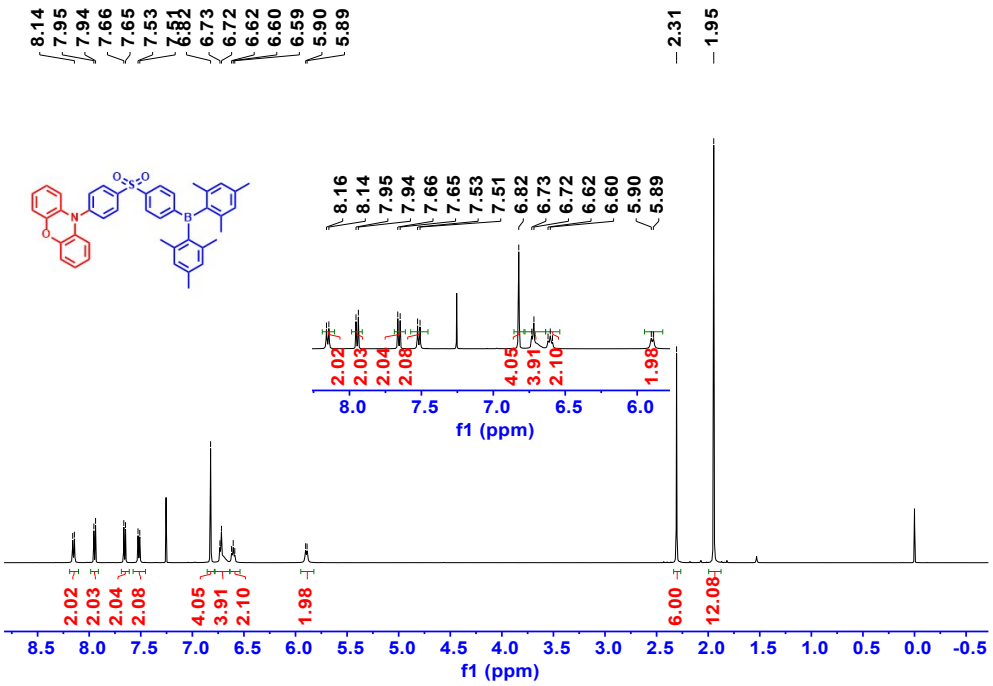


**Fig. S16** $^{1}$H NMR spectrum of PX-SF-B in $CDCl_3$ (400 MHz).

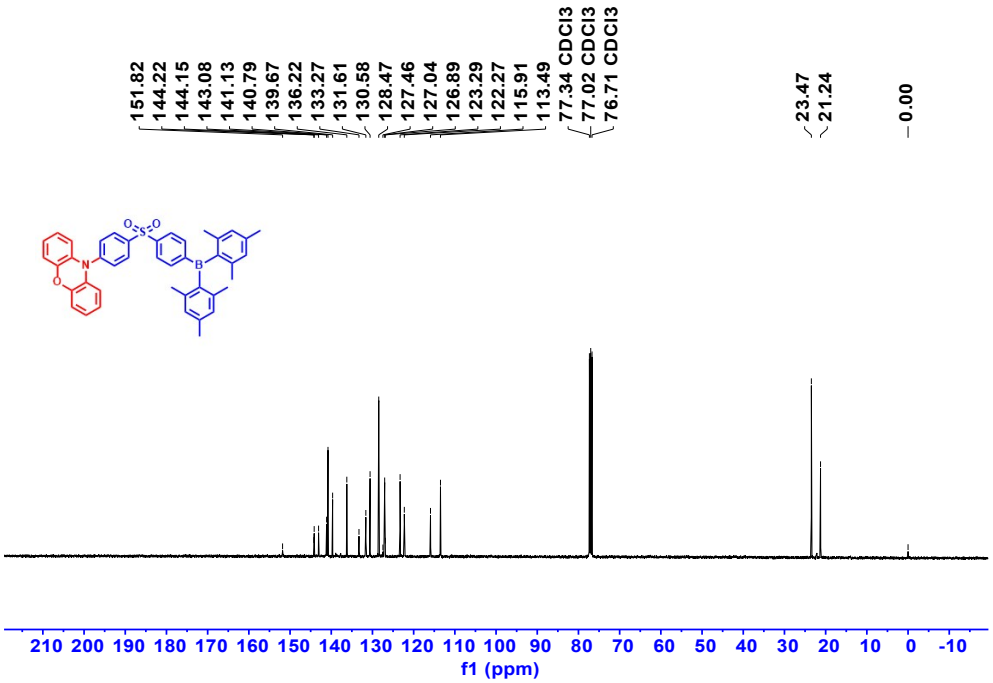


**Fig. S17** $^{13}C\{^{1}H\}$ NMR spectrum of PX-SF-B in $CDCl_3$ (100 MHz).

## 4. Cartesian coordinates of DFT-optimized geometries

## PX-TRZ-B:

| Element | X | Y | Z |
|---|---|---|---|
| C | 4.01868 | 1.17763 | -0.18444 |
| C | 4.07923 | -0.21932 | -0.01269 |
| C | 2.86073 | -0.90867 | 0.14323 |
| C | 1.64217 | -0.24248 | 0.13298 |
| C | 1.60368 | 1.14763 | -0.05622 |
| C | 2.80579 | 1.85386 | -0.21713 |
| C | -3.22914 | 1.0554 | 0.03858 |
| C | -4.46155 | 1.72291 | -0.01165 |
| C | -5.65037 | 1.00662 | 0.06248 |
| C | -5.62185 | -0.38668 | 0.17779 |
| C | -4.39652 | -1.05867 | 0.22683 |
| C | -3.20733 | -0.34138 | 0.16326 |
| N | -6.8429 | -1.11917 | 0.23654 |
| B | 5.44704 | -0.97869 | -0.01184 |
| C | -7.6012 | -1.32121 | -0.9318 |
| C | -8.81982 | -2.01756 | -0.84346 |
| O | -9.29393 | -2.51252 | 0.35483 |
| C | -8.51776 | -2.35007 | 1.48513 |
| C | -7.29511 | -1.65522 | 1.45664 |
| C | -7.18346 | -0.87496 | -2.18875 |
| C | -7.96973 | -1.09817 | -3.32227 |
| C | -9.17878 | -1.77712 | -3.21778 |
| C | -9.59911 | -2.24094 | -1.96786 |
| C | -9.00457 | -2.89331 | 2.66378 |
| C | -8.28558 | -2.74932 | 3.8539 |
| C | -7.08184 | -2.05337 | 3.8434 |
| C | -6.5903 | -1.50748 | 2.6545 |
| C | 5.47961 | -2.48385 | -0.4559 |
| C | 6.74602 | -0.21425 | 0.42497 |
| C | 7.89253 | -0.20521 | -0.41034 |
| C | 9.03427 | 0.49744 | -0.02166 |
| C | 9.10387 | 1.17439 | 1.19834 |
| C | 7.9816 | 1.14602 | 2.02654 |
| C | 6.8096 | 0.47992 | 1.65807 |
| C | 6.07152 | -3.46916 | 0.37578 |
| C | 6.07197 | -4.80754 | -0.01907 |
| C | 5.53406 | -5.21534 | -1.24277 |
| C | 4.97301 | -4.24086 | -2.0674 |
| C | 4.92473 | -2.89509 | -1.69193 |
| C | 5.59074 | -6.66061 | -1.66914 |
| C | 6.69732 | -3.1148 | 1.7075 |

| | | | |
|---|---|---|---|
| C | 4.29449 | -1.91922 | -2.665 |
| C | 7.91615 | -0.92929 | -1.73914 |
| C | 5.65027 | 0.5087 | 2.6335 |
| C | 10.36619 | 1.88256 | 1.62097 |
| N | 0.32746 | 3.1941 | -0.23361 |
| C | 0.30803 | 1.86013 | -0.09398 |
| N | -0.81381 | 1.12958 | 0.00756 |
| C | -1.9633 | 1.81764 | -0.04827 |
| N | -2.04254 | 3.14916 | -0.18447 |
| C | -0.87023 | 3.79826 | -0.27003 |
| C | -0.90075 | 5.26917 | -0.41604 |
| C | -2.12612 | 5.9494 | -0.47193 |
| C | -2.15196 | 7.33381 | -0.60952 |
| C | -0.95732 | 8.05239 | -0.69193 |
| C | 0.26558 | 7.38027 | -0.63641 |
| C | 0.29606 | 5.99591 | -0.49923 |
| H | 4.9459 | 1.73155 | -0.29839 |
| H | 2.88217 | -1.98678 | 0.27163 |
| H | 0.7089 | -0.77783 | 0.25925 |
| H | 2.76467 | 2.92655 | -0.36307 |
| H | -4.46688 | 2.80199 | -0.10306 |
| H | -6.6092 | 1.51259 | 0.02827 |
| H | -4.39097 | -2.13991 | 0.31289 |
| H | -2.25036 | -0.84737 | 0.19654 |
| H | -6.23936 | -0.35217 | -2.27792 |
| H | -7.62291 | -0.73785 | -4.28521 |
| H | -9.79402 | -1.95306 | -4.09352 |
| H | -10.53083 | -2.78187 | -1.84339 |
| H | -9.95147 | -3.42095 | 2.6291 |
| H | -8.67207 | -3.17613 | 4.77305 |
| H | -6.51325 | -1.92443 | 4.75853 |
| H | -5.65564 | -0.96063 | 2.65517 |
| H | 9.89623 | 0.51077 | -0.68482 |
| H | 8.01807 | 1.65634 | 2.9866 |
| H | 6.51066 | -5.55231 | 0.64126 |
| H | 4.56057 | -4.53467 | -3.03017 |
| H | 5.40524 | -7.3329 | -0.82575 |
| H | 4.85313 | -6.8769 | -2.44683 |
| H | 6.57866 | -6.91439 | -2.07288 |
| H | 6.01418 | -2.54577 | 2.34578 |
| H | 6.98146 | -4.01905 | 2.25202 |
| H | 7.59203 | -2.49975 | 1.5774 |
| H | 4.39285 | -2.28649 | -3.69056 |
| H | 3.22682 | -1.78529 | -2.46184 |

| | | | |
|---|---|---|---|
| H | 4.74641 | -0.92618 | -2.6196 |
| H | 7.06882 | -0.6539 | -2.3744 |
| H | 8.83106 | -0.69453 | -2.28957 |
| H | 7.86876 | -2.01339 | -1.60454 |
| H | 6.01467 | 0.64951 | 3.65504 |
| H | 4.96026 | 1.32931 | 2.4113 |
| H | 5.0588 | -0.40934 | 2.61251 |
| H | 10.89547 | 2.30271 | 0.76059 |
| H | 10.15347 | 2.69497 | 2.32163 |
| H | 11.05666 | 1.19203 | 2.12098 |
| H | -3.0436 | 5.37741 | -0.40646 |
| H | -3.10365 | 7.85422 | -0.65261 |
| H | -0.97936 | 9.13269 | -0.79905 |
| H | 1.19542 | 7.9368 | -0.70003 |
| H | 1.23576 | 5.45913 | -0.45399 |

## PX-TRZ:

| Element | X | Y | Z |
|---|---|---|---|
| N | 4.49103 | 2.13E-5 | -8.3E-6 |
| C | 3.77986 | -1.12057 | -0.19632 |
| N | 2.43801 | -1.16846 | -0.20302 |
| C | 1.81266 | -5.9E-6 | -4.73E-5 |
| N | 2.43798 | 1.16846 | 0.20295 |
| C | 3.77983 | 1.12059 | 0.19628 |
| C | 4.51954 | -2.38146 | -0.41932 |
| C | 0.33235 | -2.5E-5 | -4.37E-5 |
| C | 4.51948 | 2.38151 | 0.41931 |
| C | -0.37542 | 1.19548 | 0.19157 |
| C | -1.76548 | 1.19466 | 0.19669 |
| C | -2.46502 | -5.99E-5 | -4.17E-5 |
| C | -1.76545 | -1.19476 | -0.19677 |
| C | -0.37539 | -1.19555 | -0.19165 |
| C | 3.82479 | -3.57945 | -0.64159 |
| C | 4.52312 | -4.76443 | -0.85218 |
| C | 5.9196 | -4.76611 | -0.84269 |
| C | 6.61648 | -3.57625 | -0.62159 |
| C | 5.92207 | -2.389 | -0.41098 |
| C | 3.8247 | 3.57947 | 0.64158 |
| C | 4.523 | 4.76447 | 0.85219 |
| C | 5.91948 | 4.76618 | 0.84275 |
| C | 6.61639 | 3.57634 | 0.62165 |
| C | 5.92201 | 2.38907 | 0.41101 |

| | | | |
|---|---|---|---|
| N | -3.89002 | -8.2E-5 | -3.7E-5 |
| C | -4.59946 | 0.50385 | -1.10631 |
| C | -6.00549 | 0.49482 | -1.07762 |
| O | -6.71246 | -5.01E-5 | 1.49E-5 |
| C | -6.00547 | -0.49486 | 1.07765 |
| C | -4.59943 | -0.50393 | 1.1063 |
| C | -3.96425 | 0.99614 | -2.24997 |
| C | -4.71028 | 1.48478 | -3.32588 |
| C | -6.09995 | 1.48186 | -3.27791 |
| C | -6.74587 | 0.97931 | -2.14468 |
| C | -6.74581 | -0.97928 | 2.14478 |
| C | -6.09986 | -1.48179 | 3.27801 |
| C | -4.71019 | -1.48474 | 3.32592 |
| C | -3.96419 | -0.99618 | 2.24995 |
| H | 0.18087 | 2.11224 | 0.34297 |
| H | -2.32282 | 2.11234 | 0.35067 |
| H | -2.32277 | -2.11246 | -0.35075 |
| H | 0.18092 | -2.11229 | -0.34305 |
| H | 2.74183 | -3.56086 | -0.64616 |
| H | 3.97938 | -5.68811 | -1.0241 |
| H | 6.463 | -5.69168 | -1.00715 |
| H | 7.702 | -3.57528 | -0.61365 |
| H | 6.44682 | -1.45737 | -0.23803 |
| H | 2.74174 | 3.56087 | 0.64612 |
| H | 3.97923 | 5.68814 | 1.02411 |
| H | 6.46285 | 5.69176 | 1.00723 |
| H | 7.70191 | 3.57538 | 0.61375 |
| H | 6.44678 | 1.45745 | 0.23808 |
| H | -2.88243 | 0.99465 | -2.29673 |
| H | -4.19104 | 1.86334 | -4.2002 |
| H | -6.68487 | 1.8604 | -4.10916 |
| H | -7.82743 | 0.95091 | -2.0696 |
| H | -7.82737 | -0.95084 | 2.06974 |
| H | -6.68476 | -1.86027 | 4.1093 |
| H | -4.19093 | -1.86328 | 4.20023 |
| H | -2.88236 | -0.99471 | 2.29667 |

## PX-SF-B:

| Element | X | Y | Z |
|---|---|---|---|

| | | | |
|---|---|---|---|
| C | 2.20473 | 1.93831 | -0.62124 |
| C | 2.54921 | 1.14297 | 0.48742 |
| C | 1.9168 | 1.40878 | 1.71645 |
| C | 0.94251 | 2.39419 | 1.83214 |
| C | 0.57719 | 3.10848 | 0.69044 |
| C | 1.20744 | 2.90601 | -0.53688 |
| S | -0.87557 | 4.15986 | 0.75894 |
| C | -2.13528 | 2.94235 | 0.3552 |
| C | -2.47976 | 2.74229 | -0.98001 |
| C | -3.32875 | 1.68694 | -1.30556 |
| C | -3.80288 | 0.83781 | -0.30238 |
| C | -3.47315 | 1.06982 | 1.03774 |
| C | -2.63782 | 2.13054 | 1.3725 |
| O | -0.80719 | 5.12633 | -0.34762 |
| O | -1.07878 | 4.5815 | 2.15323 |
| N | -4.59168 | -0.29424 | -0.65773 |
| B | 3.53574 | -0.06417 | 0.32599 |
| C | -3.94401 | -1.47578 | -1.07541 |
| C | -4.71587 | -2.62783 | -1.30745 |
| O | -6.08523 | -2.63495 | -1.13659 |
| C | -6.67792 | -1.52561 | -0.56597 |
| C | -5.95899 | -0.34286 | -0.32122 |
| C | -2.56145 | -1.55411 | -1.26741 |
| C | -1.96892 | -2.74353 | -1.70151 |
| C | -2.74601 | -3.87312 | -1.93446 |
| C | -4.12696 | -3.81039 | -1.72865 |
| C | -8.02739 | -1.61725 | -0.26254 |
| C | -8.69987 | -0.52018 | 0.28328 |
| C | -8.00408 | 0.66092 | 0.51789 |
| C | -6.64243 | 0.75066 | 0.21687 |
| C | 3.30063 | -1.3302 | 1.21918 |
| C | 4.68258 | 0.02208 | -0.73587 |
| C | 4.36878 | -1.88441 | 1.97017 |
| C | 4.14835 | -3.00024 | 2.7792 |
| C | 2.89954 | -3.62184 | 2.85276 |
| C | 1.85787 | -3.09035 | 2.09137 |
| C | 2.02987 | -1.95478 | 1.29557 |
| C | 4.86313 | -1.00879 | -1.69433 |
| C | 5.87246 | -0.90069 | -2.65167 |
| C | 6.75116 | 0.18589 | -2.6779 |
| C | 6.58394 | 1.18654 | -1.72056 |
| C | 5.56408 | 1.13076 | -0.7669 |
| C | 7.86421 | 0.25414 | -3.69243 |

| | | | |
|---|---|---|---|
| C | 2.68077 | -4.8183 | 3.74338 |
| C | 5.76116 | -1.29173 | 1.93204 |
| C | 0.83042 | -1.4707 | 0.50468 |
| C | 3.9746 | -2.23392 | -1.72788 |
| C | 5.46859 | 2.26698 | 0.23077 |
| H | 2.70975 | 1.76728 | -1.56725 |
| H | 2.17841 | 0.80934 | 2.58322 |
| H | 0.44883 | 2.59949 | 2.77547 |
| H | 0.91117 | 3.49586 | -1.3972 |
| H | -2.08454 | 3.40559 | -1.74076 |
| H | -3.614 | 1.49578 | -2.33413 |
| H | -3.86476 | 0.4069 | 1.80153 |
| H | -2.36193 | 2.32548 | 2.40248 |
| H | -1.94701 | -0.68222 | -1.08107 |
| H | -0.89544 | -2.7725 | -1.8545 |
| H | -2.29205 | -4.79867 | -2.27147 |
| H | -4.76812 | -4.66966 | -1.8919 |
| H | -8.53464 | -2.5537 | -0.46712 |
| H | -9.75648 | -0.59646 | 0.51569 |
| H | -8.51163 | 1.52485 | 0.93394 |
| H | -6.10783 | 1.67572 | 0.39468 |
| H | 4.9751 | -3.4025 | 3.36012 |
| H | 0.88399 | -3.57414 | 2.11533 |
| H | 5.98234 | -1.68934 | -3.3926 |
| H | 7.26521 | 2.03434 | -1.71585 |
| H | 7.52636 | -0.08076 | -4.67804 |
| H | 8.25258 | 1.27124 | -3.7918 |
| H | 8.70156 | -0.39193 | -3.40173 |
| H | 2.42507 | -4.50662 | 4.76366 |
| H | 1.86111 | -5.44377 | 3.37881 |
| H | 3.58058 | -5.43703 | 3.80992 |
| H | 5.75757 | -0.21548 | 2.1304 |
| H | 6.40062 | -1.76362 | 2.6825 |
| H | 6.22793 | -1.429 | 0.95258 |
| H | 0.11022 | -2.28091 | 0.36748 |
| H | 0.31079 | -0.65372 | 1.01591 |
| H | 1.10323 | -1.09441 | -0.48498 |
| H | 2.912 | -1.97346 | -1.7574 |
| H | 4.19063 | -2.84037 | -2.61126 |
| H | 4.12026 | -2.85796 | -0.84202 |
| H | 6.43681 | 2.7634 | 0.3393 |
| H | 4.74387 | 3.02271 | -0.08941 |
| H | 5.15342 | 1.93102 | 1.22152 |

## PX-SF:

| Element | X | Y | Z |
|---|---|---|---|
| C | 5.33567 | 1.54785 | -1.6094 |
| C | 5.65912 | 2.39139 | -0.54453 |
| C | 5.35552 | 2.02198 | 0.76759 |
| C | 4.71865 | 0.80865 | 1.02178 |
| C | 4.39488 | -0.01841 | -0.0533 |
| C | 4.69878 | 0.33181 | -1.3684 |
| S | 3.55154 | -1.56995 | 0.26314 |
| C | 1.81469 | -1.11617 | 0.19446 |
| C | 1.17357 | -0.70317 | 1.36211 |
| C | -0.16738 | -0.33441 | 1.30055 |
| C | -0.8476 | -0.37159 | 0.07901 |
| C | -0.19295 | -0.79411 | -1.08241 |
| C | 1.14493 | -1.17541 | -1.02725 |
| O | 3.84691 | -1.96395 | 1.64947 |
| N | -2.21554 | 0.01779 | 0.01948 |
| C | -2.56458 | 1.38125 | 0.05187 |
| C | -3.92418 | 1.73742 | 0.00486 |
| O | -4.92606 | 0.79204 | -0.07822 |
| C | -4.57053 | -0.54176 | -0.11628 |
| C | -3.22843 | -0.95728 | -0.06535 |
| C | -5.60136 | -1.46478 | -0.19879 |
| C | -5.31837 | -2.8334 | -0.22615 |
| C | -3.99606 | -3.25886 | -0.16423 |
| C | -2.95702 | -2.32795 | -0.08112 |
| C | -1.61267 | 2.40296 | 0.10814 |
| C | -2.0066 | 3.74356 | 0.13639 |
| C | -3.35505 | 4.08096 | 0.10181 |
| C | -4.31497 | 3.06714 | 0.03265 |
| O | 3.81587 | -2.46191 | -0.87662 |
| H | 5.58523 | 1.83369 | -2.62609 |
| H | 6.1561 | 3.33696 | -0.73731 |
| H | 5.62057 | 2.67513 | 1.59269 |
| H | 4.49153 | 0.48915 | 2.03242 |
| H | 4.45662 | -0.35012 | -2.17545 |
| H | 1.71517 | -0.70125 | 2.30094 |
| H | -0.70005 | -0.0184 | 2.19072 |
| H | -0.74321 | -0.82484 | -2.01638 |
| H | 1.66716 | -1.52566 | -1.91005 |
| H | -6.61884 | -1.09143 | -0.23718 |

| | | | |
|---|---|---|---|
| H | -6.12932 | -3.55061 | -0.29117 |
| H | -3.75746 | -4.31715 | -0.17643 |
| H | -1.93012 | -2.66754 | -0.0254 |
| H | -0.56044 | 2.14734 | 0.12811 |
| H | -1.24707 | 4.51704 | 0.18237 |
| H | -3.66792 | 5.11919 | 0.12415 |
| H | -5.37615 | 3.28776 | -0.00371 |

## 5. References

1. K. Goushi, K. Yoshida, K. Sato and C. Adachi, *Nat. Photon.*, 2012, **6**, 253-258.