Electronic Supplementary Information

Significance of dimer models describing physical properties in a triclinic solid of tin(II) phthalocyanine

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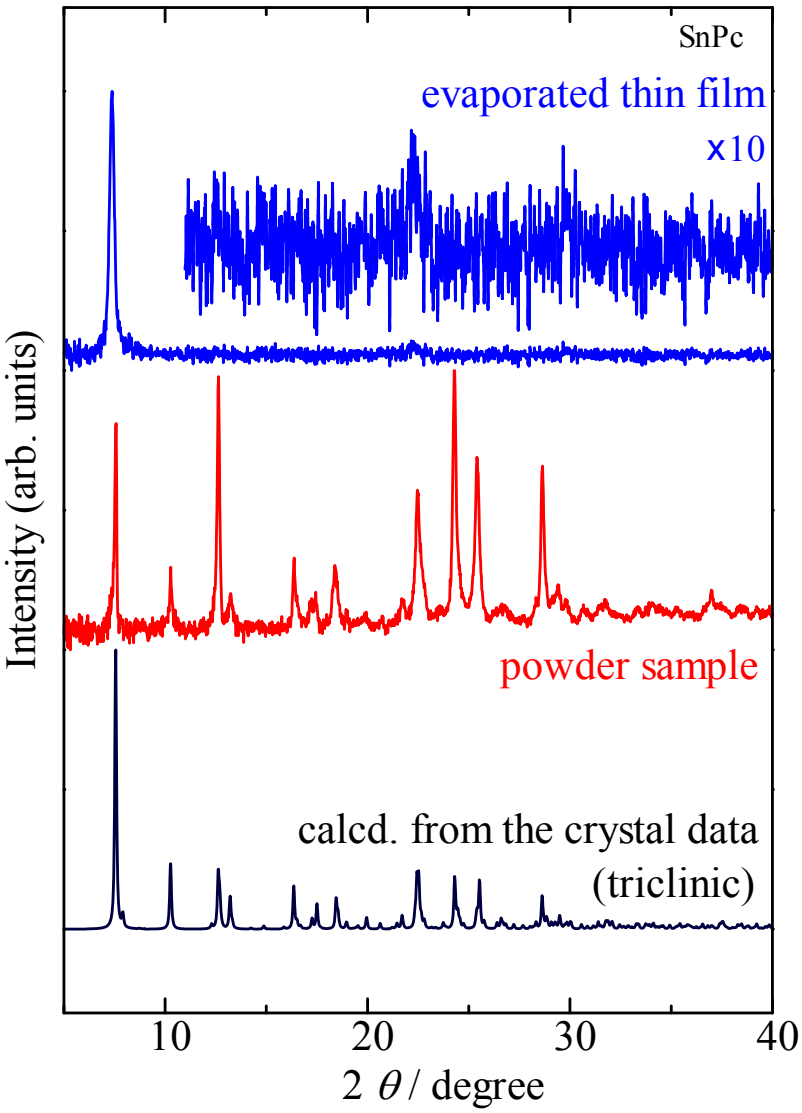


Fig. SI1. The X-ray powder pattern of the evaporated thin film of SnPc in a triclinic system.

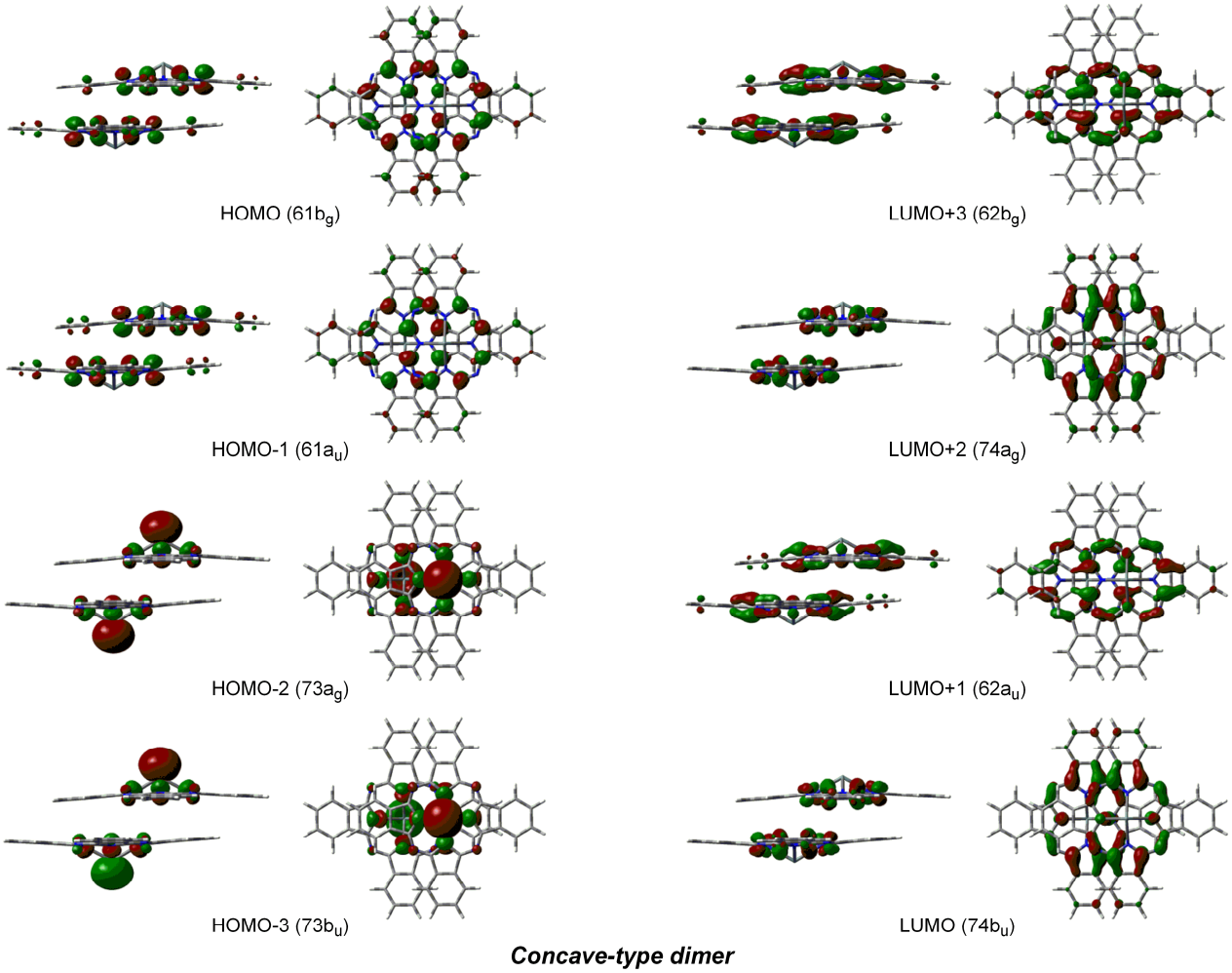


Fig. SI2. Several molecular orbitals near the HOMO and LUMO of the concave-type SnPc dimer. The orbital symmetries are labeled under the C_{2h} symmetry.

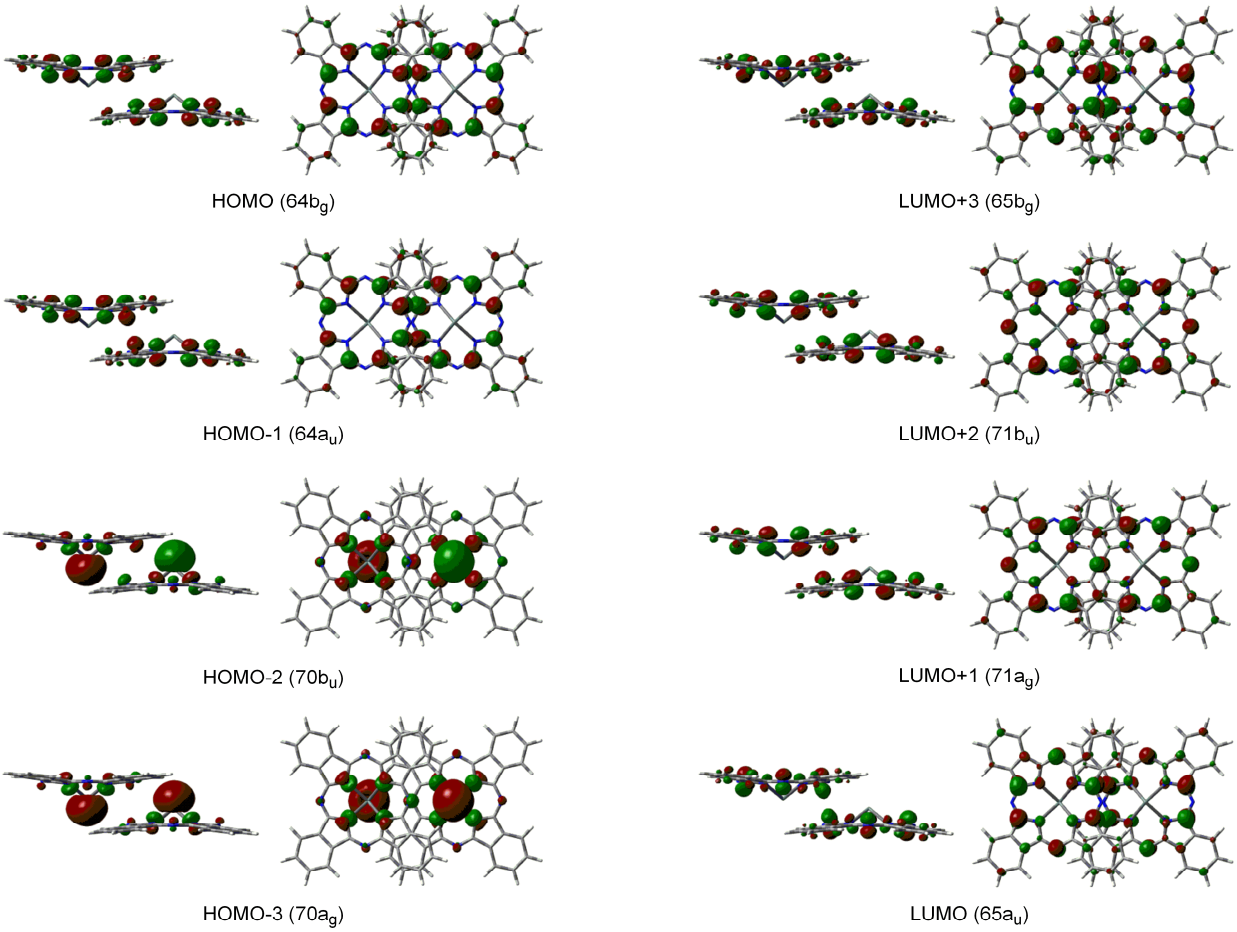
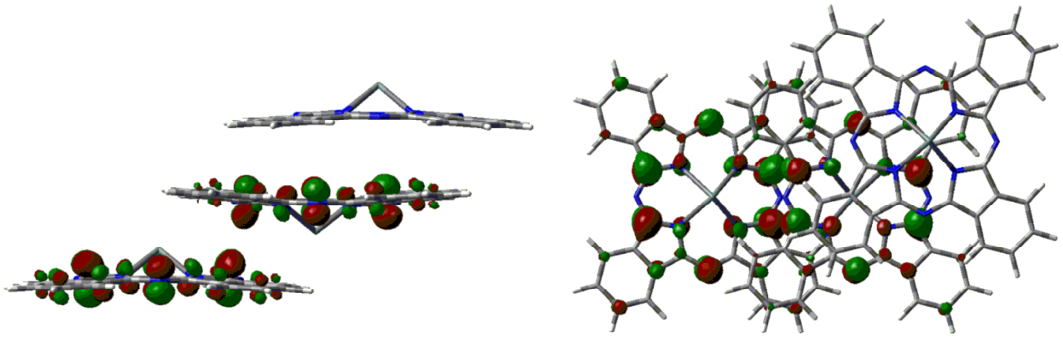
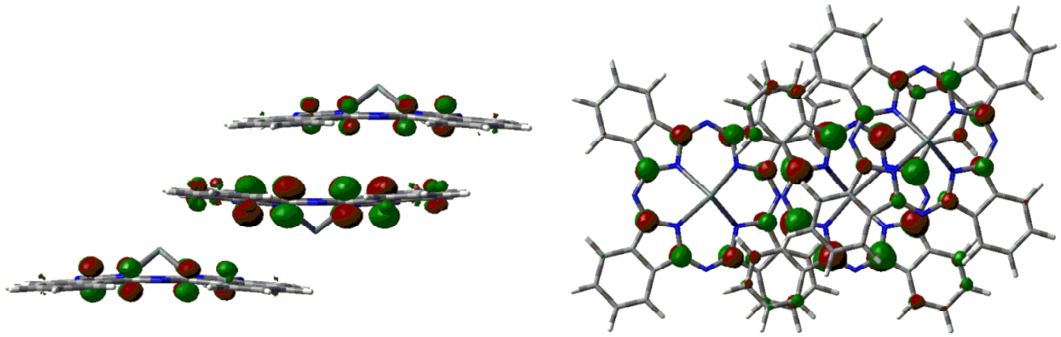


Fig. SI3. Several molecular orbitals near the HOMO and LUMO of the convex-type SnPc dimer. The orbital symmetries are labeled under the C_{2h} symmetry.



LUMO (403a)



HOMO (402a)

Trimer

Fig. SI4. HOMO and LUMO of the SnPc trimer. The orbital symmetries are labeled under the C_1 symmetry.

Table SI1. Symmetry-allowed TD-M06 excited states of the SnPc trimer.

	state	main configuration ($\|C\| \geq 0.30$)	E^a	f^b
C_1	1^1A	+0.62(402a→403a) [77 %]	1.48	0.202
	2^1A	+0.52(402a→404a) [54 %]	1.50	0.062
	5^1A	+0.57(402a→407a) [65 %]	1.62	0.064
	6^1A	+0.58(401a→403a) [67 %]	1.66	0.107
	9^1A	+0.45(400a→403a) [41 %]	1.83	0.109
	11^1A	+0.38(401a→405a) [29 %] –0.36(401a→406a) [26 %]	1.85	0.054
	12^1A	+0.34(401a→406a) [23 %]	1.89	0.062
	13^1A	+0.40(398a→403a) [32 %] +0.33(399a→408a) [22 %]	1.90	0.115
	17^1A	+0.51(401a→408a) [52 %]	2.02	0.051
	21^1A	–0.49(400a→404a) [48 %] –0.38(400a→407a) [29 %]	2.05	0.119
	23^1A	–0.39(400a→405a) [30 %] +0.39(400a→407a) [30 %]	2.10	0.210
	24^1A	+0.66(400a→408a) [87 %]	2.17	0.261
	1^3A	–0.30(400a→408a) [18 %] +0.59(402a→403a) [70 %]	0.75	0.000

[a] Excitation energy in eV.

[b] Oscillator strength.

Table SI2. Symmetry-allowed TD-M06 excited states of the concave-type SnPc dimer.

	state	main configuration ($\|C\| \geq 0.30$)	E^a	f^b	p^c
C_{2h}	$1B_u$	$+0.65(61b_g \rightarrow 62a_u)$ [85 %]	1.59	0.106	$x+y$
	$1A_u$	$+0.65(61b_g \rightarrow 74b_u)$ [85 %]	1.60	0.069	z
	$2B_u$	$+0.34(73b_u \rightarrow 74a_g)$ [23 %] $-0.37(73a_g \rightarrow 74b_u)$ [27 %] $+0.46(61a_u \rightarrow 62b_g)$ [42 %]	1.92	0.177	$x+y$
	$2A_u$	$-0.35(73b_u \rightarrow 62b_g)$ [25 %] $+0.37(73a_g \rightarrow 62a_u)$ [27 %] $+0.46(61a_u \rightarrow 74a_g)$ [42 %]	1.93	0.172	z
	$3B_u$	$-0.32(73b_u \rightarrow 74a_g)$ [20 %] $+0.37(73a_g \rightarrow 74b_u)$ [27 %] $+0.45(61a_u \rightarrow 62b_g)$ [41 %]	2.07	0.255	$x+y$
	$3A_u$	$+0.31(73b_u \rightarrow 62b_g)$ [19 %] $-0.37(73a_g \rightarrow 62a_u)$ [27 %] $+0.45(61a_u \rightarrow 74a_g)$ [41 %]	2.08	0.256	z
	$4A_u$	$+0.53(73b_u \rightarrow 62b_g)$ [56 %] $+0.47(73a_g \rightarrow 62a_u)$ [44 %]	2.38	0.001	z
	$4B_u$	$+0.52(73b_u \rightarrow 74a_g)$ [54 %] $+0.47(73a_g \rightarrow 74b_u)$ [44 %]	2.41	0.001	$x+y$
	$5B_u$	$+0.69(61b_g \rightarrow 63a_u)$ [95 %]	3.22	0.004	$x+y$
	$5A_u$	$+0.67(72b_u \rightarrow 62b_g)$ [90 %]	3.27	0.0001	z
	$6A_u$	$+0.65(72a_g \rightarrow 62a_u)$ [85 %]	3.31	0.005	z
	$6B_u$	$+0.61(72b_u \rightarrow 74a_g)$ [74 %]	3.36	0.001	$x+y$
	$7B_u$	$+0.58(72a_g \rightarrow 74b_u)$ [67 %]	3.38	0.042	$x+y$
	$7A_u$	$+0.38(59b_g \rightarrow 74b_u)$ [29 %] $+0.45(60b_g \rightarrow 74b_u)$ [41 %]	3.44	0.0002	z
	$8B_u$	$+0.40(57b_g \rightarrow 62a_u)$ [32 %] $-0.40(57a_u \rightarrow 62b_g)$ [32 %] $-0.36(60b_g \rightarrow 62a_u)$ [26 %]	3.50	0.004	$x+y$

[a] Excitation energy in eV.

[b] Oscillator strength.

[c] Transition moment direction.

Table SI3. Symmetry-allowed TD-M06 excited states of the convex-type SnPc dimer.

	state	main configuration ($\|C\| \geq 0.30$)	E^a	f^b	p^c
C_{2h}	$1B_u$	$+0.69(64b_g \rightarrow 65a_u)$ [95 %]	1.57	0.483	$x+y$
	$1A_u$	$+0.67(64b_g \rightarrow 71b_u)$ [90 %]	1.69	0.106	z
	$2A_u$	$+0.48(70a_g \rightarrow 65a_u)$ [46 %] $-0.35(70b_u \rightarrow 65b_g)$ [25 %] $-0.37(64a_u \rightarrow 71a_g)$ [27 %]	1.93	0.091	z
	$2B_u$	$+0.36(70a_g \rightarrow 71b_u)$ [26 %] $+0.55(70b_u \rightarrow 71a_g)$ [61 %]	1.95	0.003	$x+y$
	$3A_u$	$+0.34(70a_g \rightarrow 65a_u)$ [23 %] $+0.55(64a_u \rightarrow 71a_g)$ [61 %]	2.07	0.342	z
	$3B_u$	$+0.66(64a_u \rightarrow 65b_g)$ [87 %]	2.15	0.300	$x+y$
	$4A_u$	$+0.38(70a_g \rightarrow 65a_u)$ [29 %] $+0.59(70b_u \rightarrow 65b_g)$ [70 %]	2.37	0.009	z
	$4B_u$	$+0.59(70a_g \rightarrow 71b_u)$ [70 %] $-0.38(70b_u \rightarrow 71a_g)$ [29 %]	2.37	0.017	$x+y$
	$5B_u$	$+0.63(63b_g \rightarrow 65a_u)$ [79 %]	3.32	0.004	$x+y$
	$6B_u$	$+0.43(62b_g \rightarrow 65a_u)$ [37 %]	3.41	0.012	$x+y$
	$5A_u$	$+0.58(64b_g \rightarrow 72b_u)$ [67 %]	3.42	0.007	z
	$6A_u$	$+0.31(62b_g \rightarrow 71b_u)$ [19 %] $+0.34(69a_g \rightarrow 65a_u)$ [23 %] $-0.30(64b_g \rightarrow 72b_u)$ [18 %]	3.44	0.002	z
	$7B_u$	$+0.63(64b_g \rightarrow 66a_u)$ [79 %]	3.48	0.007	$x+y$
	$7A_u$	$+0.46(65a_g \rightarrow 65a_u)$ [42 %] $+0.34(65b_u \rightarrow 65b_g)$ [23 %]	3.51	0.003	z
	$8B_u$	$+0.48(69b_u \rightarrow 71a_g)$ [46 %]	3.51	0.086	$x+y$
	$9B_u$	$-0.33(65a_g \rightarrow 71b_u)$ [22 %] $+0.41(65b_u \rightarrow 71a_g)$ [34 %]	3.54	0.103	$x+y$
	$10B_u$	$+0.48(64b_g \rightarrow 67a_u)$ [46 %]	3.61	0.005	$x+y$
	$8A_u$	$+0.35(69b_u \rightarrow 65b_g)$ [25 %] $+0.34(64a_u \rightarrow 72a_g)$ [23 %]	3.62	0.034	z

[a] Excitation energy in eV.

[b] Oscillator strength.

[c] Transition moment direction.

Table SI4. Geometry optimized coordinates for the concave-type dimer.

50	0	0.000000	0.000000	0.000000
7	0	1.967384	0.000000	-1.115604
7	0	-1.967384	0.000000	-1.115604
7	0	0.000000	-1.967384	-1.115604
7	0	0.000000	1.967384	-1.115604
7	0	2.377087	-2.377087	-1.211230
7	0	-2.377087	2.377087	-1.211230
7	0	-2.377087	-2.377087	-1.211230
7	0	2.377087	2.377087	-1.211230
6	0	2.757127	-1.111181	-1.207389
6	0	-2.757127	1.111181	-1.207389
6	0	-1.111181	-2.757127	-1.207389
6	0	1.111181	2.757127	-1.207389
6	0	2.757127	1.111181	-1.207389
6	0	-2.757127	-1.111181	-1.207389
6	0	1.111181	-2.757127	-1.207389
6	0	-1.111181	2.757127	-1.207389
6	0	4.142872	-0.699740	-1.321041
6	0	4.142872	0.699740	-1.321041
6	0	5.326313	-1.419676	-1.409528
6	0	5.326313	1.419676	-1.409528
6	0	6.509232	-0.700529	-1.480048
6	0	6.509232	0.700529	-1.480048
1	0	5.314875	-2.507252	-1.418006
1	0	5.314875	2.507252	-1.418006
1	0	7.458029	-1.229501	-1.540008
1	0	7.458029	1.229501	-1.540008
6	0	-4.142872	0.699740	-1.321041
6	0	-4.142872	-0.699740	-1.321041
6	0	-5.326313	1.419676	-1.409528
6	0	-5.326313	-1.419676	-1.409528
6	0	-6.509232	0.700529	-1.480048
6	0	-6.509232	-0.700529	-1.480048
1	0	-5.314875	2.507252	-1.418006
1	0	-5.314875	-2.507252	-1.418006
1	0	-7.458029	1.229501	-1.540008
1	0	-7.458029	-1.229501	-1.540008

6	0	-0.699740	-4.142872	-1.321041
6	0	0.699740	-4.142872	-1.321041
6	0	-1.419676	-5.326313	-1.409528
6	0	1.419676	-5.326313	-1.409528
6	0	-0.700529	-6.509232	-1.480048
6	0	0.700529	-6.509232	-1.480048
1	0	-2.507252	-5.314875	-1.418006
1	0	2.507252	-5.314875	-1.418006
1	0	-1.229501	-7.458029	-1.540008
1	0	1.229501	-7.458029	-1.540008
6	0	0.699740	4.142872	-1.321041
6	0	-0.699740	4.142872	-1.321041
6	0	1.419676	5.326313	-1.409528
6	0	-1.419676	5.326313	-1.409528
6	0	0.700529	6.509232	-1.480048
6	0	-0.700529	6.509232	-1.480048
1	0	2.507252	5.314875	-1.418006
1	0	-2.507252	5.314875	-1.418006
1	0	1.229501	7.458029	-1.540008
1	0	-1.229501	7.458029	-1.540008
50	0	-3.469060	0.000000	-5.854162
7	0	-1.501676	0.000000	-4.738558
7	0	-5.436443	0.000000	-4.738558
7	0	-3.469060	1.967384	-4.738558
7	0	-3.469060	-1.967384	-4.738558
7	0	-1.091973	2.377087	-4.642932
7	0	-5.846147	-2.377087	-4.642932
7	0	-5.846147	2.377087	-4.642932
7	0	-1.091973	-2.377087	-4.642932
6	0	-0.711932	1.111181	-4.646772
6	0	-6.226187	-1.111181	-4.646772
6	0	-4.580241	2.757127	-4.646772
6	0	-2.357879	-2.757127	-4.646772
6	0	-0.711932	-1.111181	-4.646772
6	0	-6.226187	1.111181	-4.646772
6	0	-2.357879	2.757127	-4.646772
6	0	-4.580241	-2.757127	-4.646772
6	0	0.673812	0.699740	-4.533120
6	0	0.673812	-0.699740	-4.533120

6	0	1.857254	1.419676	-4.444633
6	0	1.857254	-1.419676	-4.444633
6	0	3.040172	0.700529	-4.374113
6	0	3.040172	-0.700529	-4.374113
1	0	1.845815	2.507252	-4.436156
1	0	1.845815	-2.507252	-4.436156
1	0	3.988970	1.229501	-4.314154
1	0	3.988970	-1.229501	-4.314154
6	0	-7.611932	-0.699740	-4.533120
6	0	-7.611932	0.699740	-4.533120
6	0	-8.795373	-1.419676	-4.444633
6	0	-8.795373	1.419676	-4.444633
6	0	-9.978291	-0.700529	-4.374113
6	0	-9.978291	0.700529	-4.374113
1	0	-8.783935	-2.507252	-4.436156
1	0	-8.783935	2.507252	-4.436156
1	0	-10.927089	-1.229501	-4.314154
1	0	-10.927089	1.229501	-4.314154
6	0	-4.168800	4.142872	-4.533120
6	0	-2.769319	4.142872	-4.533120
6	0	-4.888736	5.326313	-4.444633
6	0	-2.049383	5.326313	-4.444633
6	0	-4.169589	6.509232	-4.374113
6	0	-2.768530	6.509232	-4.374113
1	0	-5.976312	5.314875	-4.436156
1	0	-0.961808	5.314875	-4.436156
1	0	-4.698561	7.458029	-4.314154
1	0	-2.239559	7.458029	-4.314154
6	0	-2.769319	-4.142872	-4.533120
6	0	-4.168800	-4.142872	-4.533120
6	0	-2.049383	-5.326313	-4.444633
6	0	-4.888736	-5.326313	-4.444633
6	0	-2.768530	-6.509232	-4.374113
6	0	-4.169589	-6.509232	-4.374113
1	0	-0.961808	-5.314875	-4.436156
1	0	-5.976312	-5.314875	-4.436156
1	0	-2.239559	-7.458029	-4.314154
1	0	-4.698561	-7.458029	-4.314154

Table SI5. Geometry optimized coordinates for the convex-type dimer.

50	0	0.000000	0.000000	0.000000
7	0	1.971349	0.000000	-1.131478
7	0	-1.971349	0.000000	-1.131478
7	0	0.000000	-1.971349	-1.131478
7	0	0.000000	1.971349	-1.131478
7	0	2.375983	-2.375983	-1.268318
7	0	-2.375983	2.375983	-1.268318
7	0	-2.375983	-2.375983	-1.268318
7	0	2.375983	2.375983	-1.268318
6	0	2.757095	-1.110553	-1.255959
6	0	-2.757095	1.110553	-1.255959
6	0	-1.110553	-2.757095	-1.255959
6	0	1.110553	2.757095	-1.255959
6	0	2.757095	1.110553	-1.255959
6	0	-2.757095	-1.110553	-1.255959
6	0	1.110553	-2.757095	-1.255959
6	0	-1.110553	2.757095	-1.255959
6	0	4.137287	-0.699749	-1.433601
6	0	4.137287	0.699749	-1.433601
6	0	5.312828	-1.418891	-1.603255
6	0	5.312828	1.418891	-1.603255
6	0	6.488948	-0.700575	-1.747656
6	0	6.488948	0.700575	-1.747656
1	0	5.300696	-2.506373	-1.616585
1	0	5.300696	2.506373	-1.616585
1	0	7.431309	-1.230094	-1.868321
1	0	7.431309	1.230094	-1.868321
6	0	-4.137287	0.699749	-1.433601
6	0	-4.137287	-0.699749	-1.433601
6	0	-5.312828	1.418891	-1.603255
6	0	-5.312828	-1.418891	-1.603255
6	0	-6.488948	0.700575	-1.747656
6	0	-6.488948	-0.700575	-1.747656
1	0	-5.300696	2.506373	-1.616585
1	0	-5.300696	-2.506373	-1.616585
1	0	-7.431309	1.230094	-1.868321
1	0	-7.431309	-1.230094	-1.868321

6	0	-0.699749	-4.137287	-1.433601
6	0	0.699749	-4.137287	-1.433601
6	0	-1.418891	-5.312828	-1.603255
6	0	1.418891	-5.312828	-1.603255
6	0	-0.700575	-6.488948	-1.747656
6	0	0.700575	-6.488948	-1.747656
1	0	-2.506373	-5.300696	-1.616585
1	0	2.506373	-5.300696	-1.616585
1	0	-1.230094	-7.431309	-1.868321
1	0	1.230094	-7.431309	-1.868321
6	0	0.699749	4.137287	-1.433601
6	0	-0.699749	4.137287	-1.433601
6	0	1.418891	5.312828	-1.603255
6	0	-1.418891	5.312828	-1.603255
6	0	0.700575	6.488948	-1.747656
6	0	-0.700575	6.488948	-1.747656
1	0	2.506373	5.300696	-1.616585
1	0	-2.506373	5.300696	-1.616585
1	0	1.230094	7.431309	-1.868321
1	0	-1.230094	7.431309	-1.868321
50	0	4.485471	4.485471	0.625939
7	0	2.514122	4.485471	1.757418
7	0	6.456820	4.485471	1.757418
7	0	4.485471	2.514122	1.757418
7	0	4.485471	6.456820	1.757418
7	0	2.109487	2.109487	1.894258
7	0	6.861454	6.861454	1.894258
7	0	6.861454	2.109487	1.894258
7	0	2.109487	6.861454	1.894258
6	0	1.728376	3.374918	1.881898
6	0	7.242566	5.596023	1.881898
6	0	5.596023	1.728376	1.881898
6	0	3.374918	7.242566	1.881898
6	0	1.728376	5.596023	1.881898
6	0	7.242566	3.374918	1.881898
6	0	3.374918	1.728376	1.881898
6	0	5.596023	7.242566	1.881898
6	0	0.348184	3.785722	2.059541
6	0	0.348184	5.185220	2.059541

6	0	-0.827357	3.066580	2.229194
6	0	-0.827357	5.904362	2.229194
6	0	-2.003477	3.784895	2.373596
6	0	-2.003477	5.186046	2.373596
1	0	-0.815225	1.979097	2.242524
1	0	-0.815225	6.991844	2.242524
1	0	-2.945839	3.255376	2.494260
1	0	-2.945839	5.715565	2.494260
6	0	8.622758	5.185220	2.059541
6	0	8.622758	3.785722	2.059541
6	0	9.798299	5.904362	2.229194
6	0	9.798299	3.066580	2.229194
6	0	10.974418	5.186046	2.373596
6	0	10.974418	3.784895	2.373596
1	0	9.786167	6.991844	2.242524
1	0	9.786167	1.979097	2.242524
1	0	11.916780	5.715565	2.494260
1	0	11.916780	3.255376	2.494260
6	0	5.185220	0.348184	2.059541
6	0	3.785722	0.348184	2.059541
6	0	5.904362	-0.827357	2.229194
6	0	3.066580	-0.827357	2.229194
6	0	5.186046	-2.003477	2.373596
6	0	3.784895	-2.003477	2.373596
1	0	6.991844	-0.815225	2.242524
1	0	1.979097	-0.815225	2.242524
1	0	5.715565	-2.945839	2.494260
1	0	3.255376	-2.945839	2.494260
6	0	3.785722	8.622758	2.059541
6	0	5.185220	8.622758	2.059541
6	0	3.066580	9.798299	2.229194
6	0	5.904362	9.798299	2.229194
6	0	3.784895	10.974418	2.373596
6	0	5.186046	10.974418	2.373596
1	0	1.979097	9.786167	2.242524
1	0	6.991844	9.786167	2.242524
1	0	3.255376	11.916780	2.494260
1	0	5.715565	11.916780	2.494260

Table SI6. Geometry optimized coordinates for the trimer.

50	0	0.000000	0.000000	0.000000
7	0	1.968348	0.000000	-1.120027
7	0	-1.968348	0.000000	-1.120027
7	0	0.000000	-1.968348	-1.120027
7	0	0.000000	1.968348	-1.120027
7	0	2.376969	-2.376969	-1.221409
7	0	-2.376969	2.376969	-1.221409
7	0	-2.376969	-2.376969	-1.221409
7	0	2.376969	2.376969	-1.221409
6	0	2.757206	-1.110986	-1.218234
6	0	-2.757206	1.110986	-1.218234
6	0	-1.110986	-2.757206	-1.218234
6	0	1.110986	2.757206	-1.218234
6	0	2.757206	1.110986	-1.218234
6	0	-2.757206	-1.110986	-1.218234
6	0	1.110986	-2.757206	-1.218234
6	0	-1.110986	2.757206	-1.218234
6	0	4.141636	-0.699771	-1.352466
6	0	4.141636	0.699771	-1.352466
6	0	5.323468	-1.419257	-1.464396
6	0	5.323468	1.419257	-1.464396
6	0	6.505146	-0.700545	-1.556446
6	0	6.505146	0.700545	-1.556446
1	0	5.311670	-2.507051	-1.473975
1	0	5.311670	2.507051	-1.473975
1	0	7.452318	-1.230260	-1.631644
1	0	7.452318	1.230260	-1.631644
6	0	-4.141636	0.699771	-1.352466
6	0	-4.141636	-0.699771	-1.352466
6	0	-5.323468	1.419257	-1.464396
6	0	-5.323468	-1.419257	-1.464396
6	0	-6.505146	0.700545	-1.556446
6	0	-6.505146	-0.700545	-1.556446
1	0	-5.311670	2.507051	-1.473975
1	0	-5.311670	-2.507051	-1.473975
1	0	-7.452318	1.230260	-1.631644
1	0	-7.452318	-1.230260	-1.631644

6	0	-0.699771	-4.141636	-1.352466
6	0	0.699771	-4.141636	-1.352466
6	0	-1.419257	-5.323468	-1.464396
6	0	1.419257	-5.323468	-1.464396
6	0	-0.700545	-6.505146	-1.556446
6	0	0.700545	-6.505146	-1.556446
1	0	-2.507051	-5.311670	-1.473975
1	0	2.507051	-5.311670	-1.473975
1	0	-1.230260	-7.452318	-1.631644
1	0	1.230260	-7.452318	-1.631644
6	0	0.699771	4.141636	-1.352466
6	0	-0.699771	4.141636	-1.352466
6	0	1.419257	5.323468	-1.464396
6	0	-1.419257	5.323468	-1.464396
6	0	0.700545	6.505146	-1.556446
6	0	-0.700545	6.505146	-1.556446
1	0	2.507051	5.311670	-1.473975
1	0	-2.507051	5.311670	-1.473975
1	0	1.230260	7.452318	-1.631644
1	0	-1.230260	7.452318	-1.631644
50	0	4.532734	4.532734	0.777034
7	0	2.564386	4.532734	1.897061
7	0	6.501081	4.532734	1.897061
7	0	4.532734	2.564386	1.897061
7	0	4.532734	6.501081	1.897061
7	0	2.155765	2.155765	1.998443
7	0	6.909703	6.909703	1.998443
7	0	6.909703	2.155765	1.998443
7	0	2.155765	6.909703	1.998443
6	0	1.775528	3.421748	1.995268
6	0	7.289939	5.643719	1.995268
6	0	5.643719	1.775528	1.995268
6	0	3.421748	7.289939	1.995268
6	0	1.775528	5.643719	1.995268
6	0	7.289939	3.421748	1.995268
6	0	3.421748	1.775528	1.995268
6	0	5.643719	7.289939	1.995268
6	0	0.391098	3.832962	2.129501
6	0	0.391098	5.232505	2.129501

6	0	-0.790735	3.113477	2.241431
6	0	-0.790735	5.951990	2.241431
6	0	-1.972413	3.832188	2.333481
6	0	-1.972413	5.233279	2.333481
1	0	-0.778936	2.025683	2.251010
1	0	-0.778936	7.039785	2.251010
1	0	-2.919584	3.302474	2.408679
1	0	-2.919584	5.762993	2.408679
6	0	8.674370	5.232505	2.129501
6	0	8.674370	3.832962	2.129501
6	0	9.856202	5.951990	2.241431
6	0	9.856202	3.113477	2.241431
6	0	11.037880	5.233279	2.333481
6	0	11.037880	3.832188	2.333481
1	0	9.844403	7.039785	2.251010
1	0	9.844403	2.025683	2.251010
1	0	11.985051	5.762993	2.408679
1	0	11.985051	3.302474	2.408679
6	0	5.232505	0.391098	2.129501
6	0	3.832962	0.391098	2.129501
6	0	5.951990	-0.790735	2.241431
6	0	3.113477	-0.790735	2.241431
6	0	5.233279	-1.972413	2.333481
6	0	3.832188	-1.972413	2.333481
1	0	7.039785	-0.778936	2.251010
1	0	2.025683	-0.778936	2.251010
1	0	5.762993	-2.919584	2.408679
1	0	3.302474	-2.919584	2.408679
6	0	3.832962	8.674370	2.129501
6	0	5.232505	8.674370	2.129501
6	0	3.113477	9.856202	2.241431
6	0	5.951990	9.856202	2.241431
6	0	3.832188	11.037880	2.333481
6	0	5.233279	11.037880	2.333481
1	0	2.025683	9.844403	2.251010
1	0	7.039785	9.844403	2.251010
1	0	3.302474	11.985051	2.408679
1	0	5.762993	11.985051	2.408679
50	0	-3.624190	0.000000	-5.940560

7	0	-5.592537	0.000000	-4.820533
7	0	-1.655842	0.000000	-4.820533
7	0	-3.624190	-1.968348	-4.820533
7	0	-3.624190	1.968348	-4.820533
7	0	-6.001159	-2.376969	-4.719151
7	0	-1.247221	2.376969	-4.719151
7	0	-1.247221	-2.376969	-4.719151
7	0	-6.001159	2.376969	-4.719151
6	0	-6.381395	-1.110986	-4.722326
6	0	-0.866984	1.110986	-4.722326
6	0	-2.513204	-2.757206	-4.722326
6	0	-4.735176	2.757206	-4.722326
6	0	-6.381395	1.110986	-4.722326
6	0	-0.866984	-1.110986	-4.722326
6	0	-4.735176	-2.757206	-4.722326
6	0	-2.513204	2.757206	-4.722326
6	0	-7.765826	-0.699771	-4.588094
6	0	-7.765826	0.699771	-4.588094
6	0	-8.947658	-1.419257	-4.476163
6	0	-8.947658	1.419257	-4.476163
6	0	-10.129336	-0.700545	-4.384113
6	0	-10.129336	0.700545	-4.384113
1	0	-8.935859	-2.507051	-4.466585
1	0	-8.935859	2.507051	-4.466585
1	0	-11.076507	-1.230260	-4.308915
1	0	-11.076507	1.230260	-4.308915
6	0	0.517446	0.699771	-4.588094
6	0	0.517446	-0.699771	-4.588094
6	0	1.699279	1.419257	-4.476163
6	0	1.699279	-1.419257	-4.476163
6	0	2.880957	0.700545	-4.384113
6	0	2.880957	-0.700545	-4.384113
1	0	1.687480	2.507051	-4.466585
1	0	1.687480	-2.507051	-4.466585
1	0	3.828128	1.230260	-4.308915
1	0	3.828128	-1.230260	-4.308915
6	0	-2.924418	-4.141636	-4.588094
6	0	-4.323961	-4.141636	-4.588094
6	0	-2.204933	-5.323468	-4.476163

6	0	-5.043446	-5.323468	-4.476163
6	0	-2.923644	-6.505146	-4.384113
6	0	-4.324735	-6.505146	-4.384113
1	0	-1.117139	-5.311670	-4.466585
1	0	-6.131241	-5.311670	-4.466585
1	0	-2.393930	-7.452318	-4.308915
1	0	-4.854449	-7.452318	-4.308915
6	0	-4.323961	4.141636	-4.588094
6	0	-2.924418	4.141636	-4.588094
6	0	-5.043446	5.323468	-4.476163
6	0	-2.204933	5.323468	-4.476163
6	0	-4.324735	6.505146	-4.384113
6	0	-2.923644	6.505146	-4.384113
1	0	-6.131241	5.311670	-4.466585
1	0	-1.117139	5.311670	-4.466585
1	0	-4.854449	7.452318	-4.308915
1	0	-2.393930	7.452318	-4.308915