Supporting Information

Purely organic phosphorescent organic light emitting diodes using alkyl modified phenoselenazine

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1. General Information

Materials and measurements

Selenium, diphenylamine, sulforane, sodium tert-butoxide, iodobenzene, 1-iodo-4-methyl benzene, 1-bromo-4-tert-butyl benzene (Alfa aesar Co.), seleniumdioxide (Sigma aldrich Co.), iodine, toluene (Samchun pure chemical Co.), palladium(Ⅱ) acetate (GOM tech Co), tri-tert-butyl phosphine (INCO), and aluminum chloride (TCI chem. Co.) were used as received.

The ^{1}H and ^{13}C spectra were recorded using an Advance-500 (Bruker). Solvents for the NMR analysis were dimethylsulfoxide-d_6 (DMSO-d_6) and chloroform-d ($CDCl_3$). Ultraviolet-visible (UV- vis) spectra were measured by UV-vis spectrophotometer (JASCO, V-730). PL spectra were recorded on fluorescence spectrophotometer (PerkinElmer, LS-55).

Transient PL decay was mesured by using Hamamatsu Quantaurus-Tau system (Hamamatsu, C11367-31) and temperature was cotrolled by cryostat (Oxford, Optistat DN2).

PL quantum yield data were measured by Quantaurus-QY Absolute system (Hamamatsu, C11347-11). Mass spectra was obtained using a high-resolution mass spectrometer (JEOL, JMS-700).

2. Synthesis and analysis

The synthetic routes of 10H-phenoselenazine have been described in previously reported paper.[1]

Synthesis of 10-Phenyl-10H-phenoselenazine:

10H-phenoselenazine (0.50 g, 2.03 mmol), iodobenzene (0.50 g, 2.44 mmol), sodium tert-butoxide (0.49 g, 5.08 mmol), palladium(Ⅱ) acetate (0.046 g, 0.20 mmol) and tri-tert-butyl phosphine (0.21 g, 1.02 mmol) were dissolved in toluene (10 mL). The reaction mixture was refluxed under nitrogen at 300 °C for 12 h. Then, the mixture was cooled to room temperature and extracted with methylene chloride (MC). The organic layer was dried over anhydrous magnesium sulfate ($MgSO_4$) and the reaction product was purified by column chromatography using an MC:n-hexane (HEX) (1:6) as an eluent. The product was obtained as a yellow powder (0.50 g, yield 76%). HRMS (FAB): calcd for 323.0213 m/z, found 323.0214 m/z. Elemental analysis: calcd for C,67.48; H,4.00; N,4.43; found C,67.09; H,4.07; N,4.35.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.45 (t, 2H, J=8.8 Hz), 7.29 (m, 5H), 6.99 (t, 2H, J=8.5 HZ), 6.89 (t, 2H, J=8.0 HZ), 6.64 (d, 2H, J=9.5 HZ).

^{3}C NMR (125 MHz, $CDCl_3$): δ 144.15, 143.06, 130.30, 130.03, 127.48, 127.43, 126.39, 123.86, 120.24, 119.95.

Synthesis of 10-(*P*-tolyl)-10H-phenoselenazine:

10-(*P*-tolyl)-10H-phenoselenazine was synthesized by the same synthetic route of 10-phenyl-10H-phenoselenazine. However, 1-bromo-4-tert-butyl benzene was used instead of iodobenzene. The product was obtained as a yellow powder (0.50 g, yield 73%). HRMS (FAB): calcd for 337.0370 m/z, found 337.0370 m/z. Elemental analysis: calcd for C,68.05; H,4.50; N,4.27; found C,67.86; H,4.50; N,4.17.

^{1}H NMR (500 MHz, DMSO-d_6): δ 7.38 (d, 2H, J=8.0 HZ), 7.30 (d, 2H, J=9.0 HZ), 7.24 (d, 2H, J=8.5 HZ), 7.01 (t, 2H, J=8.5 HZ), 6.90 (d, 2H, J=8 HZ), 6.47 (d, 2H, J=9.0 HZ), 2.38 (s, 3H).

^{3}C NMR (125 MHz, DMSO-d_6): δ 143.75, 139.17, 136.82, 131.04, 129.55, 128.85, 127.46, 123.32, 118.45, 117.07, 20.64.

Synthesis of 10-(4-(Tert-butyl)phenyl)-10H-phenoselenazine:

10-(4-(Tert-butyl)phenyl)-10H-phenoselenazine was synthesized by the same synthetic route of 10-phenyl-10H-phenoselenazine. However, 1-bromo-4-tert-butyl benzene was used instead of iodobenzene. The product was obtained as a yellow powder (0.40 g, yield 52%). HRMS (FAB): calcd for 379.0839 m/z, found 379.0840 m/z. Elemental analysis: calcd for C,70.56; H,5.54; N,3.90; found C,69.84; H,5.59; N,3.70.

^{1}H NMR (500 MHz, DMSO-d_6): δ 7.57 (d, 2H, J=14 HZ), 7.34 (d, 2H, J=9.5 HZ), 7.25 (d, 2H, J=14.5 HZ), 7.06 (t, 2H, J=8.5 HZ), 6.93 (t, 2H, J=8 HZ), 6.55 (d, 2H, J=9.5 HZ), 1.33 (s, 9H).

^{3}C NMR (125 MHz, DMSO-d_6): δ 149.27, 143.60, 139.50, 129.72, 127.54, 127.46, 127.15, 123.59, 119.22, 118.14, 34.35, 31.14.

3. Device fabrication and measurement

POPhOLEDs were produced using the device stack of the indium tin oxide (ITO, 150 nm)/PEDOT:PSS (60 nm)/TAPC (10 nm)/TCTA (10 nm)/PCZAC (10 nm)/mCP (10 nm)/emitting layer (30 nm)/TSPO1 (5 nm)/TPBI (40 nm)/LiF (1 nm)/Al (200 nm). In the device structure, PEDOT:PSS, TAPC, TCTA, PCZAc, mCP, TSPO1 and TPBi represent poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate), 4,4'-cyclohexylidenebis[*N*,*N*-bis(4-methylphenyl)aniline], tris(4-(9*H*-carbazol-9-yl)phenyl)amine, 9,9-dimethyl-10-(9-phenyl-9*H*-carbazol-3-yl)-9,10-dihydroacridine, 1,3-bis(*N*-carbazolyl)benzene, diphenylphosphine oxide-4-(triphenylsilyl)phenyl and 1,3,5-tris(*N*-phenylbenzimidazole-2-yl)benzene, respectively. Device analysis was performed using CS2000 spectroradiometer for optical measurement and Keithley 2400 for electrical measurement.

4. H1 NMR, C13 NMR spectrums

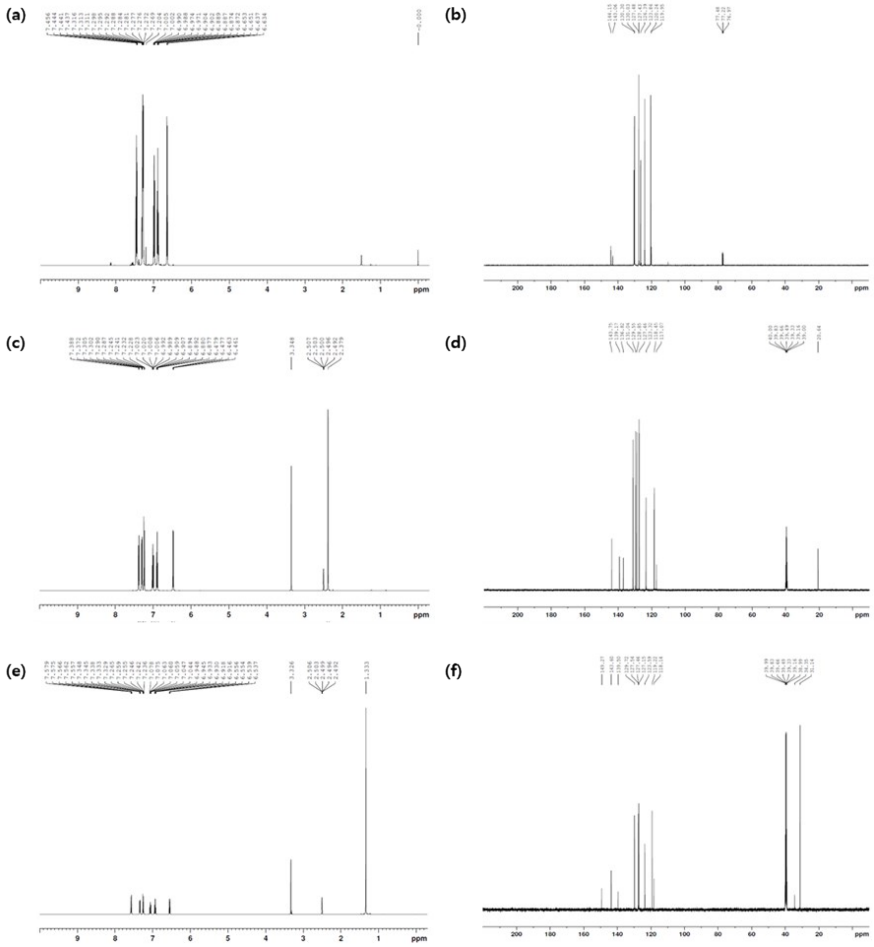

Figure S1. H1 NMR, C13 NMR spectrums of PhSe (a),(b), mPhSe (c),(d), and BuPhSe (e),(f).

5. Mass spectrum

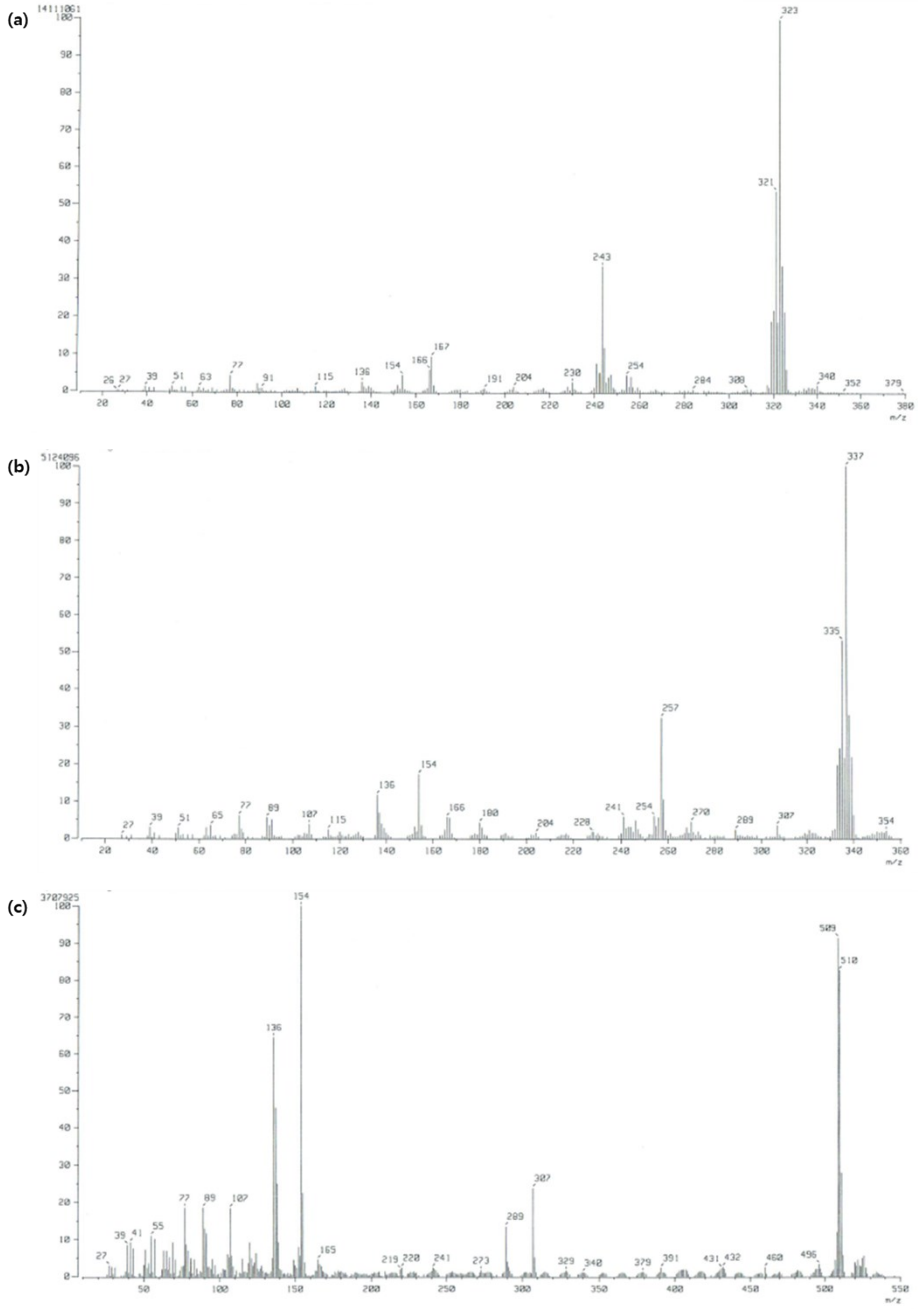

Figure S2. Mass spectrums of PhSe (a), mPhSe (b), and BuPhSe (c).

6. HPLC data

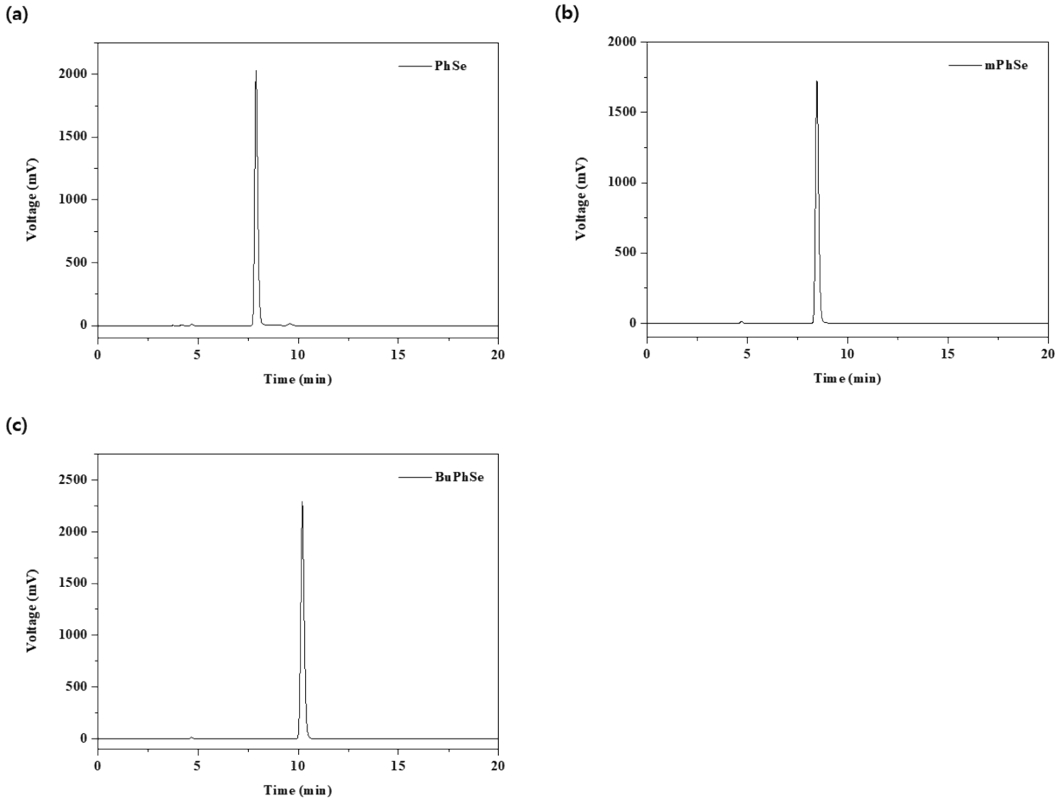

Figure S3. HPLC spectra of PhSe (a), mPhSe (b), and BuPhSe (c).

7. UV-vis spectra

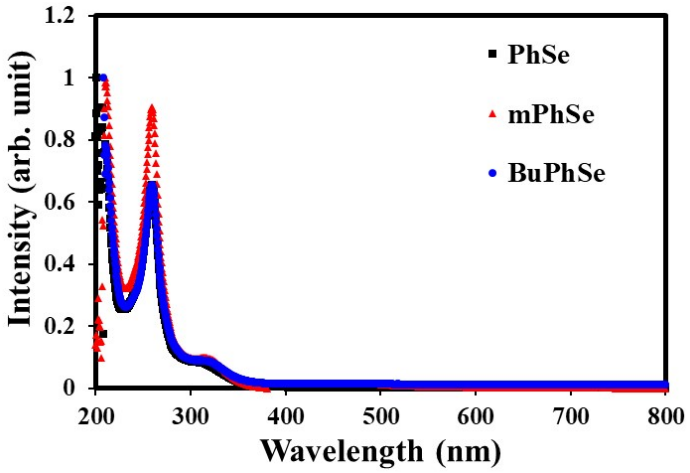

Figure S4. UV-vis spectra of PhSe, mPhSe, and BuPhSe in the solution state (THF).

8. EL spectra

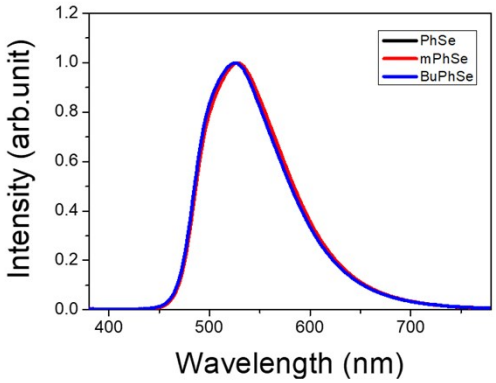

Figure S5. The EL spectra of the purely organic based PhOLEDs at doping concentration of 20 wt%.

The EL spectra of the purely organic based PhOLEDs are shown in **Figure 6**. The EL spectra were quite similar in the three emitters because the same phenoselenazine chromophore was shared in the three emitters. The alkyl blocking group did not affect the EL spectra and thus, indicate that those are only involved in managing intermolecular interaction and triplet exciton quenching. The peak wavelengths of the **PhSe**, **mPhSe**, and **BuPhSe** devices were 526, 529, and 525 nm, and color coordinates were (0.32, 0.57), (0.33, 0.57), and (0.32, 0.57), respectively.

9. Current density and luminance

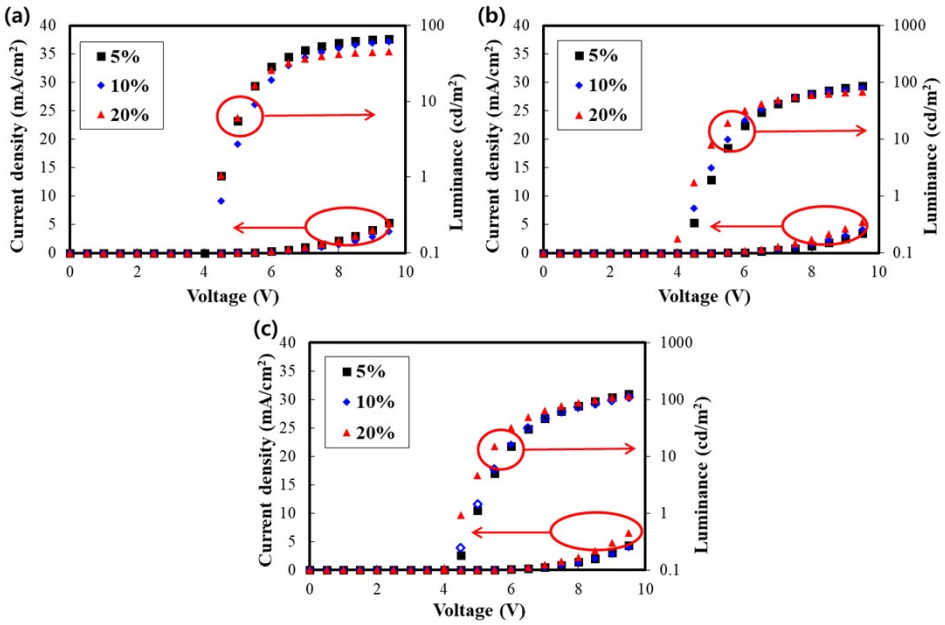

Figure S6. The data of current density and luminance according to driving voltage. ((a) PhSe, (b) mPhSe, and (c) BuPhSe.)

10. Computational studies

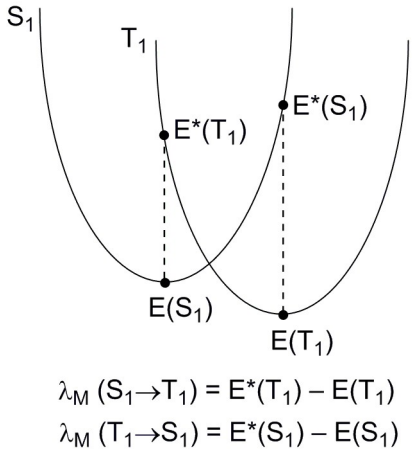

Figure S7. Marcus reorganization energy.

For ISC, Marcus reorganization energy λM is expressed as E*(T1)–E(T1) as illustrated in Figure S3. This energy for RISC is expressed as E*(S1)–E(S1). E*(S1) denotes S1 state energy at T1 geometry and E*(T1) indicates T1 state energy at S1 geometry. E(S1) and E(T1) are the electronic energies at their equilibrium states. The reorganization energy for S1↔T2 is derived in the same way.

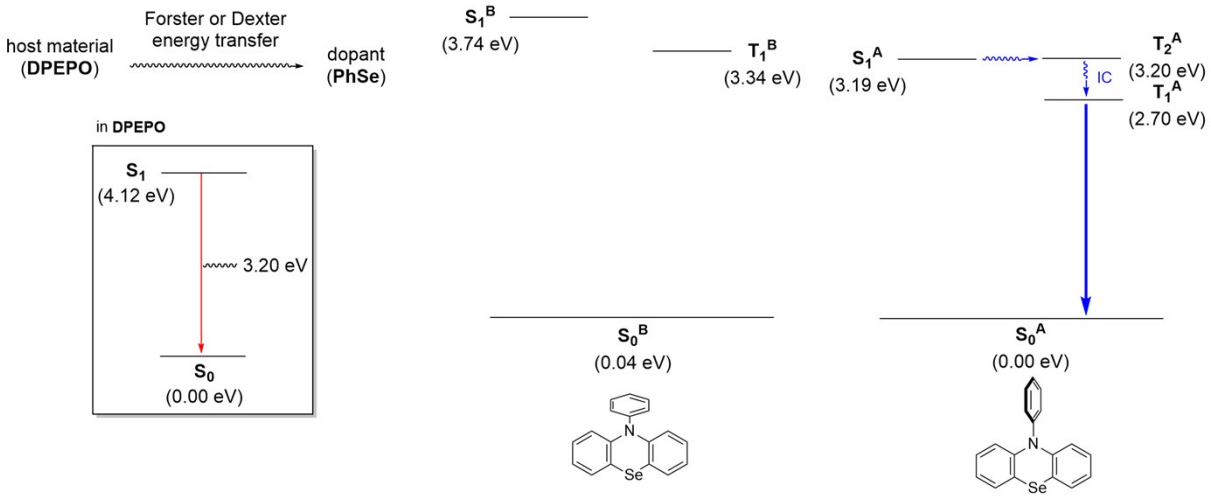

Figure S8. Jablonski diagram of $PhSe_A$, $PhSe_B$, and DPEPO host material

Förster resonance energy transfer from DPEPO host material to the conformer PhSeB would be difficult to occur, because the fluorescence energy of 3.20 eV is lower than both S1 and T1 energy of PhSeB. In addition, the spin-orbit coupling matrix element (SOCME) of

<S0|ĤSO|T1B> in this conformer is small at 9 cm–1, indicating that the phosphorescence from T1B would not occur.

Table S1. Calculated spin-orbit coupling matrix elements (SOCMEs), energy difference ΔE between S_1 and T_n (n=1,2), Marcus reorganization energy λ_M, effective Huang-Rhys factor S_{eff}, effective frequency ω_{eff}, density of state ρ_{FCWD}, and ISC and RISC rates.

	$PhSe_A$						
*n = 1 or 2	$\langle S_1\|\hat{H}_{SO}\|T_n\rangle$ (cm^{-1})	ΔE (eV)	λ_M (eV)	S_{eff} (-)	ω_{eff} (cm^{-1})	ρ_{FCWD} (-)	k (s^{-1})
$S_1 \rightarrow T_1$	3.38	–0.490	0.011	0.034	1330.9	3.54×10^{-4}	5.93×10^{5}
$T_1 \rightarrow S_1$	2.81	0.490	0.004	0.034	1305.0	6.47×10^{-294}	7.50×10^{-285}
$S_1 \rightarrow T_2$	66.02	0.011	0.299	1.566	1462.3	2.99×10^{-2}	1.91×10^{10}
$T_2 \rightarrow S_1$	3.33	–0.011	0.228	1.395	1466.4	1.24×10^{-1}	2.02×10^{8}

Table S2. Cartersian coordinates of the optimized geometries

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S_0 state of **$PhSe_A$**

==========

Se	0.929403	1.279411	-3.339976
C	-0.539503	0.136412	-3.734753
C	-0.635633	-0.440900	-4.988569
C	-1.558138	-0.017343	-2.791091
C	-1.781473	-1.122426	-5.363701
C	-2.711531	-0.694910	-3.186798
C	-2.822801	-1.227634	-4.460358
H	0.187532	-0.333865	-5.683830
H	-1.858835	-1.554274	-6.352756
H	-3.542153	-0.792082	-2.503984
H	-3.736219	-1.738535	-4.736862
C	0.988263	0.802717	-1.498649
C	-0.207665	0.568242	-0.815650
C	2.201912	0.797387	-0.834207
C	-0.143745	0.414238	0.569388
C	2.251665	0.632297	0.540054
C	1.069462	0.458740	1.235646
H	3.113846	0.946811	-1.398627
H	-1.050161	0.278547	1.140143
H	1.080710	0.345620	2.312195
N	-1.438508	0.525808	-1.497684
C	-2.619476	0.554124	-0.697600
C	-3.077281	-0.587111	-0.054344
C	-3.302910	1.750108	-0.574134
C	-4.226340	-0.526434	0.714713
C	-4.453221	1.807968	0.197301
C	-4.914872	0.671572	0.840843
H	-2.526478	-1.514229	-0.163332
H	-2.921201	2.623498	-1.087289
H	-4.586486	-1.415223	1.217827
H	-4.989490	2.743530	0.295087
H	-5.813768	0.718085	1.442876
H	3.202254	0.649456	1.056522

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S_1 state of **$PhSe_A$**

==========

Se	1.183885	0.669611	-3.330282
C	-0.448929	-0.160549	-3.708744
C	-0.669657	-0.575525	-5.027721
C	-1.539376	-0.119147	-2.778514
C	-1.915453	-0.936579	-5.461192
C	-2.826130	-0.412820	-3.280739
C	-3.010921	-0.815066	-4.575828
H	0.174961	-0.607619	-5.707824
H	-2.060762	-1.297734	-6.470312
H	-3.682993	-0.345769	-2.626126
H	-4.012078	-1.041975	-4.917563
C	1.082128	0.490516	-1.470104
C	-0.181537	0.468091	-0.793005
C	2.263281	0.675887	-0.741334
C	-0.175564	0.740850	0.592217
C	2.242430	0.850442	0.614768
C	0.995648	0.919926	1.277924
H	3.206615	0.677884	-1.277242
H	-1.110230	0.783465	1.132456
H	0.957279	1.115332	2.341324
N	-1.366431	0.195390	-1.446198
C	-2.559468	0.297744	-0.661258
C	-3.030106	-0.823178	-0.005130
C	-3.208745	1.513717	-0.582272
C	-4.187754	-0.720565	0.754096
C	-4.365144	1.609502	0.179033
C	-4.850902	0.493339	0.844229
H	-2.488417	-1.756265	-0.095599
H	-2.805227	2.366659	-1.113240
H	-4.570065	-1.589355	1.274658
H	-4.885988	2.555717	0.252048
H	-5.753719	0.570980	1.437311
H	3.166528	0.946697	1.168567

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T_1 state of **$PhSe_A$**

==========

Se	1.198164136	0.627885478	-3.328563245
C	-0.443680120	-0.176566451	-3.714746507
C	-0.668121025	-0.590077761	-5.030304311
C	-1.540039380	-0.121070111	-2.780154620
C	-1.917834323	-0.942906820	-5.463602228
C	-2.832676674	-0.402403244	-3.283329394
C	-3.020691357	-0.808057931	-4.573511396
H	0.175998072	-0.635132980	-5.711119295
H	-2.065198553	-1.308532951	-6.470714563
H	-3.691383371	-0.317706851	-2.631887241
H	-4.023941271	-1.025867152	-4.916318113
C	1.091074555	0.499400863	-1.468640666
C	-0.180554412	0.464929267	-0.792704949
C	2.265669598	0.697536171	-0.739630700
C	-0.178982460	0.731983037	0.597602961
C	2.242081382	0.867208633	0.618756183
C	0.986105403	0.917824206	1.284981193
H	3.211131541	0.707014185	-1.272332248
H	-1.115431660	0.769806033	1.136515855
H	0.944598319	1.106438970	2.349918398
N	-1.361181541	0.196170058	-1.450863014
C	-2.555053125	0.295609506	-0.664068487
C	-3.033679235	-0.827507492	-0.015892434
C	-3.199914848	1.514644295	-0.573514523
C	-4.188959951	-0.724813563	0.743073748
C	-4.354288425	1.610499344	0.186767469
C	-4.847125821	0.492008808	0.843613066
H	-2.498653263	-1.764605885	-0.113374208
H	-2.792047345	2.370936802	-1.097174531
H	-4.575398059	-1.596771535	1.256620927
H	-4.869645121	2.559926277	0.266323045
H	-5.749478154	0.569693403	1.437205564
H	3.164556585	0.970014795	1.173838109

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T_2 state of **$PhSe_A$**

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Se	1.335567	-0.106211	-3.190670
C	-0.448772	-0.320939	-3.694325
C	-0.680943	-0.649202	-5.029507
C	-1.524761	-0.174010	-2.790715
C	-1.957119	-0.836283	-5.500696
C	-2.823085	-0.364750	-3.304005
C	-3.029974	-0.688696	-4.621133
H	0.163459	-0.752654	-5.700411
H	-2.123901	-1.087942	-6.539408
H	-3.672260	-0.245958	-2.648907
H	-4.043835	-0.824034	-4.974721
C	1.077474	0.411167	-1.424171
C	-0.167336	0.458351	-0.812046
C	2.289919	0.705113	-0.739759
C	-0.244283	0.833258	0.571131
C	2.186937	1.062017	0.614630
C	0.960621	1.118481	1.239190
H	3.239442	0.642927	-1.247838
H	-1.184065	0.868684	1.088637
H	0.915058	1.393967	2.285604
N	-1.358909	0.152430	-1.466117
C	-2.552482	0.243273	-0.670471
C	-3.066804	-0.900397	-0.096116
C	-3.139109	1.485047	-0.483875
C	-4.214303	-0.811600	0.680308
C	-4.285471	1.566161	0.301185
C	-4.818061	0.426969	0.876898
H	-2.563902	-1.845959	-0.255820
H	-2.697174	2.360335	-0.941124

H -4.624993 -1.699915 1.141767
H -4.755663 2.527367 0.466381
H -5.708370 0.500076 1.489165
H 3.084259 1.292530 1.175340

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S_0 state of **$PhSe_B$**

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Se 0.624575 1.573204 -3.132798
C -0.623136 0.174893 -3.509967
C -0.612208 -0.503085 -4.719307
C -1.538533 -0.168893 -2.521420
C -1.528862 -1.517391 -4.941759
C -2.421155 -1.215524 -2.735105
C -2.427655 -1.879756 -3.949457
H 0.116693 -0.251042 -5.478989
H -1.523842 -2.043356 -5.888199
H -3.112828 -1.477429 -1.944340
H -3.128609 -2.686764 -4.120017
C 0.809613 1.075234 -1.296628
C -0.315267 0.601331 -0.630702
C 2.028857 1.154690 -0.641460
C -0.208730 0.179732 0.685011
C 2.116515 0.772091 0.686872
C 1.001863 0.278831 1.348784
H 2.909288 1.499649 -1.168521
H -1.093731 -0.201902 1.178419
H 1.079262 -0.037724 2.381009
N -1.568979 0.554124 -1.298202
C -2.386447 1.700272 -1.236603
C -2.189589 2.661318 -0.244711
C -3.422584 1.885247 -2.152306
C -3.019567 3.765822 -0.168831
C -4.243638 2.995312 -2.062379
C -4.055892 3.943572 -1.070415
H -1.378359 2.556259 0.461799
H -3.581448 1.169869 -2.946751
H -2.844165 4.499761 0.608145
H -5.038890 3.118275 -2.787331
H -4.700646 4.810031 -1.006162
H 3.067595 0.838650 1.200085

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S_1 state of **$PhSe_B$**

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Se 0.570055 1.801342 -3.193260
C -0.614041 0.328172 -3.553166
C -0.463667 -0.539717 -4.609809
C -1.577546 0.035133 -2.556343
C -1.276065 -1.671767 -4.719724
C -2.301956 -1.164413 -2.592048
C -2.166400 -1.989178 -3.684104
H 0.302832 -0.348843 -5.350330
H -1.184671 -2.320298 -5.579740
H -2.978890 -1.410610 -1.784115
H -2.757639 -2.894346 -3.741065
C 0.797359 1.218150 -1.372950
C -0.372689 0.792585 -0.696136
C 2.020554 1.026788 -0.773676
C -0.283961 0.102080 0.520737
C 2.105813 0.458083 0.500303
C 0.946794 -0.031633 1.119463
H 2.922540 1.304538 -1.304350
H -1.179992 -0.285312 0.988387
H 1.017072 -0.522188 2.082024
N -1.592750 0.904343 -1.425843
C -2.432745 1.923817 -1.297218
C -2.262187 2.864084 -0.239544
C -3.524356 2.071557 -2.201808
C -3.151635 3.891594 -0.105197
C -4.394826 3.111090 -2.038944
C -4.223527 4.024139 -0.993578
H -1.420619 2.745676 0.427694
H -3.629704 1.358618 -3.006844
H -3.024849 4.610816 0.693264
H -5.222525 3.231253 -2.725492
H -4.923654 4.840729 -0.873001
H 3.067375 0.359019 0.984174

==========

T_1 state of **$PhSe_B$**

==========

Se 1.256715 1.125598 -3.359479
C -0.272218 0.024962 -3.653731
C -0.334377 -0.881755 -4.688761
C -1.348230 0.148305 -2.759070
C -1.470273 -1.676036 -4.857252
C -2.456715 -0.708017 -2.885914
C -2.510127 -1.598564 -3.934959
H 0.506613 -0.986212 -5.361802
H -1.521239 -2.374317 -5.681701
H -3.249545 -0.663616 -2.151354
H -3.367635 -2.252479 -4.031947
C 1.139955 0.908344 -1.469695
C -0.140091 0.908732 -0.889589
C 2.256675 0.741725 -0.681774
C -0.275472 0.672276 0.491375
C 2.121936 0.582864 0.699653
C 0.852031 0.523175 1.267562
H 3.237491 0.721011 -1.138609
H -1.264326 0.598349 0.923549
H 0.744092 0.345741 2.330189
N -1.270525 1.085333 -1.710099
C -2.283382 1.942589 -1.403331
C -2.181187 2.825981 -0.273623
C -3.461493 2.016491 -2.223297
C -3.265793 3.551028 0.116523
C -4.528414 2.752887 -1.807127
C -4.479351 3.485699 -0.601031
H -1.235990 2.937316 0.235873
H -3.481440 1.517486 -3.180310
H -3.182200 4.215742 0.967145
H -5.412569 2.805909 -2.429907
H -5.336467 4.059360 -0.276325
H 3.003052 0.469395 1.316579

==========

S_0 state of **DPEPO**

==========

P -1.397327 -0.170672 -2.658782
O -2.519475 -1.122280 -2.460770
C -1.165087 0.292354 -4.395646
C -0.405469 1.377651 -4.825437
C -1.770490 -0.535003 -5.335319
C -0.243901 1.621288 -6.178531
C -1.608002 -0.287046 -6.688936
C -0.842344 0.787147 -7.110904
H 0.042734 2.054285 -4.107657
H -2.373650 -1.365743 -4.989335
H 0.344666 2.468703 -6.507358
H -2.082800 -0.934406 -7.415555
H -0.715768 0.980343 -8.168973
C 0.195224 -0.829873 -2.094732
C 0.151722 -1.913005 -1.222451
C 1.421774 -0.272231 -2.439651
C 1.320821 -2.399019 -0.663248
C 2.590720 -0.772038 -1.888362
C 2.539557 -1.826056 -0.990191
H -0.800105 -2.347916 -0.945784
H 1.480592 0.543948 -3.147612
H 1.268124 -3.220226 0.040080
H 3.543651 -0.335904 -2.161740
H 3.452779 -2.204496 -0.547823
C -1.618455 1.422494 -1.797996
C -2.206393 2.517483 -2.426396
C -1.307633 1.537626 -0.443675
C -2.429461 3.697178 -1.738217
C -1.512102 2.714873 0.253594
C -2.068731 3.796407 -0.403012
H -2.491610 2.446736 -3.468610

H -2.886747 4.538135 -2.243282
H -1.266080 2.762910 1.306362
H -2.244915 4.716476 0.140162
O -0.911571 0.396309 0.185101
O -1.639939 -2.697489 1.528897
P -1.630532 -1.458935 2.347456
C -1.771609 -1.789150 4.124278
C -1.481913 -0.862420 5.122757
C -2.235662 -3.052106 4.475951
C -1.667108 -1.193560 6.454085
H -1.085253 0.113495 4.869351
C -2.418605 -3.380515 5.809637
H -2.441035 -3.770874 3.691843
C -2.138466 -2.451640 6.798027
H -1.436348 -0.470687 7.226655
H -2.779061 -4.366013 6.076773
H -2.281110 -2.709091 7.840253
C -2.990515 -0.331004 1.936804
C -3.389671 0.718044 2.757871
C -3.610354 -0.515514 0.704574
C -4.375675 1.594850 2.334037
H -2.950084 0.853967 3.737181
C -4.584738 0.370986 0.280039
H -3.301723 -1.327888 0.059080
C -4.963979 1.429422 1.090433
H -4.685230 2.408324 2.978605
H -5.035557 0.233957 -0.694563
H -5.723817 2.124273 0.754674
C -0.098126 -0.481281 2.196592
C 0.970337 -0.658224 3.071881
C 0.076890 0.389205 1.121212
C 2.150097 0.045834 2.905493
H 0.877150 -1.354132 3.896261
C 1.243980 1.112543 0.952021
C 2.277555 0.940079 1.853587
H 2.969779 -0.103896 3.596207
H 1.345343 1.775078 0.102450
H 3.199491 1.491870 1.718602

==========

S_1 state of **DPEPO**

==========

P -1.208507 0.217041 -2.353218
O -2.243322 -0.789436 -1.961644
C -0.998496 0.303010 -4.155360
C -0.150010 1.180289 -4.826620
C -1.713554 -0.641363 -4.884795
C -0.021647 1.111758 -6.203070
C -1.584153 -0.707795 -6.263337
C -0.737342 0.166482 -6.923285
H 0.394197 1.942133 -4.283711
H -2.370595 -1.317553 -4.351293
H 0.634441 1.802590 -6.717869
H -2.147411 -1.444687 -6.822232
H -0.635787 0.115704 -8.000326
C 0.409768 -0.477381 -1.794586
C 0.398876 -1.676945 -1.082488
C 1.639930 0.108120 -2.115396
C 1.587905 -2.254112 -0.666376
C 2.824829 -0.485219 -1.730058
C 2.801255 -1.664623 -0.991590
H -0.552629 -2.147240 -0.862212
H 1.666245 1.036853 -2.670763
H 1.564575 -3.179952 -0.104130
H 3.771605 -0.034318 -2.002010
H 3.730919 -2.134238 -0.692191
C -1.327260 1.852161 -1.766764
C -1.598426 3.008679 -2.588539
C -1.452029 2.135485 -0.369856
C -1.805078 4.247356 -2.052752
C -1.691950 3.348714 0.178373
C -1.818623 4.475813 -0.658331
H -1.662379 2.888299 -3.660284
H -1.993732 5.074257 -2.727024
H -1.810270 3.427075 1.251176
H -1.996601 5.455129 -0.244267
O -1.442988 1.013212 0.528060
O -1.922626 -2.773718 1.424063
P -1.968668 -1.537317 2.240210
C -1.826531 -1.840470 4.019280
C -1.401389 -0.878747 4.931793
C -2.178787 -3.108505 4.466296
C -1.341185 -1.181955 6.280850
H -1.108312 0.108581 4.593386
C -2.115313 -3.408786 5.818063
H -2.489588 -3.855417 3.745410
C -1.700201 -2.446654 6.723698
H -1.011614 -0.431888 6.988975
H -2.389170 -4.397743 6.163555
H -1.651418 -2.682587 7.779592
C -3.422466 -0.507321 2.009624
C -4.043719 0.147511 3.069230
C -3.931808 -0.388594 0.716964
C -5.151311 0.945594 2.831590
H -3.685207 0.026835 4.082670
C -5.030670 0.418940 0.490879
H -3.448991 -0.879685 -0.121352
C -5.637201 1.088237 1.542776
H -5.634750 1.453615 3.656495
H -5.402456 0.534192 -0.519002
H -6.494242 1.723765 1.356492
C -0.440274 -0.551689 1.920138
C 0.725114 -1.039377 2.449095
C -0.340938 0.575465 1.034755
C 1.967039 -0.464405 2.141696
H 0.696906 -1.895027 3.112771
C 0.921405 1.172654 0.748281
C 2.051919 0.645746 1.297786
H 2.866541 -0.882210 2.575488
H 0.941252 2.036875 0.100731
H 3.015660 1.082730 1.074809

11. . References

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