

Electronic Supplementary Information (ESI)

Theoretical and experimental investigation on the electronic properties of the shuttlecock shaped and the double-decker structured metal phthalocyanines, MPc and M(Pc)₂ (M = Sn and Pb)

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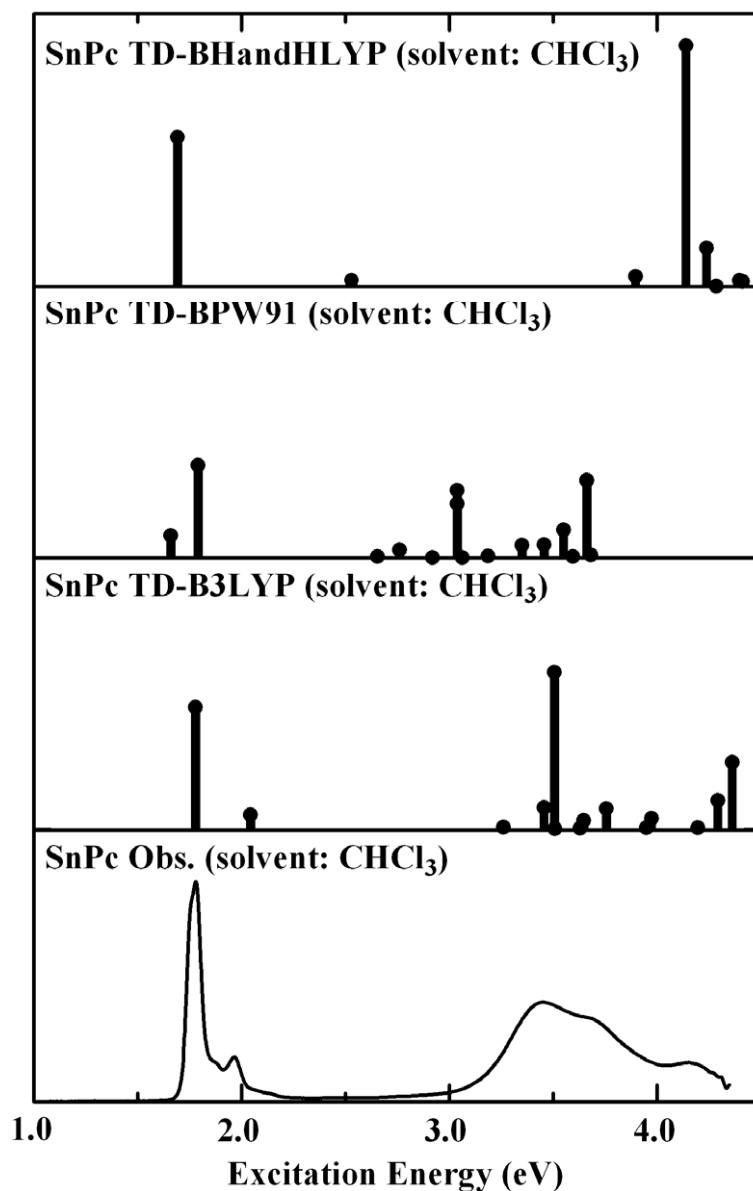


Fig. S1. Excited states of a SnPc monomer obtained by the TD-B3LYP, TD-BWP91 and TD-BHandHLYP calculations with the CPCM method (solvent: CH_3Cl). The vertical line depicts the oscillator strength of each state.

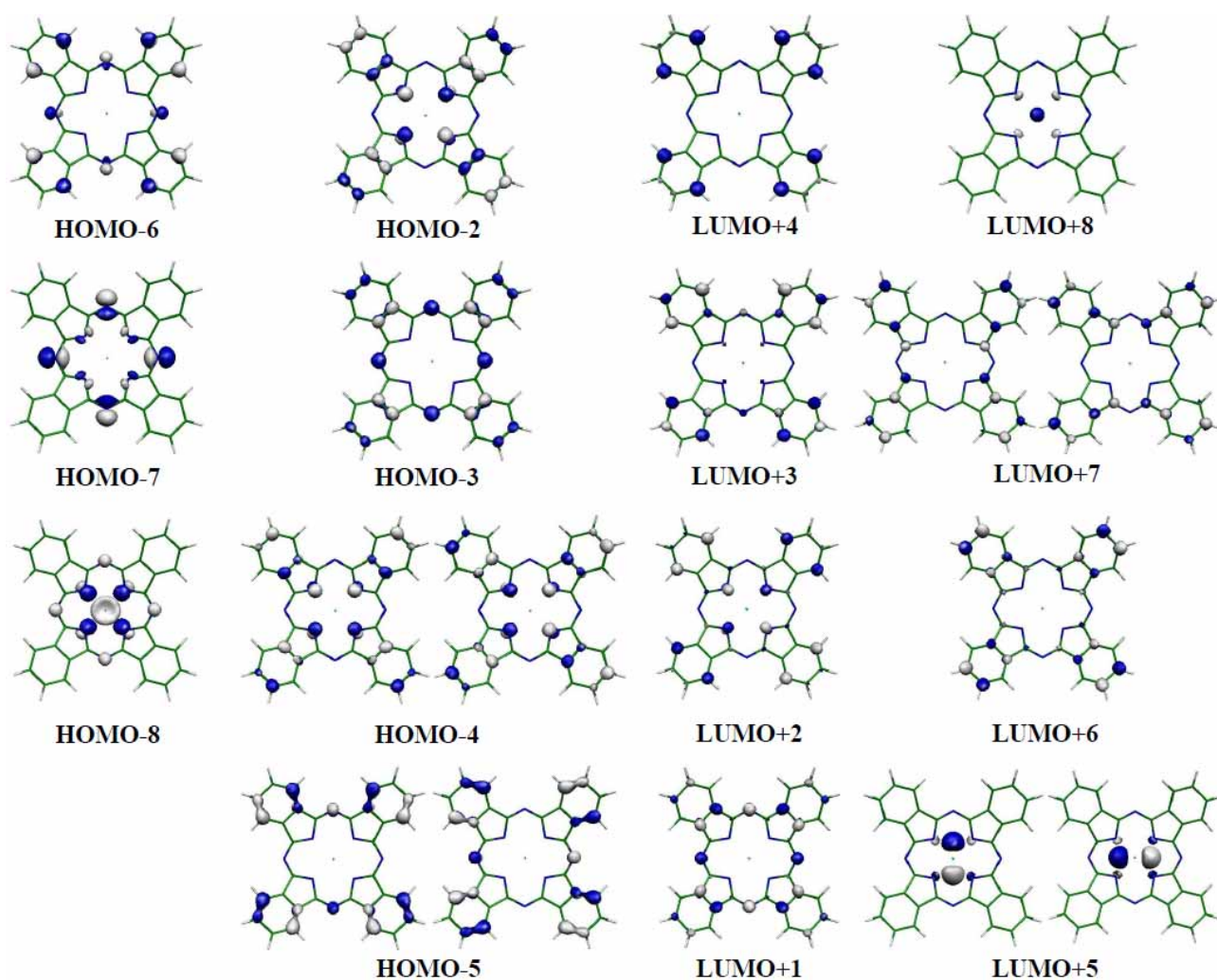


Fig. S2. Several molecular orbitals of SnPc.

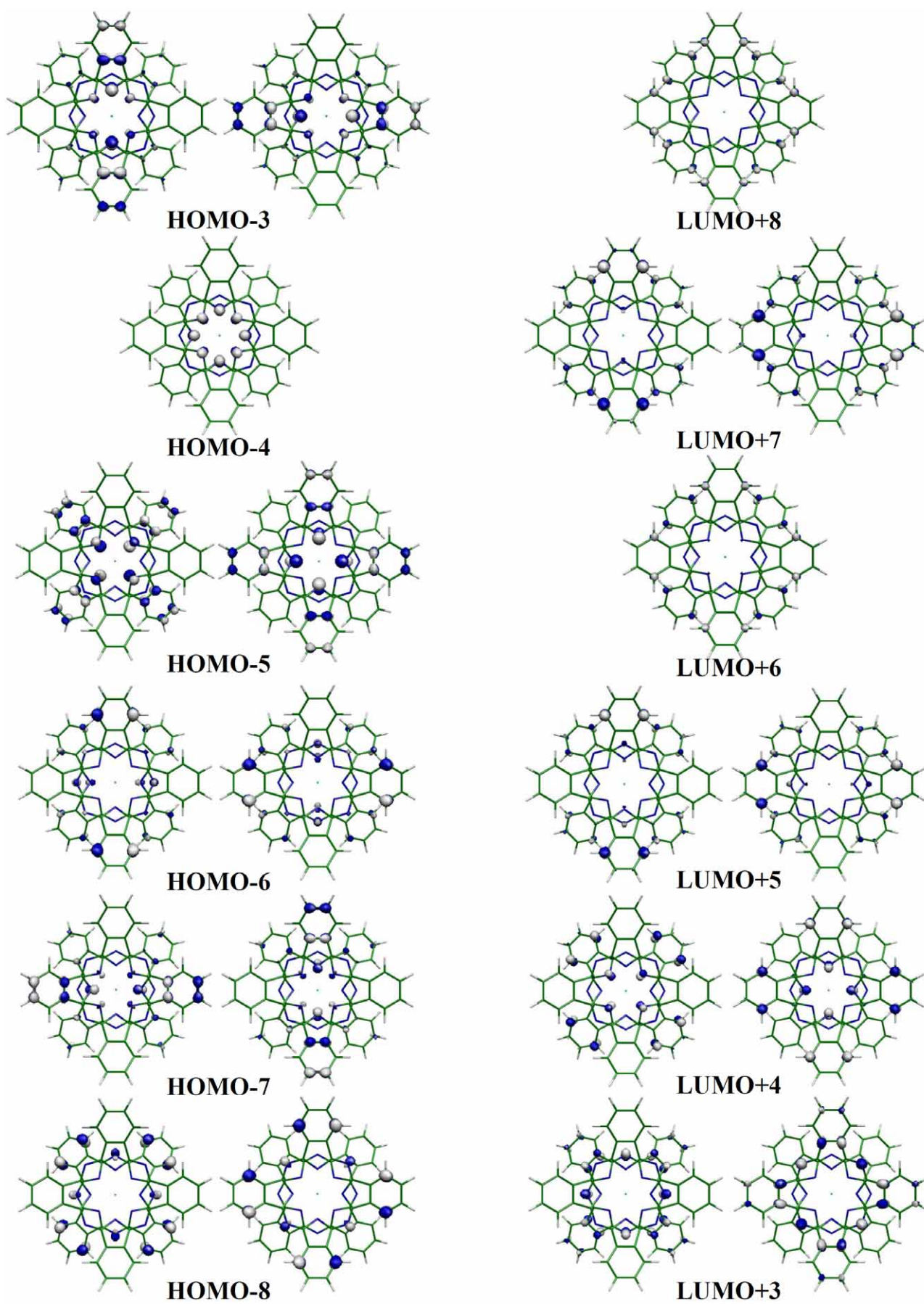


Fig. S3. Several molecular orbitals of $\text{Sn}(\text{Pc})_2$.

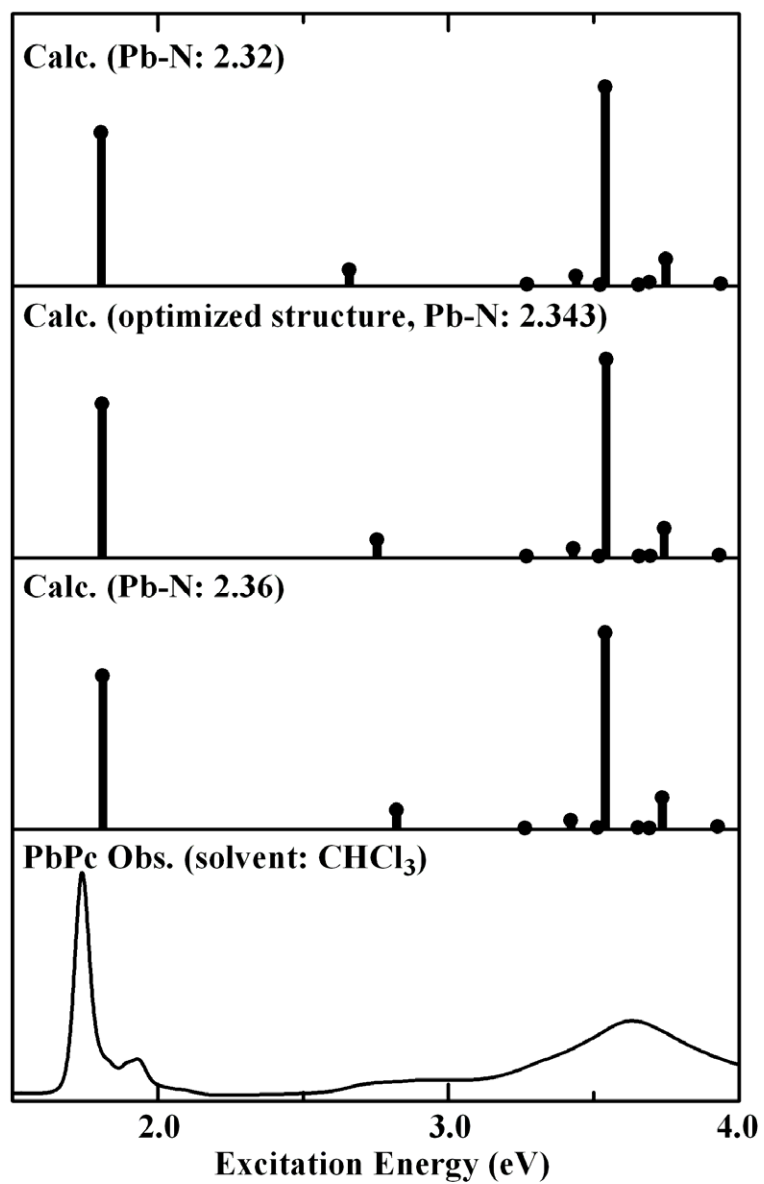


Fig. S4. Dependence of the excitation energy on the Pb-N atomic distance.

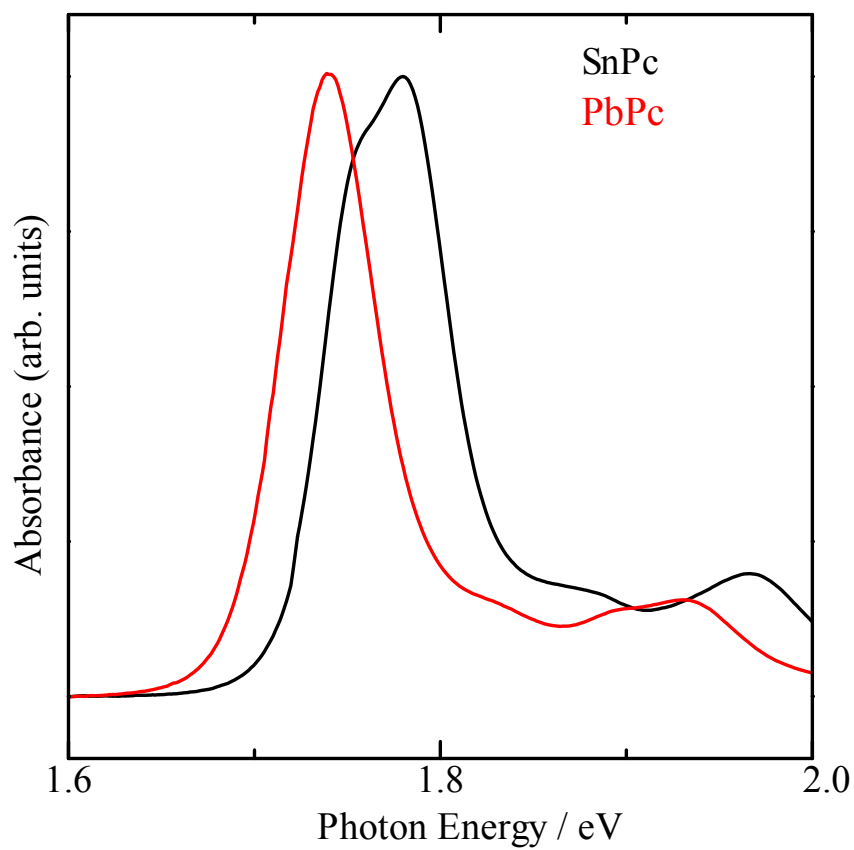


Fig. S5. Absorption spectra in the Q-band region of SnPc and PbPc.

Table S1. Symmetry-allowed TD-B3LYP excited states of SnPc with the CPCM method (solvent: CHCl₃).

	state	main configuration ($ C \geq 0.30$)	E^a	f^b	p^c
C_{4v}	1E	+0.62(13a ₂ →34e)	1.78	0.639	$x+y$
	2E	+0.66(22a ₁ →34e)	2.04	0.078	$x+y$
	3E	+0.68(18b ₁ →34e)	3.26	0.014	$x+y$
	4E	+0.56(14b ₂ →34e)+0.39(15b ₂ →34e)	3.46	0.116	$x+y$
	5E	+0.65(21a ₁ →34e)	3.51	0.825	$x+y$
	1A ₂	+0.44(33e→34e)+0.44(33e→34e)	3.51	0.004	z
	2A ₂	+0.43(32e→34e)+0.43(32e→34e)	3.63	0.009	z
	6E	−0.37(14b ₂ →34e)+0.56(15b ₂ →34e)	3.65	0.047	$x+y$
	7E	+0.68(13a ₂ →35e)	3.76	0.110	$x+y$
	3A ₂	−0.45(31e→34e)+0.45(31e→34e)	3.95	0.010	z
	8E	+0.63(20a ₁ →34e)	3.97	0.060	$x+y$
C_{2v}	9E	+0.62(12a ₂ →34e)	4.20	0.010	$x+y$
	10E	+0.65(17b ₁ →34e)	4.29	0.154	$x+y$
	11E	+0.66(22a ₁ →35e)	4.36	0.352	$x+y$

^a Excitation energy in eV.

^b Oscillator strength.

^c Transition moment direction.

Table S2. Symmetry-allowed TD-B3LYP excited states of PbPc with the CPCM method (solvent: CHCl₃).

	state	main configuration ($ C \geq 0.30$)	E^a	f^b	p^c
C_{4v}	1E	+0.62(13a ₂ →34e)	1.81	0.706	$x+y$
	2E	±0.39(22a ₁ →34e)+0.55(22a ₁ →34e)	2.75	0.082	$x+y$
	3E	+0.67(18b ₂ →34e)	3.27	0.007	$x+y$
	4E	+0.43(14b ₁ →34e)−0.39(15b ₁ →34e)	3.43	0.043	$x+y$
	1A ₂	−0.46(33e→34e)+0.46(33e→34e)	3.52	0.008	z
	5E	+0.61(21a ₁ →34e)	3.54	0.909	$x+y$
	2A ₂	+0.45(32e→34e)+0.45(32e→34e)	3.66	0.008	z
	6E	+0.36(14b ₁ →34e)+0.40(15b ₁ →34e)	3.70	0.008	$x+y$
	7E	+0.62(13a ₂ →35e)	3.74	0.135	$x+y$
	3A ₂	+0.48(31e→34e)+0.48(31e→34e)	3.93	0.012	z
	8E	+0.51(17b ₂ →34e)±0.35(17b ₂ →34e)	4.07	0.002	$x+y$
	9E	+0.43(20a ₁ →34e)±0.39(12a ₂ →34e)	4.14	0.048	$x+y$
C_{4v}	10E	±0.34(20a ₁ →34e)+0.45(12a ₂ →34e)	4.26	0.121	$x+y$
	11E	+0.61(13a ₂ →36e)±0.36(13a ₂ →36e)	4.58	0.017	$x+y$
	12E	+0.54(19a ₁ →34e)±0.41(19a ₁ →34e)	4.77	0.035	$x+y$

^a Excitation energy in eV.

^b Oscillator strength.

^c Transition moment direction.

Table S3. Symmetry-allowed TD-B3LYP excited states of Sn(Pc)₂ with the CPCM method (solvent: CHCl₃).

	state	main configuration ($ C \geq 0.30$)	E^a	f^b	p^c
<i>D</i> _{4d}	1E ₁	+0.64(13a ₂ →34e ₁)	1.49	0.158	<i>x+y</i>
	2E ₁	+0.61(13b ₁ →34e ₃)	1.97	1.011	<i>x+y</i>
	3E ₁	+0.45(21b ₂ →34e ₃)±0.37(33e ₂ →34e ₃)+0.37(33e ₂ →34e ₃)	3.08	0.005	<i>x+y</i>
	4E ₁	+0.52(21b ₂ →34e ₃)±0.32(33e ₂ →34e ₃)−0.32(33e ₂ →34e ₃)	3.18	0.001	<i>x+y</i>
	5E ₁	+0.67(13a ₂ →35e ₁)	3.35	0.003	<i>x+y</i>
	1B ₂	−0.48(33e ₁ →34e ₃)+0.48(33e ₁ →34e ₃)	3.37	0.014	<i>z</i>
	6E ₁	+0.37(32e ₂ →34e ₃)±0.37(32e ₂ →34e ₃)	3.40	0.160	<i>x+y</i>
	2B ₂	+0.48(32e ₁ →34e ₃)+0.48(32e ₁ →34e ₃)	3.45	0.001	<i>z</i>
	7E ₁	±0.45(20b ₂ →34e ₃)+0.53(21a ₁ →34e ₁)	3.50	0.022	<i>x+y</i>
	8E ₁	±0.30(31e ₂ →34e ₃)+0.30(31e ₂ →34e ₃)	3.54	0.120	<i>x+y</i>
	9E ₁	±0.40(33e ₂ →34e ₁)+0.40(33e ₂ →34e ₁)	3.57	0.649	<i>x+y</i>
	3B ₂	−0.49(33e ₃ →34e ₁)+0.49(33e ₃ →34e ₁)	3.59	0.137	<i>z</i>
	10E ₁	+0.48(20b ₂ →34e ₃)±0.37(21a ₁ →34e ₁)	3.66	1.658	<i>x+y</i>
	11E ₁	±0.46(32e ₂ →34e ₁)+0.46(32e ₂ →34e ₁)	3.84	0.015	<i>x+y</i>
	4B ₂	+0.41(32e ₃ →34e ₁)+0.41(32e ₃ →34e ₁)	3.94	0.030	<i>z</i>

^a Excitation energy in eV.

^b Oscillator strength.

^c Transition moment direction.

Table S4. Symmetry-allowed TD-B3LYP excited states of Pb(Pc)₂.

	state	main configuration ($ C \geq 0.30$)	E^a	f^b	p^c
D_{4d}	1E ₁	$\pm 0.49(13a_2 \rightarrow 34e_1) + 0.36(13a_2 \rightarrow 34e_1)$	1.54	0.040	$x+y$
	2E ₁	$\pm 0.37(13b_1 \rightarrow 34e_3) + 0.42(13b_1 \rightarrow 34e_3)$	2.10	0.468	$x+y$
	1B ₂	$+0.66(21b_2 \rightarrow 22a_1)$	2.71	0.048	z
	3E ₁	$\pm 0.38(32e_1 \rightarrow 22a_1) + 0.58(33e_1 \rightarrow 22a_1)$	2.98	0.001	$x+y$
	4E ₁	$+0.44(21b_2 \rightarrow 34e_3) \pm 0.36(33e_2 \rightarrow 34e_3) + 0.36(33e_2 \rightarrow 34e_3)$	3.11	0.005	$x+y$
	2B ₂	$+0.66(20b_2 \rightarrow 22a_1)$	3.15	0.001	z
	5E ₁	$+0.55(32e_1 \rightarrow 22a_1) \pm 0.38(33e_1 \rightarrow 22a_1)$	3.15	0.002	$x+y$
	6E ₁	$+0.40(21b_2 \rightarrow 34e_3) \pm 0.31(21b_2 \rightarrow 34e_3)$	3.21	0.001	$x+y$
	7E ₁	$+0.55(13a_2 \rightarrow 35e_1)$	3.38	0.001	$x+y$
	8E ₁	$+0.39(13a_2 \rightarrow 35e_1)$	3.41	0.019	$x+y$
	3B ₂	$-0.46(33e_1 \rightarrow 34e_3) + 0.46(33e_1 \rightarrow 34e_3)$	3.43	0.003	z
	9E ₁	$\pm 0.47(20b_2 \rightarrow 34e_3) + 0.49(21a_1 \rightarrow 34e_1)$	3.50	0.003	$x+y$
	10E ₁	$-0.34(33e_2 \rightarrow 34e_1) \pm 0.34(33e_2 \rightarrow 34e_1)$	3.54	0.002	$x+y$
	11E ₁	$+0.44(31e_1 \rightarrow 22a_1)$	3.60	0.115	$x+y$
	12E ₁	$+0.46(31e_1 \rightarrow 22a_1)$	3.60	0.001	$x+y$
	4B ₂	$-0.47(33e_3 \rightarrow 34e_1) + 0.47(33e_3 \rightarrow 34e_1)$	3.61	0.081	z
D_{4d}	13E ₁	$+0.37(20b_2 \rightarrow 34e_3) \pm 0.35(21a_1 \rightarrow 34e_1)$	3.82	0.946	$x+y$
	14E ₁	$+0.39(32e_2 \rightarrow 34e_1) \pm 0.39(32e_2 \rightarrow 34e_1)$	3.83	0.293	$x+y$

^a Excitation energy in eV.

^b Oscillator strength.

^c Transition moment direction.

Table S5. Geometry optimized coordinates for SnPc.

Sn	0.00000000	0.00000000	1.28918900
N	-1.40539900	1.40539900	0.17476000
N	1.40539900	-1.40539900	0.17476000
N	1.40539900	1.40539900	0.17476000
N	-1.40539900	-1.40539900	0.17476000
N	0.00000000	3.37174200	-0.00015100
N	0.00000000	-3.37174200	-0.00015100
N	3.37174200	0.00000000	-0.00015100
N	-3.37174200	0.00000000	-0.00015100
C	-1.16995800	2.74867900	0.01918900
C	1.16995800	-2.74867900	0.01918900
C	2.74867900	1.16995800	0.01918900
C	-2.74867900	-1.16995800	0.01918900
C	-2.74867900	1.16995800	0.01918900
C	2.74867900	-1.16995800	0.01918900
C	1.16995800	2.74867900	0.01918900
C	-1.16995800	-2.74867900	0.01918900
C	-2.43779900	3.43190000	-0.20313700
C	-3.43190000	2.43779900	-0.20313700
C	-2.75765700	4.77034700	-0.42476900
C	-4.77034700	2.75765700	-0.42476900
C	-4.09571300	5.09015100	-0.63088600
C	-5.09015100	4.09571300	-0.63088600
H	-1.98423100	5.52989700	-0.43274500
H	-5.52989700	1.98423100	-0.43274500
H	-4.38078100	6.12381900	-0.79820100
H	-6.12381900	4.38078100	-0.79820100
C	2.43779900	-3.43190000	-0.20313700
C	3.43190000	-2.43779900	-0.20313700
C	2.75765700	-4.77034700	-0.42476900
C	4.77034700	-2.75765700	-0.42476900
C	4.09571300	-5.09015100	-0.63088600
C	5.09015100	-4.09571300	-0.63088600
H	1.98423100	-5.52989700	-0.43274500
H	5.52989700	-1.98423100	-0.43274500
H	4.38078100	-6.12381900	-0.79820100
H	6.12381900	-4.38078100	-0.79820100
C	3.43190000	2.43779900	-0.20313700

C	2.43779900	3.43190000	-0.20313700
C	4.77034700	2.75765700	-0.42476900
C	2.75765700	4.77034700	-0.42476900
C	5.09015100	4.09571300	-0.63088600
C	4.09571300	5.09015100	-0.63088600
H	5.52989700	1.98423100	-0.43274500
H	1.98423100	5.52989700	-0.43274500
H	6.12381900	4.38078100	-0.79820100
H	4.38078100	6.12381900	-0.79820100
C	-3.43190000	-2.43779900	-0.20313700
C	-2.43779900	-3.43190000	-0.20313700
C	-4.77034700	-2.75765700	-0.42476900
C	-2.75765700	-4.77034700	-0.42476900
C	-5.09015100	-4.09571300	-0.63088600
C	-4.09571300	-5.09015100	-0.63088600
H	-5.52989700	-1.98423100	-0.43274500
H	-1.98423100	-5.52989700	-0.43274500
H	-6.12381900	-4.38078100	-0.79820100
H	-4.38078100	-6.12381900	-0.79820100

Table S6. Geometry optimized coordinates for PbPc.

Pb	0.00000000	0.00000000	1.29918900
N	0.00000000	2.00889000	0.09247700
N	0.00000000	-2.00889000	0.09247700
N	-2.00889000	0.00000000	0.09247700
N	2.00889000	0.00000000	0.09247700
N	-2.38551800	2.38551800	-0.12125000
N	2.38551800	-2.38551800	-0.12125000
N	-2.38551800	-2.38551800	-0.12125000
N	2.38551800	2.38551800	-0.12125000
C	-1.11758600	2.77926600	-0.09409200
C	1.11758600	2.77926600	-0.09409200
C	-2.77926600	-1.11758600	-0.09409200
C	-2.77926600	1.11758600	-0.09409200
C	1.11758600	-2.77926600	-0.09409200
C	-1.11758600	-2.77926600	-0.09409200
C	2.77926600	1.11758600	-0.09409200
C	2.77926600	-1.11758600	-0.09409200
C	-0.70357600	4.15461100	-0.35662500
C	0.70357600	4.15461100	-0.35662500
C	-4.15461100	-0.70357600	-0.35662500
C	-4.15461100	0.70357600	-0.35662500
C	0.70357600	-4.15461100	-0.35662500
C	-0.70357600	-4.15461100	-0.35662500
C	4.15461100	0.70357600	-0.35662500
C	4.15461100	-0.70357600	-0.35662500
C	-1.42277000	5.31982300	-0.61564900
C	1.42277000	5.31982300	-0.61564900
C	-0.70299400	6.48589400	-0.85666400
C	0.70299400	6.48589400	-0.85666400
C	-5.31982300	-1.42277000	-0.61564900
C	-5.31982300	1.42277000	-0.61564900
C	-6.48589400	-0.70299400	-0.85666400
C	-6.48589400	0.70299400	-0.85666400
C	1.42277000	-5.31982300	-0.61564900
C	-1.42277000	-5.31982300	-0.61564900
C	0.70299400	-6.48589400	-0.85666400
C	-0.70299400	-6.48589400	-0.85666400
C	5.31982300	1.42277000	-0.61564900

C	5.31982300	-1.42277000	-0.61564900
C	6.48589400	0.70299400	-0.85666400
C	6.48589400	-0.70299400	-0.85666400
H	-2.50680400	5.30926000	-0.62545500
H	2.50680400	5.30926000	-0.62545500
H	-1.23254800	7.41276600	-1.05234300
H	1.23254800	7.41276600	-1.05234300
H	-5.30926000	-2.50680400	-0.62545500
H	-5.30926000	2.50680400	-0.62545500
H	-7.41276600	-1.23254800	-1.05234300
H	-7.41276600	1.23254800	-1.05234300
H	2.50680400	-5.30926000	-0.62545500
H	-2.50680400	-5.30926000	-0.62545500
H	1.23254800	-7.41276600	-1.05234300
H	-1.23254800	-7.41276600	-1.05234300
H	5.30926000	2.50680400	-0.62545500
H	5.30926000	-2.50680400	-0.62545500
H	7.41276600	1.23254800	-1.05234300
H	7.41276600	-1.23254800	-1.05234300

Table S7. Geometry optimized coordinates for Sn(Pc)₂.

Sn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.96133700	1.28977600
N	0.00000000	-1.96133700	1.28977600
N	1.96133700	0.00000000	1.28977600
N	-1.96133700	0.00000000	1.28977600
N	2.37030700	2.37030700	1.60161600
N	-2.37030700	-2.37030700	1.60161600
N	2.37030700	-2.37030700	1.60161600
N	-2.37030700	2.37030700	1.60161600
C	1.10782800	2.74415800	1.54009900
C	-1.10782800	2.74415800	1.54009900
C	2.74415800	-1.10782800	1.54009900
C	2.74415800	1.10782800	1.54009900
C	-1.10782800	-2.74415800	1.54009900
C	1.10782800	-2.74415800	1.54009900
C	-2.74415800	1.10782800	1.54009900
C	-2.74415800	-1.10782800	1.54009900
C	0.69955800	4.10109100	1.86490100
C	-0.69955800	4.10109100	1.86490100
C	4.10109100	-0.69955800	1.86490100
C	4.10109100	0.69955800	1.86490100
C	-0.69955800	-4.10109100	1.86490100
C	0.69955800	-4.10109100	1.86490100
C	-4.10109100	0.69955800	1.86490100
C	-4.10109100	-0.69955800	1.86490100
C	1.42367200	5.24888000	2.18506700
C	-1.42367200	5.24888000	2.18506700
C	0.70374600	6.40021100	2.48417500
C	-0.70374600	6.40021100	2.48417500
C	5.24888000	-1.42367200	2.18506700
C	5.24888000	1.42367200	2.18506700
C	6.40021100	-0.70374600	2.48417500
C	6.40021100	0.70374600	2.48417500
C	-1.42367200	-5.24888000	2.18506700
C	1.42367200	-5.24888000	2.18506700
C	-0.70374600	-6.40021100	2.48417500
C	0.70374600	-6.40021100	2.48417500
C	-5.24888000	1.42367200	2.18506700

C	-5.24888000	-1.42367200	2.18506700
C	-6.40021100	0.70374600	2.48417500
C	-6.40021100	-0.70374600	2.48417500
H	2.50739600	5.23645500	2.19396600
H	-2.50739600	5.23645500	2.19396600
H	1.23286900	7.31612400	2.72721700
H	-1.23286900	7.31612400	2.72721700
H	5.23645500	-2.50739600	2.19396600
H	5.23645500	2.50739600	2.19396600
H	7.31612400	-1.23286900	2.72721700
H	7.31612400	1.23286900	2.72721700
H	-2.50739600	-5.23645500	2.19396600
H	2.50739600	-5.23645500	2.19396600
H	-1.23286900	-7.31612400	2.72721700
H	1.23286900	-7.31612400	2.72721700
H	-5.23645500	2.50739600	2.19396600
H	-5.23645500	-2.50739600	2.19396600
H	-7.31612400	1.23286900	2.72721700
H	-7.31612400	-1.23286900	2.72721700
N	-1.38687500	1.38687500	-1.28977600
N	1.38687500	-1.38687500	-1.28977600
N	-1.38687500	-1.38687500	-1.28977600
N	1.38687500	1.38687500	-1.28977600
N	-3.35212000	0.00000000	-1.60161600
N	3.35212000	0.00000000	-1.60161600
N	0.00000000	-3.35212000	-1.60161600
N	0.00000000	3.35212000	-1.60161600
C	-2.72376500	1.15705900	-1.54009900
C	-1.15705900	2.72376500	-1.54009900
C	-1.15705900	-2.72376500	-1.54009900
C	-2.72376500	-1.15705900	-1.54009900
C	2.72376500	-1.15705900	-1.54009900
C	1.15705900	-2.72376500	-1.54009900
C	1.15705900	2.72376500	-1.54009900
C	2.72376500	1.15705900	-1.54009900
C	-3.39457100	2.40524700	-1.86490100
C	-2.40524700	3.39457100	-1.86490100
C	-2.40524700	-3.39457100	-1.86490100
C	-3.39457100	-2.40524700	-1.86490100
C	3.39457100	-2.40524700	-1.86490100

C	2.40524700	-3.39457100	-1.86490100
C	2.40524700	3.39457100	-1.86490100
C	3.39457100	2.40524700	-1.86490100
C	-4.71820700	2.70483000	-2.18506700
C	-2.70483000	4.71820700	-2.18506700
C	-5.02325600	4.02800900	-2.48417500
C	-4.02800900	5.02325600	-2.48417500
C	-2.70483000	-4.71820700	-2.18506700
C	-4.71820700	-2.70483000	-2.18506700
C	-4.02800900	-5.02325600	-2.48417500
C	-5.02325600	-4.02800900	-2.48417500
C	4.71820700	-2.70483000	-2.18506700
C	2.70483000	-4.71820700	-2.18506700
C	5.02325600	-4.02800900	-2.48417500
C	4.02800900	-5.02325600	-2.48417500
C	2.70483000	4.71820700	-2.18506700
C	4.71820700	2.70483000	-2.18506700
C	4.02800900	5.02325600	-2.48417500
C	5.02325600	4.02800900	-2.48417500
H	-5.47573000	1.92973600	-2.19396600
H	-1.92973600	5.47573000	-2.19396600
H	-6.04505100	4.30151100	-2.72721700
H	-4.30151100	6.04505100	-2.72721700
H	-1.92973600	-5.47573000	-2.19396600
H	-5.47573000	-1.92973600	-2.19396600
H	-4.30151100	-6.04505100	-2.72721700
H	-6.04505100	-4.30151100	-2.72721700
H	5.47573000	-1.92973600	-2.19396600
H	1.92973600	-5.47573000	-2.19396600
H	6.04505100	-4.30151100	-2.72721700
H	4.30151100	-6.04505100	-2.72721700
H	1.92973600	5.47573000	-2.19396600
H	5.47573000	1.92973600	-2.19396600
H	4.30151100	6.04505100	-2.72721700
H	6.04505100	4.30151100	-2.72721700

Table S8. Geometry optimized coordinates for Pb(Pc)₂.

Pb	0.00000000	0.00000000	0.00000000
N	0.00000000	1.97607700	1.33964400
N	0.00000000	-1.97607700	1.33964400
N	1.97607700	0.00000000	1.33964400
N	-1.97607700	0.00000000	1.33964400
N	2.37419300	2.37419300	1.62735200
N	-2.37419300	-2.37419300	1.62735200
N	2.37419300	-2.37419300	1.62735200
N	-2.37419300	2.37419300	1.62735200
C	1.11161400	2.75529500	1.57014800
C	-1.11161400	2.75529500	1.57014800
C	2.75529500	-1.11161400	1.57014800
C	2.75529500	1.11161400	1.57014800
C	-1.11161400	-2.75529500	1.57014800
C	1.11161400	-2.75529500	1.57014800
C	-2.75529500	1.11161400	1.57014800
C	-2.75529500	-1.11161400	1.57014800
C	0.70060200	4.11714600	1.88019100
C	-0.70060200	4.11714600	1.88019100
C	4.11714600	-0.70060200	1.88019100
C	4.11714600	0.70060200	1.88019100
C	-0.70060200	-4.11714600	1.88019100
C	0.70060200	-4.11714600	1.88019100
C	-4.11714600	0.70060200	1.88019100
C	-4.11714600	-0.70060200	1.88019100
C	1.42344700	5.26874800	2.18816900
C	-1.42344700	5.26874800	2.18816900
C	0.70349600	6.42314200	2.47687300
C	-0.70349600	6.42314200	2.47687300
C	5.26874800	-1.42344700	2.18816900
C	5.26874800	1.42344700	2.18816900
C	6.42314200	-0.70349600	2.47687300
C	6.42314200	0.70349600	2.47687300
C	-1.42344700	-5.26874800	2.18816900
C	1.42344700	-5.26874800	2.18816900
C	-0.70349600	-6.42314200	2.47687300
C	0.70349600	-6.42314200	2.47687300
C	-5.26874800	1.42344700	2.18816900

C	-5.26874800	-1.42344700	2.18816900
C	-6.42314200	0.70349600	2.47687300
C	-6.42314200	-0.70349600	2.47687300
H	2.50727400	5.25674300	2.19628000
H	-2.50727400	5.25674300	2.19628000
H	1.23276300	7.34133000	2.71110300
H	-1.23276300	7.34133000	2.71110300
H	5.25674300	-2.50727400	2.19628000
H	5.25674300	2.50727400	2.19628000
H	7.34133000	-1.23276300	2.71110300
H	7.34133000	1.23276300	2.71110300
H	-2.50727400	-5.25674300	2.19628000
H	2.50727400	-5.25674300	2.19628000
H	-1.23276300	-7.34133000	2.71110300
H	1.23276300	-7.34133000	2.71110300
H	-5.25674300	2.50727400	2.19628000
H	-5.25674300	-2.50727400	2.19628000
H	-7.34133000	1.23276300	2.71110300
H	-7.34133000	-1.23276300	2.71110300
N	-1.39729700	1.39729700	-1.33964400
N	1.39729700	-1.39729700	-1.33964400
N	-1.39729700	-1.39729700	-1.33964400
N	1.39729700	1.39729700	-1.33964400
N	-3.35761600	0.00000000	-1.62735200
N	3.35761600	0.00000000	-1.62735200
N	0.00000000	-3.35761600	-1.62735200
N	0.00000000	3.35761600	-1.62735200
C	-2.73431800	1.16225700	-1.57014800
C	-1.16225700	2.73431800	-1.57014800
C	-1.16225700	-2.73431800	-1.57014800
C	-2.73431800	-1.16225700	-1.57014800
C	2.73431800	-1.16225700	-1.57014800
C	1.16225700	-2.73431800	-1.57014800
C	1.16225700	2.73431800	-1.57014800
C	2.73431800	1.16225700	-1.57014800
C	-3.40666200	2.41586200	-1.88019100
C	-2.41586200	3.40666200	-1.88019100
C	-2.41586200	-3.40666200	-1.88019100
C	-3.40666200	-2.41586200	-1.88019100
C	3.40666200	-2.41586200	-1.88019100

C	2.41586200	-3.40666200	-1.88019100
C	2.41586200	3.40666200	-1.88019100
C	3.40666200	2.41586200	-1.88019100
C	-4.73209600	2.71903800	-2.18816900
C	-2.71903800	4.73209600	-2.18816900
C	-5.03929400	4.04440100	-2.47687300
C	-4.04440100	5.03929400	-2.47687300
C	-2.71903800	-4.73209600	-2.18816900
C	-4.73209600	-2.71903800	-2.18816900
C	-4.04440100	-5.03929400	-2.47687300
C	-5.03929400	-4.04440100	-2.47687300
C	4.73209600	-2.71903800	-2.18816900
C	2.71903800	-4.73209600	-2.18816900
C	5.03929400	-4.04440100	-2.47687300
C	4.04440100	-5.03929400	-2.47687300
C	2.71903800	4.73209600	-2.18816900
C	4.73209600	2.71903800	-2.18816900
C	4.04440100	5.03929400	-2.47687300
C	5.03929400	4.04440100	-2.47687300
H	-5.48998900	1.94416800	-2.19628000
H	-1.94416800	5.48998900	-2.19628000
H	-6.06279900	4.31940900	-2.71110300
H	-4.31940900	6.06279900	-2.71110300
H	-1.94416800	-5.48998900	-2.19628000
H	-5.48998900	-1.94416800	-2.19628000
H	-4.31940900	-6.06279900	-2.71110300
H	-6.06279900	-4.31940900	-2.71110300
H	5.48998900	-1.94416800	-2.19628000
H	1.94416800	-5.48998900	-2.19628000
H	6.06279900	-4.31940900	-2.71110300
H	4.31940900	-6.06279900	-2.71110300
H	1.94416800	5.48998900	-2.19628000
H	5.48998900	1.94416800	-2.19628000
H	4.31940900	6.06279900	-2.71110300
H	6.06279900	4.31940900	-2.71110300