Electronic Supplementary Information

Theoretical study on crystal polymorphisms and electronic structures of lead (II) phthalocyanine using model dimers

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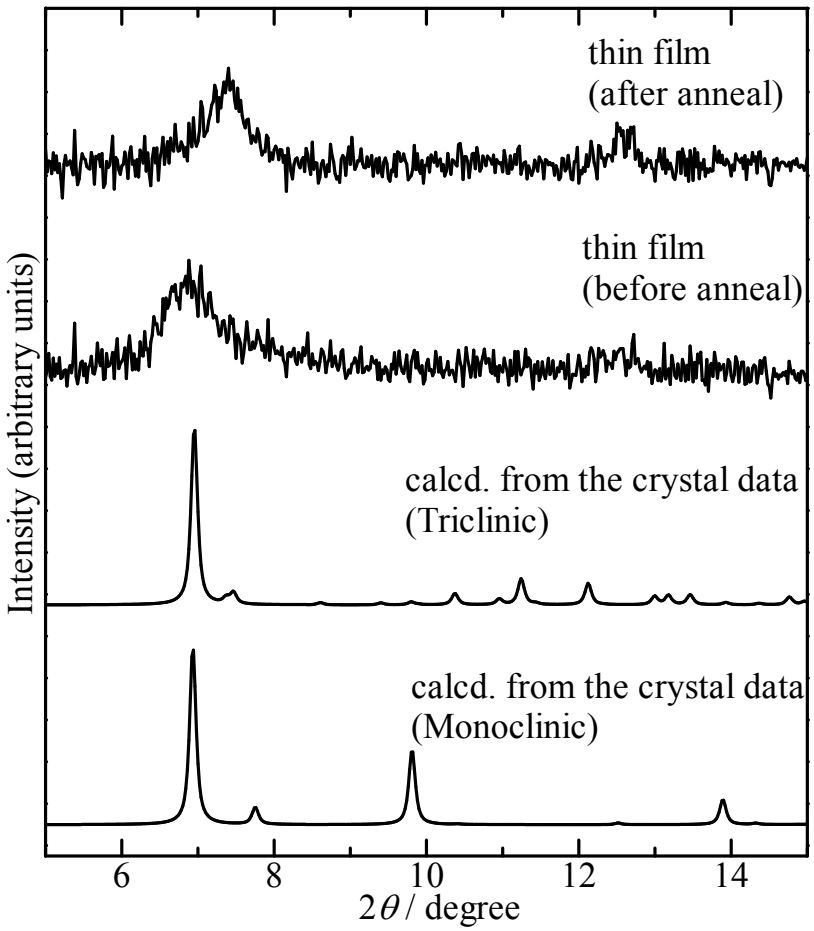


Fig. S1. The X-ray powder pattern of the evaporated thin film of PbPc. The diffraction patterns were consistent with the results reported by A. Miyamoto *et al.* (reference 36).

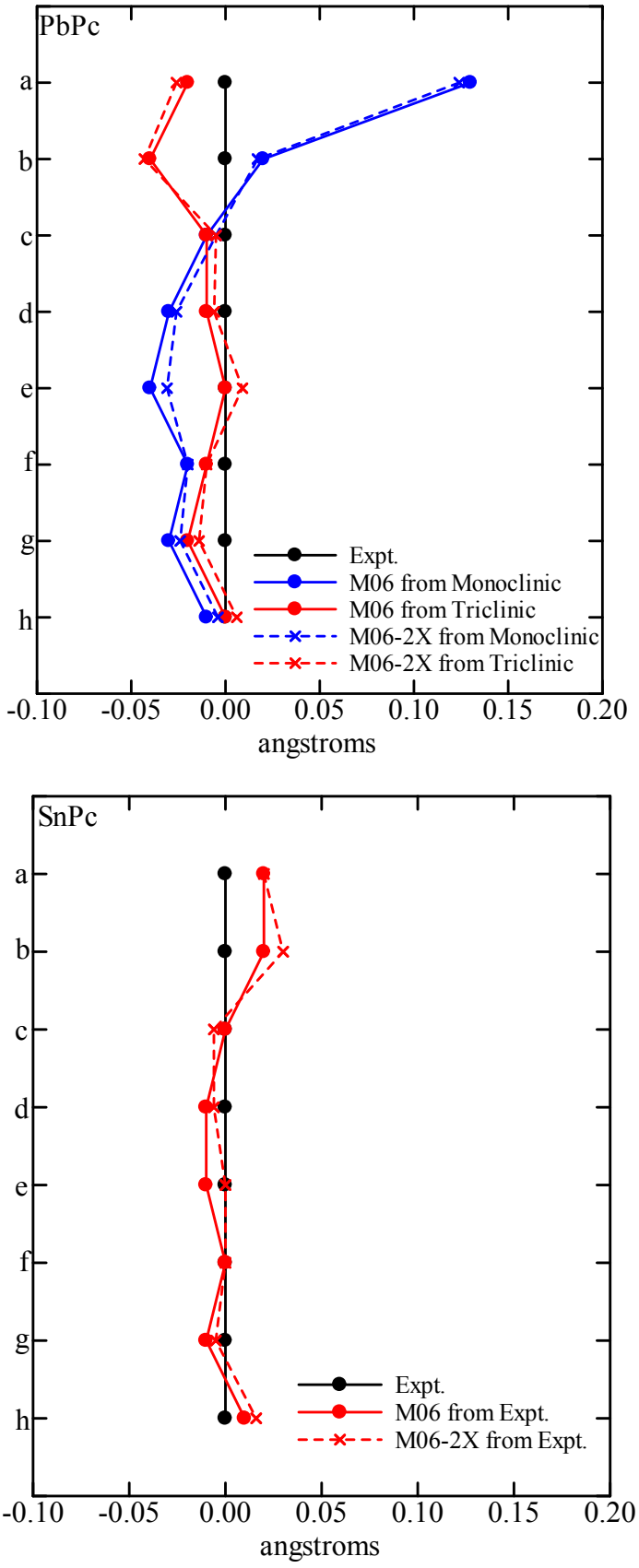
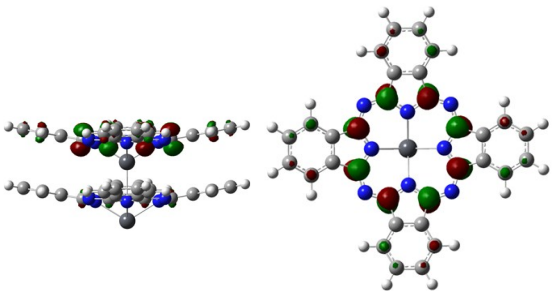
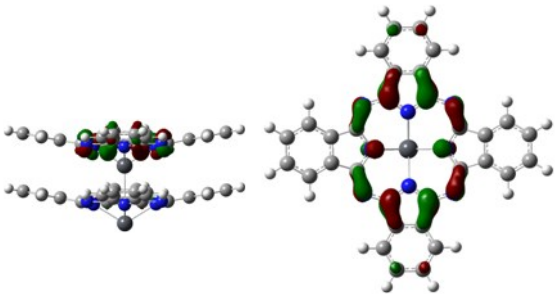


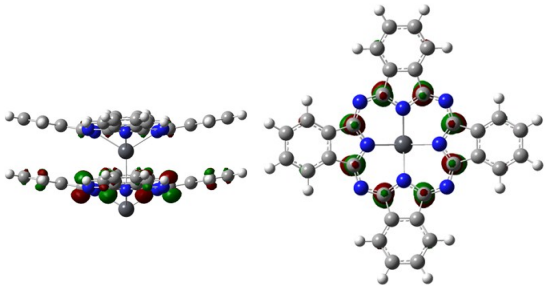
Fig. S2. Comparison of main calculated bond lengths (coloured solid and broken lines for M06 and M06-2x, respectively) with X-ray crystallographic data for PbPc (references 5 and 6 for monoclinic and triclinic, respectively) and SnPc (reference 10).



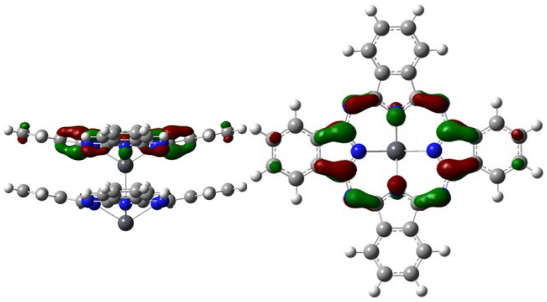
HOMO($26a_2$)



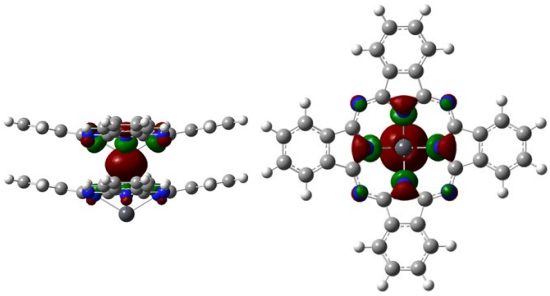
LUMO+3(68e)



HOMO-1($25a_2$)



LUMO+2(68e)



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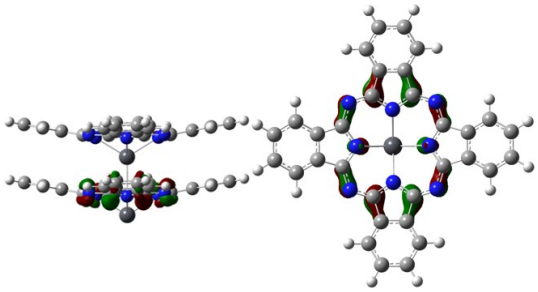
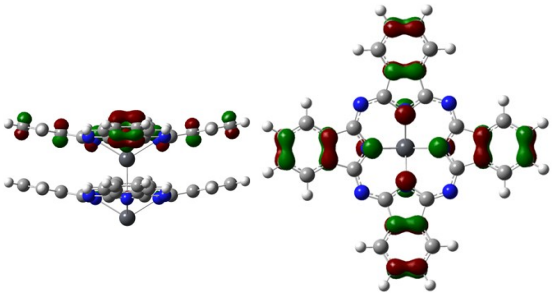
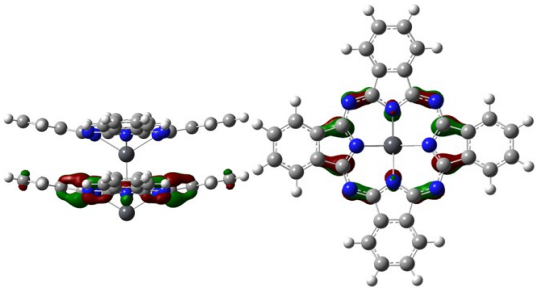


LUMO+1(67e)

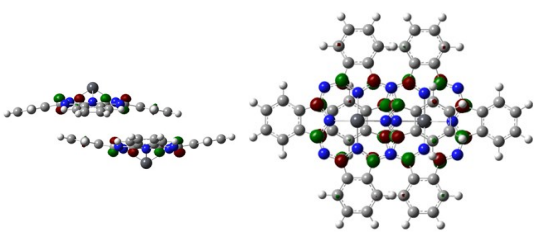


HOMO-3($36b_2$)

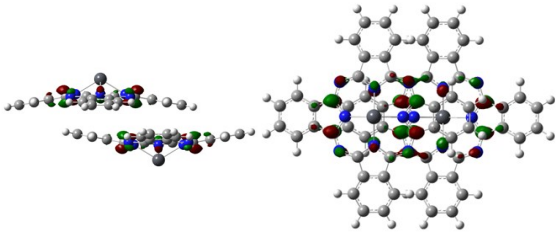


LUMO(67e)

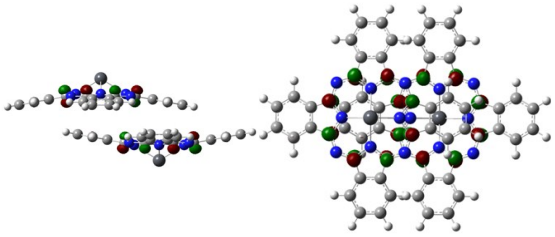
Fig. S3. Several molecular orbitals near the HOMO and LUMO of the Type 1 dimer. The orbital symmetries are labeled under the C_{4v} symmetry.



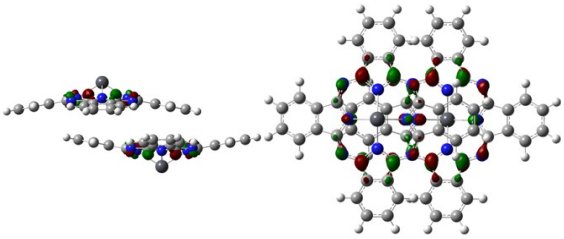
HOMO($61b_g$)



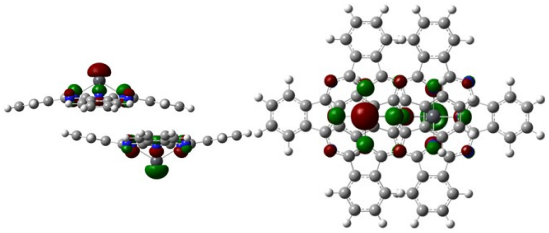
LUMO+3($62a_u$)



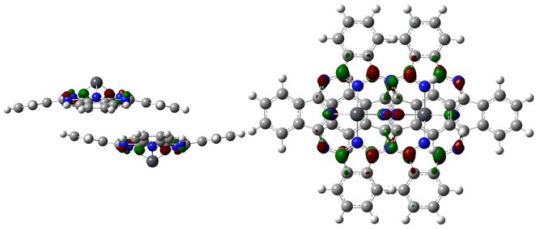
HOMO-1($61a_u$)



LUMO+2($74a_g$)



HOMO-2($73b_u$)



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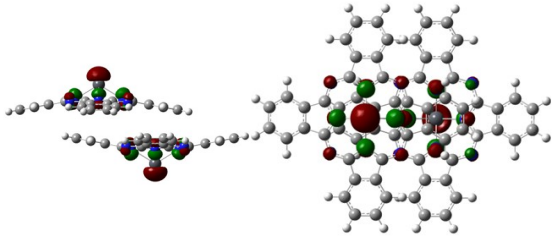

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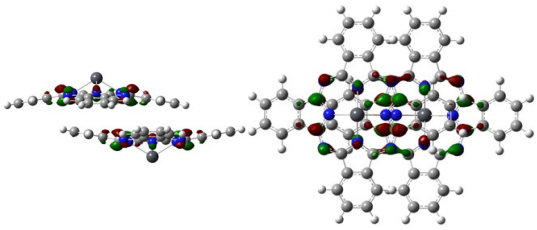
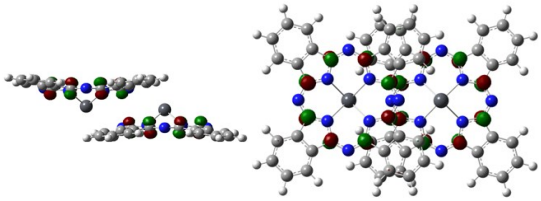
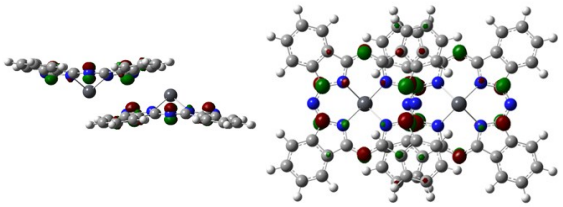


LUMO($62a_g$)

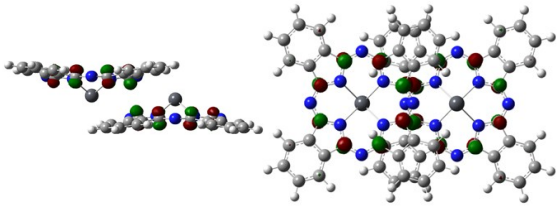
Fig. S4. Several molecular orbitals near the HOMO and LUMO of the Type 2 dimer. The orbital symmetries are labeled under the C_{2h} symmetry.



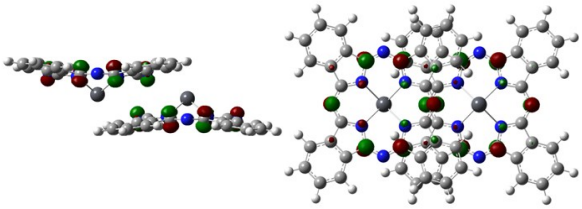
HOMO($64b_g$)



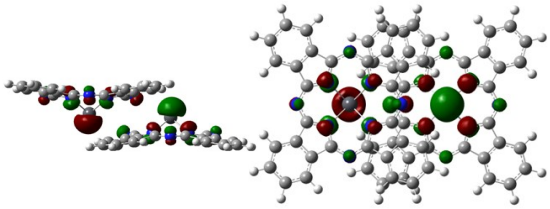
LUMO+3($65b_g$)



HOMO-1($64a_u$)



LUMO+2($71a_g$)



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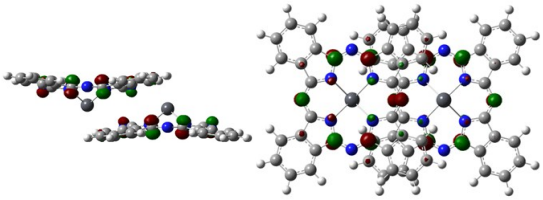
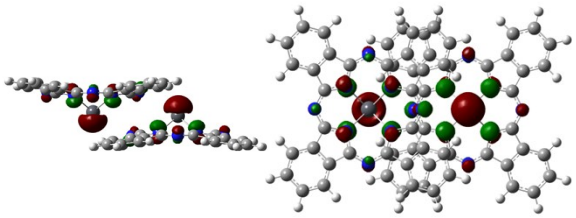
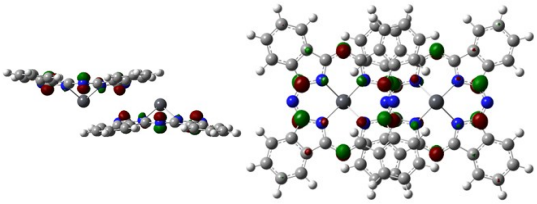


LUMO+1($71b_u$)

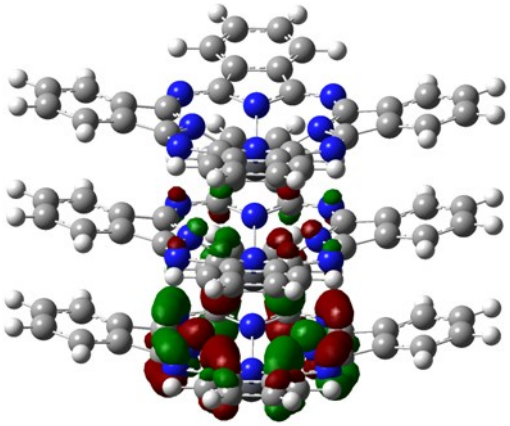


HOMO-3($70a_g$)

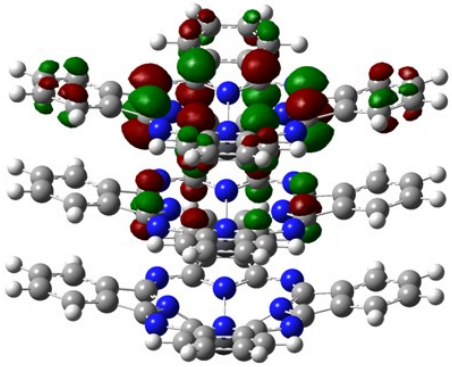


LUMO($65a_u$)

Fig. S5. Several molecular orbitals near the HOMO and LUMO of the Type 3 dimer. The orbital symmetries are labeled under the C_{2h} symmetry.

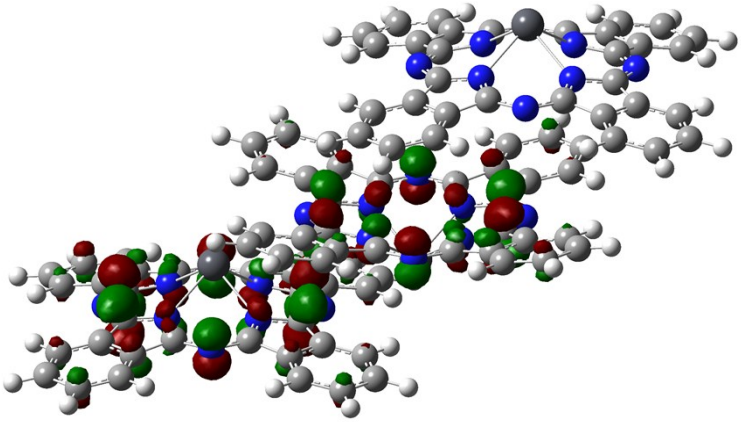


LUMO(127e)

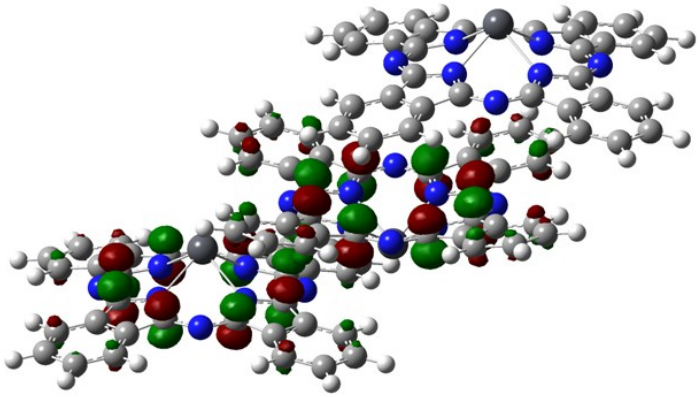


HOMO($27a_2$)

Fig. S6. HOMO and LUMO of the Type 4 PbPc trimer. The orbital symmetries are labeled under the C_{4v}



LUMO(403a)



HOMO(402a)

Fig. S7. HOMO and LUMO of the Type 5 PbPc trimer. The orbital symmetries are labeled under the C_1

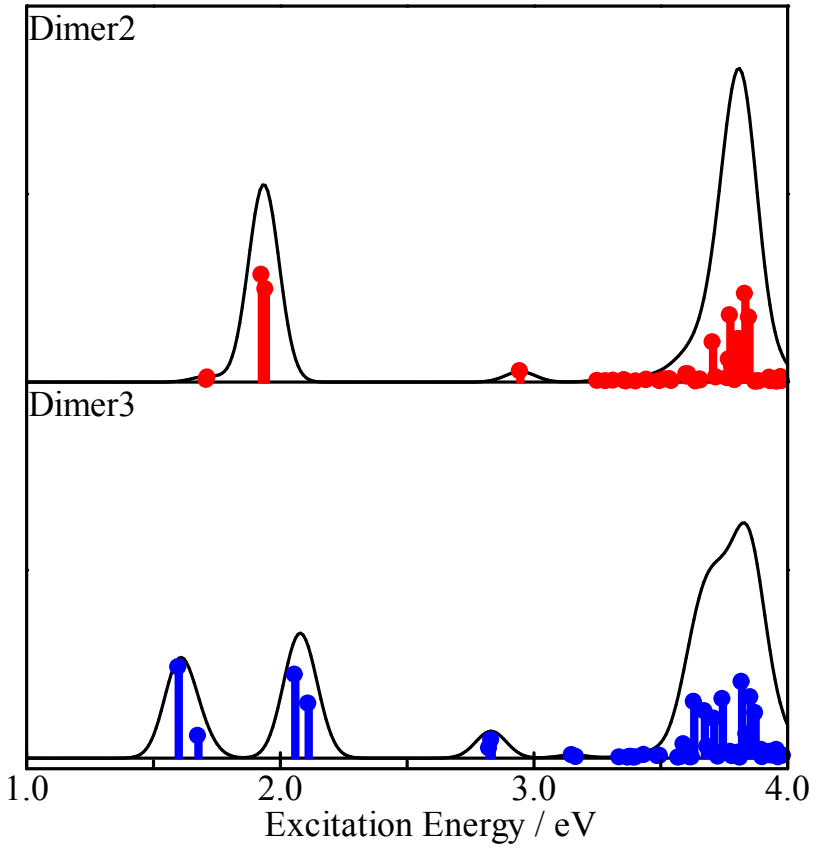


Fig. S8. Excited states of the Types 2 (red) and 3 (blue) dimers of PbPc obtained by the TD-M06 calculation.

Table S1 Differences of the total energy between the models and the corresponding components obtained by the M06 method. The values with the M06-2X method are also shown in parenthesis.

	ΔE [kcal mol^{-1}]	
	PbPc	SnPc
Type 1	-25.7 (-25.7)	-19.3 (-)
Type 2	-25.2 (-25.7)	-25.2 (-)
Type 3	-23.8 (-25.4)	-23.8 (-)
Type 4	-52.4 (-)	-38.9 (-)
Type 5	-48.7 (-)	-48.7 (-)

Table S2. Elemental analysis of PbPc.

	Analyses (%)		
	C	H	N
Measured value	53.44	2.35	15.69
Calculated value	53.40	2.24	15.57

Table S3. M06-Optimized parameters and X-ray observed bond lengths for monoclinic and triclinic systems of PbPc and triclinic systems of SnPc in Å. The results with M06-2x are also shown in parentheses.

	PbPc (C_{4v})			SnPc (C_{4v})	
	Calc.	Expt. Monoclinic[a]	Expt. Triclinic[b]	Calc.	Expt. Triclinic[c]
a	2.34 (2.33)	2.21	2.36	2.272 (2.270)	2.25
b	3.65 (3.65)	3.63	3.69	3.595 (3.596)	3.57
c	1.36 (1.36)	1.37	1.37	1.367 (1.367)	1.373
d	1.32 (1.32)	1.35	1.33	1.321 (1.322)	1.328
e	1.45 (1.46)	1.49	1.45	1.449 (1.456)	1.456
f	1.39 (1.39)	1.41	1.40	1.387 (1.390)	1.390
g	1.38 (1.39)	1.41	1.40	1.384 (1.385)	1.390
h	1.40 (1.41)	1.41	1.40	1.403 (1.406)	1.390

[a] Values from reference 5. [b] Values from reference 6. [c] Values from reference 10.

Table S4. Orbital energies near frontier orbitals optimized by the M06 method for PbPc monomer, dimers and Trimers. Corresponding orbitals are indicated by the same colors.

Monomer		Dimer						Trimer			
		Type 1		Type 2		Type 3		Type 4		Type 5	
Symmetry	Orbital energy	Symmetry	Orbital energy	Symmetry	Orbital energy	Symmetry	Orbital energy	Symmetry	Orbital energy	Symmetry	Orbital energy
34e	-2.977	68e	-2.977	$62a_u$	-2.884	$65b_g$	-2.825	129e	-2.322	408a	-2.776
$13a_2$	-5.284	67e	-5.284	$74a_g$	-2.912	$71a_g$	-2.950	128e	-2.810	407a	-2.890
$22a_1$	-6.890	$26a_2$	-4.871	$74b_u$	-2.919	$71b_u$	-2.967	127e	-3.306	406a	-2.915
		$25a_2$	-5.477	$62b_g$	-2.921	$65a_u$	-3.078	$27a_2$	-4.647	405a	-2.920
		$44a_1$	-6.077	$61b_g$	-5.166	$64b_g$	-5.107	$26a_2$	-5.099	404a	-2.932
		$36b_2$	-6.826	$61a_u$	-5.259	$64a_u$	-5.442	$25a_2$	-5.567	403a	-3.043
				$73b_u$	-6.782	$70b_u$	-6.678	$51a_1$	-5.821	402a	-5.052
				$73a_g$	-6.828	$70a_g$	-6.783	$50a_1$	-6.239	401a	-5.217
								$39b_2$	-6.615	400a	-5.408
										399a	-6.647
										398a	-6.750
										397a	-6.811

Table S5. Symmetry-allowed TD-M06 excited states of the Type 1 dimer.

	State	Main configuration(|C|≧0.30)	E^a	f^b	p^c
C_{4v}	1E	-0.32(26a2→67e)[21%]+0.63(26a2→67e)[79%]	1.01	0.0001	x+y
		+0.63(26a_2→67e)[79%]+0.32(26a_2→67e)[21%]	1.01	0.0001	x+y
	2E	-0.48(25a_2→67e)[45%]+0.37(26a_2→68e)[27%]	1.69	0.006	x+y
		+0.48(25a_2→67e)[45%]-0.37(26a_2→68e)[27%]	1.69	0.006	x+y
	3E	+0.47(44a_1→67e)[45%]-0.40(26a_2→68e)[32%]	1.90	0.219	x+y
		-0.47(44a_1→67e)[45%]-0.40(26a_2→68e)[32%]	1.90	0.219	x+y
	4E	+0.46(44a_1→67e)[42%]-0.32(26a_2→68e)[20%]	2.05	0.256	x+y
		+0.46(44a_1→67e)[42%]+0.32(26a_2→68e)[20%]	2.05	0.256	x+y
	5E	+0.68(25a_2→68e)[92%]	2.28	0.006	x+y
		+0.68(25a_2→68e)[92%]	2.28	0.006	x+y
	6E	-0.68(44a_1→68e)[92%]	2.59	0.012	x+y
		+0.68(44a_1→68e)[92%]	2.59	0.012	x+y
	7E	+0.63(42a_1→67e)[80%]	2.84	0.003	x+y
		+0.63(42a_1→67e)[80%]	2.84	0.003	x+y

[a]Excitation energy in eV. [b]Oscillator strength. [c]Transition moment direction.

Table S6. Symmetry-allowed TD-M06 excited states of the Type 2 dimer.

	State	Main Configuration(|C|≧0.30)	E^a	f^b	p^c
C_{2h}	$1B_u$	-0.44($61a_u \rightarrow 62b_g$)[39%]+0.55($61b_g \rightarrow 62a_u$)[61%]	1.71	0.009	x+y
	$1A_u$	+0.39($61a_u \rightarrow 74a_g$)[30%]+0.59($61b_g \rightarrow 74b_u$)[69%]	1.71	0.022	z
	$2B_u$	+0.54($61a_u \rightarrow 62b_g$)[58%]+0.43($61b_g \rightarrow 62a_u$)[36%]	1.93	0.568	x+y
	$2A_u$	+0.58($61a_u \rightarrow 74a_g$)[66%]-0.37($61b_g \rightarrow 74b_u$)[28%]	1.94	0.492	z
	$3A_u$	+0.43($73a_g \rightarrow 62a_u$)[37%]+0.52($73b_u \rightarrow 62b_g$)[55%]	2.94	0.049	z
	$3B_u$	-0.46($73a_g \rightarrow 74b_u$)[43%]+0.50($73b_u \rightarrow 74a_g$)[50%]	2.95	0.057	x+y
	$4A_u$	+0.53($72a_g \rightarrow 62a_u$)[57%]+0.32($73a_g \rightarrow 62a_u$)[21%]-0.30($73b_u \rightarrow 62b_g$)[19%]	3.25	0.004	z
	$4B_u$	+0.31($72a_g \rightarrow 74b_u$)[19%]+0.43($73a_g \rightarrow 74b_u$)[36%]+0.40($73b_u \rightarrow 74a_g$)[32%]	3.28	0.002	x+y
	$5A_u$	-0.36($72a_g \rightarrow 62a_u$)[26%]+0.40($73a_g \rightarrow 62a_u$)[33%]	3.31	0.005	z
	$5B_u$	-0.31($72b_u \rightarrow 74a_g$)[20%]+0.40($72a_g \rightarrow 74b_u$)[31%]-0.31($61b_g \rightarrow 63a_u$)[19%]	3.36	0.008	x+y
	$6A_u$	-0.35($60b_g \rightarrow 74b_u$)[24%]+0.43($72b_u \rightarrow 62b_g$)[38%]	3.36	0.003	z
	$6B_u$	-0.30($72b_u \rightarrow 74a_g$)[18%]+0.53($61b_g \rightarrow 63a_u$)[56%]	3.37	0.001	x+y
	$7B_u$	+0.36($72b_u \rightarrow 74a_g$)[26%]+0.40($72a_g \rightarrow 74b_u$)[31%]	3.40	0.001	x+y
	$8B_u$	-0.32($57a_u \rightarrow 62b_g$)[21%]+0.39($57b_g \rightarrow 62a_u$)[30%]	3.44	0.008	x+y
	$7A_u$	+0.31($57a_u \rightarrow 74a_g$)[19%]+0.42($57b_g \rightarrow 74b_u$)[35%]	3.45	0.010	z
	$8A_u$	+0.52($61b_g \rightarrow 75b_u$)[54%]	3.50	0.003	z
	$9B_u$	+0.32($61a_u \rightarrow 64b_g$)[21%]+0.52($61b_g \rightarrow 64a_u$)[54%]	3.52	0.012	x+y
	$10B_u$	-0.32($60a_u \rightarrow 62b_g$)[20%]+0.44($60b_g \rightarrow 62a_u$)[38%]	3.54	0.013	x+y
	$9A_u$	+0.39($69b_u \rightarrow 62b_g$)[30%]	3.54	0.004	z
	$11B_u$	+0.49($61a_u \rightarrow 63b_g$)[48%]	3.60	0.040	x+y

[a]Excitation energy in eV. [b]Oscillator strength. [c]Transition moment direction.

Table S7. Symmetry-allowed TD-M06 excited states of the Type 3 dimer.

	State	Main configuration(|C|≧0.30)	E^a	f^b	p^c
C_{2h}	$1B_u$	$+0.70(64b_g\rightarrow65a_u)[98\%]$	1.60	0.481	x+y
	$1A_u$	$+0.67(64b_g\rightarrow71b_u)[90\%]$	1.68	0.116	z
	$2A_u$	$+0.66(64a_u\rightarrow71a_g)[87\%]$	2.06	0.441	z
	$2B_u$	$+0.69(64a_u\rightarrow65b_g)[95\%]$	2.11	0.287	x+y
	$3A_u$	$+0.58(70a_g\rightarrow65a_u)[66\%]-0.37(70b_u\rightarrow65b_g)[27\%]$	2.83	0.050	z
	$3B_u$	$+0.43(70a_g\rightarrow71b_u)[37\%]+0.53(70b_u\rightarrow71a_g)[56\%]$	2.83	0.094	x+y
	$4B_u$	$+0.53(70a_g\rightarrow71b_u)[57\%]-0.44(70b_u\rightarrow71a_g)[38\%]$	3.15	0.013	x+y
	$4A_u$	$+0.38(70a_g\rightarrow65a_u)[29\%]+0.57(70b_u\rightarrow65b_g)[65\%]$	3.17	0.003	z
	$5B_u$	$+0.60(63b_g\rightarrow65a_u)[73\%]$	3.34	0.001	x+y
	$5A_u$	$+0.43(63a_u\rightarrow71a_g)[37\%]+0.48(63b_g\rightarrow71b_u)[46\%]$	3.37	0.000	z
	$6A_u$	$+0.65(64b_g\rightarrow72b_u)[84\%]$	3.38	0.004	z
	$6B_u$	$+0.37(62b_g\rightarrow65a_u)[28\%]+0.31(69a_g\rightarrow71b_u)[19\%]-0.30(64b_g\rightarrow66a_u)[19\%]$	3.40	0.000	x+y
	$7A_u$	$+0.31(62b_g\rightarrow71b_u)[20\%]+0.43(69a_g\rightarrow65a_u)[36\%]$	3.40	0.001	z
	$7B_u$	$+0.60(64b_g\rightarrow66a_u)[72\%]$	3.44	0.014	x+y
	$8A_u$	$+0.34(65a_g\rightarrow65a_u)[23\%]-0.30(65b_u\rightarrow65b_g)[18\%]$	3.49	0.009	z
	$8B_u$	$+0.39(65b_u\rightarrow71a_g)[30\%]$	3.50	0.010	x+y
	$9A_u$	$-0.35(64a_u\rightarrow72a_g)[24\%]+0.50(64b_g\rightarrow73b_u)[50\%]$	3.57	0.000	z
	$10A_u$	$-0.33(62a_u\rightarrow71a_g)[21\%]+0.34(69a_g\rightarrow65a_u)[23\%]$	3.58	0.004	z
	$9B_u$	$+0.38(62b_g\rightarrow65a_u)[30\%]+0.34(69b_u\rightarrow71a_g)[23\%]$	3.59	0.071	x+y
	$11A_u$	$+0.44(64a_u\rightarrow72a_g)[39\%]$	3.62	0.001	z

[a]Excitation energy in eV. [b]Oscillator strength. [c]Transition moment direction.

Table S8. Symmetry-allowed TD-M06 excited states of the Type 4 trimer.

	State	Main configuration(|C|≧0.30)	E^a	f^b	p^c
C_{4v}	1E	+0.69($27a_2$→127e)[96%]	0.786	0.0002	x+y
		+0.69($27a_2$→127e)[96%]	0.786	0.0002	x+y
	2E	+0.55($26a_2$→127e)[60%]+0.44($27a_2$→128e)[38%]	1.178	0.0001	x+y
		+0.55($26a_2$→127e)[60%]+0.44($27a_2$→128e)[38%]	1.178	0.0001	x+y
	3E	-0.43($26a_2$→127e)[37%]+0.54($27a_2$→128e)[59%]	1.272	0.001	x+y
		-0.43($26a_2$→127e)[37%]+0.54($27a_2$→128e)[59%]	1.272	0.001	x+y
	4E	-0.40($25a_2$→127e)[32%]+0.55($26a_2$→128e)[60%]	1.664	0.002	x+y
		-0.40($25a_2$→127e)[32%]+0.55($26a_2$→128e)[60%]	1.664	0.002	x+y
	5E	-0.45($25a_2$→127e)[40%]+0.48($27a_2$→129e)[47%]	1.736	0.007	x+y
		-0.45($25a_2$→127e)[40%]+0.48($27a_2$→129e)[47%]	1.736	0.007	x+y
	6E	+0.62($51a_1$→127e)[76%]	1.823	0.038	x+y
		+0.62($51a_1$→127e)[76%]	1.823	0.038	x+y
	7E	-0.35($50a_1$→127e)[24%]+0.31($26a_2$→128e)[19%]+0.36($27a_2$→129e)[26%]	1.964	0.318	x+y
		+0.35($50a_1$→127e)[24%]+0.31($26a_2$→128e)[19%]+0.36($27a_2$→129e)[26%]	1.964	0.318	x+y
	8E	+0.57($50a_1$→127e)[64%]	2.071	0.160	x+y
		+0.57($50a_1$→127e)[64%]	2.071	0.160	x+y
	9E	+0.58($25a_2$→128e)[67%]	2.148	0.001	x+y
		+0.58($25a_2$→128e)[67%]	2.148	0.001	x+y
	10E	-0.30($25a_2$→128e)[18%]+0.59($26a_2$→129e)[70%]	2.190	0.001	x+y
		-0.30($25a_2$→128e)[18%]+0.59($26a_2$→129e)[70%]	2.190	0.001	x+y
	11E	+0.60($51a_1$→128e)[72%]	2.233	0.079	x+y
		+0.60($51a_1$→128e)[72%]	2.233	0.079	x+y

12E	+0.66($50a_1$→$128e$)[86%]	2.538	0.0001	x+y
	+0.66($50a_1$→$128e$)[86%]	2.538	0.0001	x+y
13E	+0.67($51a_1$→$129e$)[89%]	2.583	0.005	x+y
	+0.67($51a_1$→$129e$)[89%]	2.583	0.005	x+y
14E	+0.55($49a_1$→$127e$)[60%]	2.845	0.003	x+y
	+0.55($49a_1$→$127e$)[60%]	2.845	0.003	x+y
15E	+0.51($48a_1$→$127e$)[53%]-0.35($49a_1$→$127e$)[24%]	2.857	0.001	x+y
	+0.51($48a_1$→$127e$)[53%]-0.35($49a_1$→$127e$)[24%]	2.857	0.001	x+y
$1A_1$	+0.43(126e→127e)[37%]-0.43(126e→127e)[37%]	2.884	0.001	z

[a]Excitation energy in eV. [b]Oscillator strength. [c]Transition moment direction.

Table S9. Symmetry-allowed TD-M06 excited states of the Type 5 trimer.

	State	Main configuration(|C|≧0.30)	E^a	f^b
C_1	1A	+0.69(402a→403a)[95%]	1.57	0.369
	2A	+0.42(402a→404a)[35%]+0.46(402a→405a)[43%]	1.61	0.008
	3A	+0.46(402a→404a)[42%]-0.31(402a→407a)[19%]	1.63	0.021
	4A	-0.40(402a→405a)[32%]+0.53(402a→406a)[56%]	1.64	0.018
	5A	+0.53(402a→407a)[57%]	1.67	0.046
	6A	+0.58(401a→403a)[68%]	1.68	0.063
	7A	-0.40(401a→405a)[31%]-0.31(401a→406a)[19%]+0.47(401a→407a)[44%]	1.74	0.006
	8A	+0.34(400a→403a)[23%]+0.60(402a→408a)[72%]	1.77	0.002
	9A	+0.35(400a→403a)[24%]+0.50(401a→406a)[51%]	1.85	0.213
	10A	+0.45(401a→405a)[40%]+0.46(401a→407a)[42%]	1.87	0.176
	11A	+0.49(400a→403a)[47%]-0.32(401a→406a)[20%]-0.32(402a→408a)[21%]	1.93	0.042
	12A	+0.33(400a→404a)[22%]+0.52(401a→404a)[54%]	1.95	0.005
	13A	-0.36(400a→404a)[26%]+0.47(401a→404a)[43%]	1.98	0.015
	14A	+0.64(401a→408a)[82%]	2.03	0.032
	15A	+0.46(400a→404a)[43%]+0.31(400a→405a)[19%]	2.05	0.469
	16A	+0.59(400a→406a)[70%]	2.10	0.015
	17A	+0.46(400a→405a)[42%]+0.47(400a→407a)[44%]	2.10	0.021
	18A	+0.67(400a→408a)[89%]	2.13	0.224
	19A	+0.63(399a→403a)[78%]	2.77	0.001
	20A	-0.34(399a→405a)[23%]+0.44(399a→407a)[38%]	2.82	0.015
	21A	+0.58(398a→403a)[67%]+0.32(399a→408a)[21%]	2.83	0.039
	22A	+0.51(398a→404a)[52%]-0.41(399a→404a)[33%]	2.85	0.070

23A	+0.44(397a→406a)[38%]+0.39(397a→407a)[30%]	2.94	0.024
24A	+0.48(397a→405a)[46%]-0.41(397a→406a)[33%]	2.94	0.030
25A	+0.41(398a→404a)[33%]+0.54(399a→404a)[58%]	3.14	0.004
26A	+0.32(399a→406a)[20%]+0.39(399a→407a)[30%]	3.15	0.001
27A	+0.53(399a→408a)[55%]	3.18	0.002
29A	-0.32(398a→405a)[21%]+0.35(398a→407a)[24%]	3.19	0.003
30A	+0.33(396a→403a)[21%]	3.20	0.005
31A	+0.62(402a→409a)[76%]	3.23	0.001
33A	+0.48(398a→408a)[46%]	3.26	0.003
34A	+0.44(396a→407a)[38%]+0.33(397a→403a)[22%]	3.26	0.003
35A	+0.39(397a→407a)[31%]	3.29	0.001
36A	+0.35(395a→403a)[24%]	3.33	0.005
37A	+0.43(402a→410a)[36%]	3.33	0.003
39A	+0.32(393a→403a)[21%]	3.34	0.003
40A	+0.32(393a→403a)[21%]	3.35	0.004

[a]Excitation energy in eV. [b]Oscillator strength. [c]Transition moment direction.

Table S10. Symmetry-allowed TD-M06 excited states of the Monomer.

	State	Main configuration(|C|≧0.30)	E^a	f^b	p^c
C_{4v}	1E	+0.69($13a_2$→34e)[97%]	1.82	0.547	x+y
		+0.69($13a_2$→34e)[97%]	1.82	0.547	x+y
	2E	+0.69($22a_1$→34e)[95%]	2.85	0.049	x+y
		+0.69($22a_1$→34e)[95%]	2.85	0.049	x+y
	3E	+0.60($14b_1$→34e)[72%]+0.35($15b_1$→34e)[25%]	3.52	0.019	x+y
		+0.60($14b_1$→34e)[72%]+0.35($15b_1$→34e)[25%]	3.52	0.019	x+y
	4E	+0.44($21a_1$→34e)[40%]+0.53($13a_2$→35e)[56%]	3.66	0.161	x+y
		+0.44($21a_1$→34e)[40%]+0.53($13a_2$→35e)[56%]	3.66	0.161	x+y
	$1A_1$	-0.31(32e→34e)[20%]-0.39(33e→34e)[30%]	3.67	0.001	z
	5E	+0.51($21a_1$→34e)[52%]-0.45($13a_2$→35e)[41%]	3.72	0.703	x+y
		+0.51($21a_1$→34e)[52%]-0.45($13a_2$→35e)[41%]	3.72	0.703	x+y
	$2A_1$	+0.37(32e→34e)[27%]-0.31(33e→34e)[19%]	3.76	0.007	z
	6E	-0.35($14b_1$→34e)[24%]+0.59($15b_1$→34e)[70%]	3.80	0.083	x+y
		-0.35($14b_1$→34e)[24%]+0.59($15b_1$→34e)[70%]	3.80	0.083	x+y
	$3A_1$	-0.47(31e→34e)[45%]+0.47(31e→34e)[45%]	4.02	0.010	z
	7E	+0.48($17b_2$→34e)[46%]+0.49($13a_2$→36e)[49%]	4.10	0.004	x+y
		-0.48($17b_2$→34e)[46%]+0.49($13a_2$→36e)[49%]	4.10	0.004	x+y
	8E	-0.45($17b_2$→34e)[40%]+0.50($13a_2$→36e)[49%]	4.12	0.024	x+y
		+0.45($17b_2$→34e)[40%]+0.50($13a_2$→36e)[49%]	4.12	0.024	x+y
	9E	+0.47($20a_1$→34e)[44%]+0.47($12a_2$→34e)[44%]	4.21	0.038	x+y
		+0.47($20a_1$→34e)[44%]-0.47($12a_2$→34e)[44%]	4.21	0.098	x+y
	10E	-0.45($20a_1$→34e)[40%]+0.50($12a_2$→34e)[50%]	4.37	0.098	x+y

+0.45($20a_1 \rightarrow 34e$)[40%]+0.50($12a_2 \rightarrow 34e$)[50%]	4.37	0.043	x+y

[a]Excitation energy in eV. [b]Oscillator strength. [c]Transition moment direction.

Table S11. Geometry optimized coordinates for the PbPc monomer.

82	0	0.00000000	0.00000000	1.27463300
7	0	0.00000000	1.99704600	0.05417600
7	0	1.99704600	0.00000000	0.05417600
7	0	-1.99704600	0.00000000	0.05417600
7	0	0.00000000	-1.99704600	0.05417600
7	0	2.37809400	2.37809400	-0.14132800
7	0	-2.37809400	2.37809400	-0.14132800
7	0	2.37809400	-2.37809400	-0.14132800
7	0	-2.37809400	-2.37809400	-0.14132800
6	0	1.11374100	2.76655000	-0.11911600
6	0	2.76655000	-1.11374100	-0.11911600
6	0	-2.76655000	1.11374100	-0.11911600
6	0	-1.11374100	-2.76655000	-0.11911600
6	0	-1.11374100	2.76655000	-0.11911600
6	0	2.76655000	1.11374100	-0.11911600
6	0	-2.76655000	-1.11374100	-0.11911600
6	0	1.11374100	-2.76655000	-0.11911600
6	0	0.70091600	4.13569500	-0.36824800
6	0	4.13569500	-0.70091600	-0.36824800
6	0	-4.13569500	0.70091600	-0.36824800
6	0	-0.70091600	-4.13569500	-0.36824800
6	0	-0.70091600	4.13569500	-0.36824800
6	0	4.13569500	0.70091600	-0.36824800
6	0	-4.13569500	-0.70091600	-0.36824800
6	0	0.70091600	-4.13569500	-0.36824800
6	0	1.39401700	5.31678700	-0.58316200
6	0	-1.39401700	5.31678700	-0.58316200
6	0	5.31678700	-1.39401700	-0.58316200
6	0	5.31678700	1.39401700	-0.58316200
6	0	-5.31678700	1.39401700	-0.58316200
6	0	-5.31678700	-1.39401700	-0.58316200
6	0	-1.39401700	-5.31678700	-0.58316200
6	0	1.39401700	-5.31678700	-0.58316200
6	0	0.70156800	6.49676800	-0.79787300
6	0	-0.70156800	6.49676800	-0.79787300
6	0	6.49676800	-0.70156800	-0.79787300
6	0	6.49676800	0.70156800	-0.79787300

6	0	-6.49676800	0.70156800	-0.79787300
6	0	-6.49676800	-0.70156800	-0.79787300
6	0	-0.70156800	-6.49676800	-0.79787300
6	0	0.70156800	-6.49676800	-0.79787300
1	0	1.24507400	7.42294000	-0.96640100
1	0	-1.24507400	7.42294000	-0.96640100
1	0	2.48253900	5.31678700	-0.58316200
1	0	-2.48253900	5.31678700	-0.58316200
1	0	5.31678700	-2.48253900	-0.58316200
1	0	5.31678700	2.48253900	-0.58316200
1	0	7.42294000	-1.24507400	-0.96640100
1	0	7.42294000	1.24507400	-0.96640100
1	0	-5.31678700	2.48253900	-0.58316200
1	0	-5.31678700	-2.48253900	-0.58316200
1	0	-7.42294000	1.24507400	-0.96640100
1	0	-7.42294000	-1.24507400	-0.96640100
1	0	-2.48253900	-5.31678700	-0.58316200
1	0	2.48253900	-5.31678700	-0.58316200
1	0	-1.24507400	-7.42294000	-0.96640100
1	0	1.24507400	-7.42294000	-0.96640100

Table S12. Geometry optimized coordinates for the Type 1 dimer.

82	0	0.00000000	0.00000000	3.10255100
7	0	0.00000000	1.99700000	1.88205100
7	0	1.99700000	0.00000000	1.88205100
7	0	-1.99700000	0.00000000	1.88205100
7	0	0.00000000	-1.99700000	1.88205100
7	0	2.37807100	2.37807100	1.68655100
7	0	-2.37807100	2.37807100	1.68655100
7	0	2.37807100	-2.37807100	1.68655100
7	0	-2.37807100	-2.37807100	1.68655100
6	0	1.11373300	2.76653400	1.70885100
6	0	2.76653400	-1.11373300	1.70885100
6	0	-2.76653400	1.11373300	1.70885100
6	0	-1.11373300	-2.76653400	1.70885100
6	0	-1.11373300	2.76653400	1.70885100
6	0	2.76653400	1.11373300	1.70885100
6	0	-2.76653400	-1.11373300	1.70885100
6	0	1.11373300	-2.76653400	1.70885100
6	0	0.70092400	4.13572400	1.45965100
6	0	4.13572400	-0.70092400	1.45965100
6	0	-4.13572400	0.70092400	1.45965100
6	0	-0.70092400	-4.13572400	1.45965100
6	0	-0.70092400	4.13572400	1.45965100
6	0	4.13572400	0.70092400	1.45965100
6	0	-4.13572400	-0.70092400	1.45965100
6	0	0.70092400	-4.13572400	1.45965100
6	0	1.39402400	5.31680600	1.24468800
6	0	-1.39402400	5.31680600	1.24468800
6	0	5.31680600	-1.39402400	1.24468800
6	0	5.31680600	1.39402400	1.24468800
6	0	-5.31680600	1.39402400	1.24468800
6	0	-5.31680600	-1.39402400	1.24468800
6	0	-1.39402400	-5.31680600	1.24468800
6	0	1.39402400	-5.31680600	1.24468800
6	0	0.70157400	6.49678000	1.02992600
6	0	-0.70157400	6.49678000	1.02992600
6	0	6.49678000	-0.70157400	1.02992600
6	0	6.49678000	0.70157400	1.02992600

6	0	-6.49678000	0.70157400	1.02992600
6	0	-6.49678000	-0.70157400	1.02992600
6	0	-0.70157400	-6.49678000	1.02992600
6	0	0.70157400	-6.49678000	1.02992600
1	0	1.24507400	7.42293400	0.86136100
1	0	-1.24507400	7.42293400	0.86136100
1	0	2.48252400	5.31680600	1.24468800
1	0	-2.48252400	5.31680600	1.24468800
1	0	5.31680600	-2.48252400	1.24468800
1	0	5.31680600	2.48252400	1.24468800
1	0	7.42293400	-1.24507400	0.86136100
1	0	7.42293400	1.24507400	0.86136100
1	0	-5.31680600	2.48252400	1.24468800
1	0	-5.31680600	-2.48252400	1.24468800
1	0	-7.42293400	1.24507400	0.86136100
1	0	-7.42293400	-1.24507400	0.86136100
1	0	-2.48252400	-5.31680600	1.24468800
1	0	2.48252400	-5.31680600	1.24468800
1	0	-1.24507400	-7.42293400	0.86136100
1	0	1.24507400	-7.42293400	0.86136100
82	0	0.00000000	0.00000000	-0.55321800
7	0	0.00000000	1.99700000	-1.77371800
7	0	1.99700000	0.00000000	-1.77371800
7	0	-1.99700000	0.00000000	-1.77371800
7	0	0.00000000	-1.99700000	-1.77371800
7	0	2.37807100	2.37807100	-1.96921800
7	0	-2.37807100	2.37807100	-1.96921800
7	0	2.37807100	-2.37807100	-1.96921800
7	0	-2.37807100	-2.37807100	-1.96921800
6	0	1.11373300	2.76653400	-1.94691800
6	0	2.76653400	-1.11373300	-1.94691800
6	0	-2.76653400	1.11373300	-1.94691800
6	0	-1.11373300	-2.76653400	-1.94691800
6	0	-1.11373300	2.76653400	-1.94691800
6	0	2.76653400	1.11373300	-1.94691800
6	0	-2.76653400	-1.11373300	-1.94691800
6	0	1.11373300	-2.76653400	-1.94691800
6	0	0.70092400	4.13572400	-2.19611800
6	0	4.13572400	-0.70092400	-2.19611800

6	0	-4.13572400	0.70092400	-2.19611800
6	0	-0.70092400	-4.13572400	-2.19611800
6	0	-0.70092400	4.13572400	-2.19611800
6	0	4.13572400	0.70092400	-2.19611800
6	0	-4.13572400	-0.70092400	-2.19611800
6	0	0.70092400	-4.13572400	-2.19611800
6	0	1.39402400	5.31680600	-2.41108100
6	0	-1.39402400	5.31680600	-2.41108100
6	0	5.31680600	-1.39402400	-2.41108100
6	0	5.31680600	1.39402400	-2.41108100
6	0	-5.31680600	1.39402400	-2.41108100
6	0	-5.31680600	-1.39402400	-2.41108100
6	0	-1.39402400	-5.31680600	-2.41108100
6	0	1.39402400	-5.31680600	-2.41108100
6	0	0.70157400	6.49678000	-2.62584300
6	0	-0.70157400	6.49678000	-2.62584300
6	0	6.49678000	-0.70157400	-2.62584300
6	0	6.49678000	0.70157400	-2.62584300
6	0	-6.49678000	0.70157400	-2.62584300
6	0	-6.49678000	-0.70157400	-2.62584300
6	0	-0.70157400	-6.49678000	-2.62584300
6	0	0.70157400	-6.49678000	-2.62584300
1	0	1.24507400	7.42293400	-2.79440800
1	0	-1.24507400	7.42293400	-2.79440800
1	0	2.48252400	5.31680600	-2.41108100
1	0	-2.48252400	5.31680600	-2.41108100
1	0	5.31680600	-2.48252400	-2.41108100
1	0	5.31680600	2.48252400	-2.41108100
1	0	7.42293400	-1.24507400	-2.79440800
1	0	7.42293400	1.24507400	-2.79440800
1	0	-5.31680600	2.48252400	-2.41108100
1	0	-5.31680600	-2.48252400	-2.41108100
1	0	-7.42293400	1.24507400	-2.79440800
1	0	-7.42293400	-1.24507400	-2.79440800
1	0	-2.48252400	-5.31680600	-2.41108100
1	0	2.48252400	-5.31680600	-2.41108100
1	0	-1.24507400	-7.42293400	-2.79440800
1	0	1.24507400	-7.42293400	-2.79440800

Table S13. Geometry optimized coordinates for the Type 2 dimer.

82	0	3.23963700	2.32528400	0.00000000
7	0	2.01913700	0.32828400	0.00000000
7	0	2.01913700	2.32528400	1.99700000
7	0	2.01913700	2.32528400	-1.99700000
7	0	2.01913700	4.32228400	0.00000000
7	0	1.82363700	-0.05278700	2.37807100
7	0	1.82363700	-0.05278700	-2.37807100
7	0	1.82363700	4.70335400	2.37807100
7	0	1.82363700	4.70335400	-2.37807100
6	0	1.84593700	-0.44125100	1.11373300
6	0	1.84593700	3.43901700	2.76653400
6	0	1.84593700	1.21155100	-2.76653400
6	0	1.84593700	5.09181800	-1.11373300
6	0	1.84593700	-0.44125100	-1.11373300
6	0	1.84593700	1.21155100	2.76653400
6	0	1.84593700	3.43901700	-2.76653400
6	0	1.84593700	5.09181800	1.11373300
6	0	1.59673700	-1.81044100	0.70092400
6	0	1.59673700	3.02620700	4.13572400
6	0	1.59673700	1.62436000	-4.13572400
6	0	1.59673700	6.46100800	-0.70092400
6	0	1.59673700	-1.81044100	-0.70092400
6	0	1.59673700	1.62436000	4.13572400
6	0	1.59673700	3.02620700	-4.13572400
6	0	1.59673700	6.46100800	0.70092400
6	0	1.38177400	-2.99152200	1.39402400
6	0	1.38177400	-2.99152200	-1.39402400
6	0	1.38177400	3.71930700	5.31680600
6	0	1.38177400	0.93126000	5.31680600
6	0	1.38177400	0.93126000	-5.31680600
6	0	1.38177400	3.71930700	-5.31680600
6	0	1.38177400	7.64208900	-1.39402400
6	0	1.38177400	7.64208900	1.39402400
6	0	1.16701200	-4.17149600	0.70157400
6	0	1.16701200	-4.17149600	-0.70157400
6	0	1.16701200	3.02685700	6.49678000
6	0	1.16701200	1.62371000	6.49678000

6	0	1.16701200	1.62371000	-6.49678000
6	0	1.16701200	3.02685700	-6.49678000
6	0	1.16701200	8.82206300	-0.70157400
6	0	1.16701200	8.82206300	0.70157400
1	0	0.99844700	-5.09765100	1.24507400
1	0	0.99844700	-5.09765100	-1.24507400
1	0	1.38177400	-2.99152200	2.48252400
1	0	1.38177400	-2.99152200	-2.48252400
1	0	1.38177400	4.80780700	5.31680600
1	0	1.38177400	-0.15724000	5.31680600
1	0	0.99844700	3.57035700	7.42293400
1	0	0.99844700	1.08021000	7.42293400
1	0	1.38177400	-0.15724000	-5.31680600
1	0	1.38177400	4.80780700	-5.31680600
1	0	0.99844700	1.08021000	-7.42293400
1	0	0.99844700	3.57035700	-7.42293400
1	0	1.38177400	7.64208900	-2.48252400
1	0	1.38177400	7.64208900	2.48252400
1	0	0.99844700	9.74821800	-1.24507400
1	0	0.99844700	9.74821800	1.24507400
82	0	-3.23963700	-2.32528400	0.00000000
7	0	-2.01913700	-0.32828400	0.00000000
7	0	-2.01913700	-2.32528400	1.99700000
7	0	-2.01913700	-2.32528400	-1.99700000
7	0	-2.01913700	-4.32228400	0.00000000
7	0	-1.82363700	0.05278700	2.37807100
7	0	-1.82363700	0.05278700	-2.37807100
7	0	-1.82363700	-4.70335400	2.37807100
7	0	-1.82363700	-4.70335400	-2.37807100
6	0	-1.84593700	0.44125100	1.11373300
6	0	-1.84593700	-3.43901700	2.76653400
6	0	-1.84593700	-1.21155100	-2.76653400
6	0	-1.84593700	-5.09181800	-1.11373300
6	0	-1.84593700	0.44125100	-1.11373300
6	0	-1.84593700	-1.21155100	2.76653400
6	0	-1.84593700	-3.43901700	-2.76653400
6	0	-1.84593700	-5.09181800	1.11373300
6	0	-1.59673700	1.81044100	0.70092400
6	0	-1.59673700	-3.02620700	4.13572400

6	0	-1.59673700	-1.62436000	-4.13572400
6	0	-1.59673700	-6.46100800	-0.70092400
6	0	-1.59673700	1.81044100	-0.70092400
6	0	-1.59673700	-1.62436000	4.13572400
6	0	-1.59673700	-3.02620700	-4.13572400
6	0	-1.59673700	-6.46100800	0.70092400
6	0	-1.38177400	2.99152200	1.39402400
6	0	-1.38177400	2.99152200	-1.39402400
6	0	-1.38177400	-3.71930700	5.31680600
6	0	-1.38177400	-0.93126000	5.31680600
6	0	-1.38177400	-0.93126000	-5.31680600
6	0	-1.38177400	-3.71930700	-5.31680600
6	0	-1.38177400	-7.64208900	-1.39402400
6	0	-1.38177400	-7.64208900	1.39402400
6	0	-1.16701200	4.17149600	0.70157400
6	0	-1.16701200	4.17149600	-0.70157400
6	0	-1.16701200	-3.02685700	6.49678000
6	0	-1.16701200	-1.62371000	6.49678000
6	0	-1.16701200	-1.62371000	-6.49678000
6	0	-1.16701200	-3.02685700	-6.49678000
6	0	-1.16701200	-8.82206300	-0.70157400
6	0	-1.16701200	-8.82206300	0.70157400
1	0	-0.99844700	5.09765100	1.24507400
1	0	-0.99844700	5.09765100	-1.24507400
1	0	-1.38177400	2.99152200	2.48252400
1	0	-1.38177400	2.99152200	-2.48252400
1	0	-1.38177400	-4.80780700	5.31680600
1	0	-1.38177400	0.15724000	5.31680600
1	0	-0.99844700	-3.57035700	7.42293400
1	0	-0.99844700	-1.08021000	7.42293400
1	0	-1.38177400	0.15724000	-5.31680600
1	0	-1.38177400	-4.80780700	-5.31680600
1	0	-0.99844700	-1.08021000	-7.42293400
1	0	-0.99844700	-3.57035700	-7.42293400
1	0	-1.38177400	-7.64208900	-2.48252400
1	0	-1.38177400	-7.64208900	2.48252400
1	0	-0.99844700	-9.74821800	-1.24507400
1	0	-0.99844700	-9.74821800	1.24507400

Table S14. Geometry optimized coordinates for the Type 3 dimer.

82	0	0.13747700	3.09432900	0.00000000
7	0	1.35797700	1.68223700	1.41209200
7	0	1.35797700	1.68223700	-1.41209200
7	0	1.35797700	4.50642100	1.41209200
7	0	1.35797700	4.50642100	-1.41209200
7	0	1.55347700	-0.26877100	0.00000000
7	0	1.55347700	3.09432900	3.36310000
7	0	1.55347700	3.09432900	-3.36310000
7	0	1.55347700	6.45742900	0.00000000
6	0	1.53117700	0.35056600	1.16870700
6	0	1.53117700	1.92562200	-2.74376300
6	0	1.53117700	4.26303600	2.74376300
6	0	1.53117700	5.83809200	-1.16870700
6	0	1.53117700	1.92562200	2.74376300
6	0	1.53117700	0.35056600	-1.16870700
6	0	1.53117700	5.83809200	1.16870700
6	0	1.53117700	4.26303600	-2.74376300
6	0	1.78037700	-0.32569700	2.42877100
6	0	1.78037700	0.66555800	-3.42002600
6	0	1.78037700	5.52310000	3.42002600
6	0	1.78037700	6.51435600	-2.42877100
6	0	1.78037700	0.66555800	3.42002600
6	0	1.78037700	-0.32569700	-2.42877100
6	0	1.78037700	6.51435600	2.42877100
6	0	1.78037700	5.52310000	-3.42002600
6	0	1.99534000	-1.65094400	2.77382600
6	0	1.99534000	0.32050300	4.74527300
6	0	1.99534000	0.32050300	-4.74527300
6	0	1.99534000	-1.65094400	-2.77382600
6	0	1.99534000	5.86815500	4.74527300
6	0	1.99534000	7.83960200	2.77382600
6	0	1.99534000	7.83960200	-2.77382600
6	0	1.99534000	5.86815500	-4.74527300
6	0	2.21010200	-1.99567500	4.09782900
6	0	2.21010200	-1.00350000	5.09000400
6	0	2.21010200	-1.00350000	-5.09000400
6	0	2.21010200	-1.99567500	-4.09782900

6	0	2.21010200	7.19215900	5.09000400
6	0	2.21010200	8.18433400	4.09782900
6	0	2.21010200	8.18433400	-4.09782900
6	0	2.21010200	7.19215900	-5.09000400
1	0	2.37866700	-3.03487800	4.36840700
1	0	2.37866700	-1.27407800	6.12920700
1	0	1.99534000	-2.42062900	2.00414000
1	0	1.99534000	1.09018900	5.51495900
1	0	1.99534000	1.09018900	-5.51495900
1	0	1.99534000	-2.42062900	-2.00414000
1	0	2.37866700	-1.27407800	-6.12920700
1	0	2.37866700	-3.03487800	-4.36840700
1	0	1.99534000	5.09846900	5.51495900
1	0	1.99534000	8.60928800	2.00414000
1	0	2.37866700	7.46273600	6.12920700
1	0	2.37866700	9.22353600	4.36840700
1	0	1.99534000	8.60928800	-2.00414000
1	0	1.99534000	5.09846900	-5.51495900
1	0	2.37866700	9.22353600	-4.36840700
1	0	2.37866700	7.46273600	-6.12920700
82	0	-0.13747700	-3.09432900	0.00000000
7	0	-1.35797700	-4.50642100	1.41209200
7	0	-1.35797700	-1.68223700	1.41209200
7	0	-1.35797700	-4.50642100	-1.41209200
7	0	-1.35797700	-1.68223700	-1.41209200
7	0	-1.55347700	-3.09432900	3.36310000
7	0	-1.55347700	-6.45742900	0.00000000
7	0	-1.55347700	0.26877100	0.00000000
7	0	-1.55347700	-3.09432900	-3.36310000
6	0	-1.53117700	-4.26303600	2.74376300
6	0	-1.53117700	-0.35056600	1.16870700
6	0	-1.53117700	-5.83809200	-1.16870700
6	0	-1.53117700	-1.92562200	-2.74376300
6	0	-1.53117700	-5.83809200	1.16870700
6	0	-1.53117700	-1.92562200	2.74376300
6	0	-1.53117700	-4.26303600	-2.74376300
6	0	-1.53117700	-0.35056600	-1.16870700
6	0	-1.78037700	-5.52310000	3.42002600
6	0	-1.78037700	0.32569700	2.42877100

6	0	-1.78037700	-6.51435600	-2.42877100
6	0	-1.78037700	-0.66555800	-3.42002600
6	0	-1.78037700	-6.51435600	2.42877100
6	0	-1.78037700	-0.66555800	3.42002600
6	0	-1.78037700	-5.52310000	-3.42002600
6	0	-1.78037700	0.32569700	-2.42877100
6	0	-1.99534000	-5.86815500	4.74527300
6	0	-1.99534000	-7.83960200	2.77382600
6	0	-1.99534000	1.65094400	2.77382600
6	0	-1.99534000	-0.32050300	4.74527300
6	0	-1.99534000	-7.83960200	-2.77382600
6	0	-1.99534000	-5.86815500	-4.74527300
6	0	-1.99534000	-0.32050300	-4.74527300
6	0	-1.99534000	1.65094400	-2.77382600
6	0	-2.21010200	-7.19215900	5.09000400
6	0	-2.21010200	-8.18433400	4.09782900
6	0	-2.21010200	1.99567500	4.09782900
6	0	-2.21010200	1.00350000	5.09000400
6	0	-2.21010200	-8.18433400	-4.09782900
6	0	-2.21010200	-7.19215900	-5.09000400
6	0	-2.21010200	1.00350000	-5.09000400
6	0	-2.21010200	1.99567500	-4.09782900
1	0	-2.37866700	-7.46273600	6.12920700
1	0	-2.37866700	-9.22353600	4.36840700
1	0	-1.99534000	-5.09846900	5.51495900
1	0	-1.99534000	-8.60928800	2.00414000
1	0	-1.99534000	2.42062900	2.00414000
1	0	-1.99534000	-1.09018900	5.51495900
1	0	-2.37866700	3.03487800	4.36840700
1	0	-2.37866700	1.27407800	6.12920700
1	0	-1.99534000	-8.60928800	-2.00414000
1	0	-1.99534000	-5.09846900	-5.51495900
1	0	-2.37866700	-9.22353600	-4.36840700
1	0	-2.37866700	-7.46273600	-6.12920700
1	0	-1.99534000	-1.09018900	-5.51495900
1	0	-1.99534000	2.42062900	-2.00414000
1	0	-2.37866700	1.27407800	-6.12920700
1	0	-2.37866700	3.03487800	-4.36840700

Table S15. Geometry optimized coordinates for the Type 4 trimer.

82	0	0.00000000	0.00000000	4.92956900
7	0	0.00000000	1.99700000	3.70906900
7	0	1.99700000	0.00000000	3.70906900
7	0	-1.99700000	0.00000000	3.70906900
7	0	0.00000000	-1.99700000	3.70906900
7	0	2.37807100	2.37807100	3.51356900
7	0	-2.37807100	2.37807100	3.51356900
7	0	2.37807100	-2.37807100	3.51356900
7	0	-2.37807100	-2.37807100	3.51356900
6	0	1.11373300	2.76653400	3.53586900
6	0	2.76653400	-1.11373300	3.53586900
6	0	-2.76653400	1.11373300	3.53586900
6	0	-1.11373300	-2.76653400	3.53586900
6	0	-1.11373300	2.76653400	3.53586900
6	0	2.76653400	1.11373300	3.53586900
6	0	-2.76653400	-1.11373300	3.53586900
6	0	1.11373300	-2.76653400	3.53586900
6	0	0.70092400	4.13572400	3.28666900
6	0	4.13572400	-0.70092400	3.28666900
6	0	-4.13572400	0.70092400	3.28666900
6	0	-0.70092400	-4.13572400	3.28666900
6	0	-0.70092400	4.13572400	3.28666900
6	0	4.13572400	0.70092400	3.28666900
6	0	-4.13572400	-0.70092400	3.28666900
6	0	0.70092400	-4.13572400	3.28666900
6	0	1.39402400	5.31680600	3.07170600
6	0	-1.39402400	5.31680600	3.07170600
6	0	5.31680600	-1.39402400	3.07170600
6	0	5.31680600	1.39402400	3.07170600
6	0	-5.31680600	1.39402400	3.07170600
6	0	-5.31680600	-1.39402400	3.07170600
6	0	-1.39402400	-5.31680600	3.07170600
6	0	1.39402400	-5.31680600	3.07170600
6	0	0.70157400	6.49678000	2.85694400
6	0	-0.70157400	6.49678000	2.85694400
6	0	6.49678000	-0.70157400	2.85694400
6	0	6.49678000	0.70157400	2.85694400

6	0	-6.49678000	0.70157400	2.85694400
6	0	-6.49678000	-0.70157400	2.85694400
6	0	-0.70157400	-6.49678000	2.85694400
6	0	0.70157400	-6.49678000	2.85694400
1	0	1.24507400	7.42293400	2.68837900
1	0	-1.24507400	7.42293400	2.68837900
1	0	2.48252400	5.31680600	3.07170600
1	0	-2.48252400	5.31680600	3.07170600
1	0	5.31680600	-2.48252400	3.07170600
1	0	5.31680600	2.48252400	3.07170600
1	0	7.42293400	-1.24507400	2.68837900
1	0	7.42293400	1.24507400	2.68837900
1	0	-5.31680600	2.48252400	3.07170600
1	0	-5.31680600	-2.48252400	3.07170600
1	0	-7.42293400	1.24507400	2.68837900
1	0	-7.42293400	-1.24507400	2.68837900
1	0	-2.48252400	-5.31680600	3.07170600
1	0	2.48252400	-5.31680600	3.07170600
1	0	-1.24507400	-7.42293400	2.68837900
1	0	1.24507400	-7.42293400	2.68837900
82	0	0.00000000	0.00000000	1.27518500
7	0	0.00000000	1.99700000	0.05468500
7	0	1.99700000	0.00000000	0.05468500
7	0	-1.99700000	0.00000000	0.05468500
7	0	0.00000000	-1.99700000	0.05468500
7	0	2.37807100	2.37807100	-0.14081500
7	0	-2.37807100	2.37807100	-0.14081500
7	0	2.37807100	-2.37807100	-0.14081500
7	0	-2.37807100	-2.37807100	-0.14081500
7	0	1.11373300	2.76653400	-0.11851500
7	0	2.76653400	-1.11373300	-0.11851500
6	0	-2.76653400	1.11373300	-0.11851500
6	0	-1.11373300	-2.76653400	-0.11851500
6	0	-1.11373300	2.76653400	-0.11851500
6	0	2.76653400	1.11373300	-0.11851500
6	0	-2.76653400	-1.11373300	-0.11851500
6	0	1.11373300	-2.76653400	-0.11851500
6	0	0.70092400	4.13572400	-0.36771500
6	0	4.13572400	-0.70092400	-0.36771500

6	0	-4.13572400	0.70092400	-0.36771500
6	0	-0.70092400	-4.13572400	-0.36771500
6	0	-0.70092400	4.13572400	-0.36771500
6	0	4.13572400	0.70092400	-0.36771500
6	0	-4.13572400	-0.70092400	-0.36771500
6	0	0.70092400	-4.13572400	-0.36771500
6	0	1.39402400	5.31680600	-0.58267800
6	0	-1.39402400	5.31680600	-0.58267800
6	0	5.31680600	-1.39402400	-0.58267800
6	0	5.31680600	1.39402400	-0.58267800
6	0	-5.31680600	1.39402400	-0.58267800
6	0	-5.31680600	-1.39402400	-0.58267800
6	0	-1.39402400	-5.31680600	-0.58267800
6	0	1.39402400	-5.31680600	-0.58267800
6	0	0.70157400	6.49678000	-0.79744000
6	0	-0.70157400	6.49678000	-0.79744000
6	0	6.49678000	-0.70157400	-0.79744000
6	0	6.49678000	0.70157400	-0.79744000
6	0	-6.49678000	0.70157400	-0.79744000
6	0	-6.49678000	-0.70157400	-0.79744000
6	0	-0.70157400	-6.49678000	-0.79744000
6	0	0.70157400	-6.49678000	-0.79744000
1	0	1.24507400	7.42293400	-0.96600500
1	0	-1.24507400	7.42293400	-0.96600500
1	0	2.48252400	5.31680600	-0.58267800
1	0	-2.48252400	5.31680600	-0.58267800
1	0	5.31680600	-2.48252400	-0.58267800
1	0	5.31680600	2.48252400	-0.58267800
1	0	7.42293400	-1.24507400	-0.96600500
1	0	7.42293400	1.24507400	-0.96600500
1	0	-5.31680600	2.48252400	-0.58267800
1	0	-5.31680600	-2.48252400	-0.58267800
1	0	-7.42293400	1.24507400	-0.96600500
1	0	-7.42293400	-1.24507400	-0.96600500
1	0	-2.48252400	-5.31680600	-0.58267800
1	0	2.48252400	-5.31680600	-0.58267800
1	0	-1.24507400	-7.42293400	-0.96600500
1	0	1.24507400	-7.42293400	-0.96600500
82	0	0.00000000	0.00000000	-2.38075400

7	0	0.00000000	1.99700000	-3.60125400
7	0	1.99700000	0.00000000	-3.60125400
7	0	-1.99700000	0.00000000	-3.60125400
7	0	0.00000000	-1.99700000	-3.60125400
7	0	2.37807100	2.37807100	-3.79675400
7	0	-2.37807100	2.37807100	-3.79675400
7	0	2.37807100	-2.37807100	-3.79675400
7	0	-2.37807100	-2.37807100	-3.79675400
6	0	1.11373300	2.76653400	-3.77445400
6	0	2.76653400	-1.11373300	-3.77445400
6	0	-2.76653400	1.11373300	-3.77445400
6	0	-1.11373300	-2.76653400	-3.77445400
6	0	-1.11373300	2.76653400	-3.77445400
6	0	2.76653400	1.11373300	-3.77445400
6	0	-2.76653400	-1.11373300	-3.77445400
6	0	1.11373300	-2.76653400	-3.77445400
6	0	0.70092400	4.13572400	-4.02365400
6	0	4.13572400	-0.70092400	-4.02365400
6	0	-4.13572400	0.70092400	-4.02365400
6	0	-0.70092400	-4.13572400	-4.02365400
6	0	-0.70092400	4.13572400	-4.02365400
6	0	4.13572400	0.70092400	-4.02365400
6	0	-4.13572400	-0.70092400	-4.02365400
6	0	0.70092400	-4.13572400	-4.02365400
6	0	1.39402400	5.31680600	-4.23861800
6	0	-1.39402400	5.31680600	-4.23861800
6	0	5.31680600	-1.39402400	-4.23861800
6	0	5.31680600	1.39402400	-4.23861800
6	0	-5.31680600	1.39402400	-4.23861800
6	0	-5.31680600	-1.39402400	-4.23861800
6	0	-1.39402400	-5.31680600	-4.23861800
6	0	1.39402400	-5.31680600	-4.23861800
6	0	0.70157400	6.49678000	-4.45337900
6	0	-0.70157400	6.49678000	-4.45337900
6	0	6.49678000	-0.70157400	-4.45337900
6	0	6.49678000	0.70157400	-4.45337900
6	0	-6.49678000	0.70157400	-4.45337900
6	0	-6.49678000	-0.70157400	-4.45337900
6	0	-0.70157400	-6.49678000	-4.45337900

6	0	0.70157400	-6.49678000	-4.45337900
1	0	1.24507400	7.42293400	-4.62194400
1	0	-1.24507400	7.42293400	-4.62194400
1	0	2.48252400	5.31680600	-4.23861800
1	0	-2.48252400	5.31680600	-4.23861800
1	0	5.31680600	-2.48252400	-4.23861800
1	0	5.31680600	2.48252400	-4.23861800
1	0	7.42293400	-1.24507400	-4.62194400
1	0	7.42293400	1.24507400	-4.62194400
1	0	-5.31680600	2.48252400	-4.23861800
1	0	-5.31680600	-2.48252400	-4.23861800
1	0	-7.42293400	1.24507400	-4.62194400
1	0	-7.42293400	-1.24507400	-4.62194400
1	0	-2.48252400	-5.31680600	-4.23861800
1	0	2.48252400	-5.31680600	-4.23861800
1	0	-1.24507400	-7.42293400	-4.62194400
1	0	1.24507400	-7.42293400	-4.62194400

Table S16. Geometry optimized coordinates for the Type 5 trimer.

82	0	-0.21688300	1.47701500	1.63116100
7	0	-0.48234900	-0.40053300	0.25931200
7	0	-1.29444900	2.24615900	-0.29883800
7	0	1.92563400	0.57232000	1.36890400
7	0	1.11353400	3.21901200	0.81075300
7	0	-2.46659400	0.23988900	-0.96187100
7	0	1.36795000	-1.75335500	1.02411200
7	0	-0.56618100	4.55012200	-0.30520300
7	0	3.26836300	2.55687700	1.68078100
6	0	-1.61219400	-0.64078500	-0.46753900
6	0	-1.39429300	3.56836000	-0.62194700
6	0	2.17660400	-0.76911700	1.38091100
6	0	2.39450500	3.44002800	1.22650300
6	0	0.18365600	-1.57429100	0.46256600
6	0	-2.28432200	1.54972900	-0.92948700
6	0	3.06663300	1.24951400	1.68845200
6	0	0.59865500	4.37353400	0.29639800
6	0	-1.71774200	-2.06845000	-0.70801200
6	0	-2.55440100	3.75422700	-1.47447000
6	0	3.55415200	-0.98266100	1.78582200
6	0	2.71749300	4.84001600	1.01936400
6	0	-0.58753100	-2.65594800	-0.12265400
6	0	-3.11453800	2.48380900	-1.66801900
6	0	4.11428900	0.28775700	1.97937200
6	0	1.58728200	5.42751400	0.43400600
6	0	-2.65468200	-2.86026600	-1.35355100
6	0	-0.40687500	-4.02870500	-0.18936800
6	0	-3.13589900	4.86538600	-2.06500800
6	0	-4.24992000	2.33873100	-2.44994600
6	0	4.32321700	-2.11769400	1.99024400
6	0	5.43723700	0.40896100	2.37518300
6	0	3.84199900	5.60795800	1.27878700
6	0	1.59419200	6.77639700	0.11460500
6	0	-2.47419500	-4.23173600	-1.42020300
6	0	-1.34293500	-4.81977900	-0.83430200
6	0	-4.27021700	4.72044400	-2.84620200
6	0	-4.83087200	3.44884800	-3.03993100

6	0	5.64492500	-1.99660400	2.38568400
6	0	6.20558100	-0.72500800	2.57941300
6	0	3.84890300	6.95557600	0.95968600
6	0	2.71764400	7.54361900	0.37378500
1	0	-3.20890400	-4.85264600	-1.92640800
1	0	-1.20127200	-5.89623800	-0.88661700
1	0	-3.53226300	-2.40408800	-1.80806700
1	0	0.47070700	-4.48488300	0.26514800
1	0	-2.70096700	5.85183500	-1.91472100
1	0	-4.68485200	1.35228200	-2.60023300
1	0	-4.72620300	5.59176900	-3.30927700
1	0	-5.72119200	3.33508400	-3.65308500
1	0	3.88828500	-3.10414300	1.83995800
1	0	5.87217000	1.39540900	2.52546900
1	0	6.24799300	-2.88665000	2.54598300
1	0	7.24298200	-0.62996500	2.88979200
1	0	4.71958100	5.15178000	1.73330300
1	0	0.71661100	7.23257500	-0.33991100
1	0	4.73069400	7.55776500	1.16311400
1	0	2.72306300	8.60135700	0.12332400
82	0	-5.67593000	-0.66696500	-0.59254900
7	0	-7.00634700	-2.40896100	0.22785900
7	0	-4.59836400	-1.43610900	1.33745100
7	0	-7.81844600	0.23773100	-0.33029100
7	0	-5.41046300	1.21058300	0.77930000
7	0	-5.32663100	-3.74007100	1.34381500
7	0	-9.16117500	-1.74682600	-0.64216800
7	0	-3.42621900	0.57016100	2.00048400
7	0	-7.26076300	2.56340600	0.01450000
6	0	-6.49146800	-3.56348300	0.74221400
6	0	-3.60849100	-0.73967800	1.96810000
6	0	-8.95944600	-0.43946400	-0.64983900
6	0	-6.07646800	2.38434100	0.57604600
6	0	-8.28731800	-2.62997800	-0.18789100
6	0	-4.49852000	-2.75830900	1.66055900
6	0	-8.06941700	1.57916700	-0.34229900
6	0	-4.28061900	1.45083600	1.50615100
6	0	-7.48009400	-4.61746300	0.60460600
6	0	-2.77827500	-1.67375900	2.70663200

6	0	-10.00710100	0.52229300	-0.94075900
6	0	-5.30528200	3.46599800	1.16126600
6	0	-8.61030600	-4.02996500	0.01924800
6	0	-3.33841100	-2.94417600	2.51308200
6	0	-9.44696500	1.79271100	-0.74721000
6	0	-4.17507000	2.87850000	1.74662400
6	0	-7.48700500	-5.96634700	0.92400700
6	0	-9.73481200	-4.79790800	-0.24017500
6	0	-1.64289300	-1.52868000	3.48855900
6	0	-2.75691300	-4.05533600	3.10362000
6	0	-11.33005000	0.40108900	-1.33657000
6	0	-10.21603000	2.92774500	-0.95163200
6	0	-5.48593800	4.83875600	1.22798100
6	0	-3.23813100	3.67031700	2.39216300
6	0	-8.61045700	-6.73356900	0.66482800
6	0	-9.74171600	-6.14552600	0.07892700
6	0	-1.06194000	-2.63879800	4.07854300
6	0	-1.62259600	-3.91039400	3.88481400
6	0	-12.09839300	1.53505900	-1.54080100
6	0	-11.53773800	2.80665500	-1.34707200
6	0	-4.54987700	5.62983000	1.87291500
6	0	-3.41861800	5.04178700	2.45881500
1	0	-8.61587500	-7.79130600	0.91528900
1	0	-10.62350700	-6.74771400	-0.12450200
1	0	-6.60942300	-6.42252400	1.37852300
1	0	-10.61239300	-4.34173000	-0.69469100
1	0	-1.20796100	-0.54223200	3.63884500
1	0	-3.19184500	-5.04178400	2.95333400
1	0	-0.17162100	-2.52503300	4.69169800
1	0	-1.16661000	-4.78171800	4.34788900
1	0	-11.76498200	-0.58535900	-1.48685700
1	0	-9.78109700	3.91419300	-0.80134500
1	0	-13.13579500	1.44001600	-1.85117900
1	0	-12.14080600	3.69670100	-1.50737100
1	0	-6.36351900	5.29493300	0.77346500
1	0	-2.36054900	3.21413900	2.84667900
1	0	-4.69154000	6.70628900	1.92523000
1	0	-2.68390900	5.66269600	2.96502000
82	0	6.44891900	-0.88083400	-2.18338800

7	0	7.52648600	-1.64997800	-0.25338800
7	0	6.71438600	0.99671400	-0.81153900
7	0	5.11850300	-2.62283100	-1.36298000
7	0	4.30640300	0.02386200	-1.92113000
7	0	8.69863100	0.35629200	0.40964500
7	0	6.79821800	-3.95394100	-0.24702400
7	0	4.86408600	2.34953600	-1.57633900
7	0	2.96367400	-1.96069600	-2.23300700
6	0	8.51635900	-0.95354800	0.37726100
6	0	6.04838100	2.17047200	-1.01479300
6	0	5.63338100	-3.77735300	-0.84862500
6	0	3.16540400	-0.65333300	-2.24067800
6	0	7.62633000	-2.97217900	0.06972000
6	0	7.84423100	1.23696600	-0.08468800
6	0	3.83753200	-2.84384700	-1.77873000
6	0	4.05543300	1.36529800	-1.93313800
6	0	9.34657400	-1.88762800	1.11579300
6	0	6.81956800	3.25212900	-0.42957300
6	0	4.64475500	-4.83133300	-0.98623300
6	0	2.11774800	0.30842400	-2.53159800
6	0	8.78643800	-3.15804600	0.92224300
6	0	7.94977900	2.66463100	0.15578500
6	0	3.51454400	-4.24383500	-1.57159100
6	0	2.67788400	1.57884200	-2.33804900
6	0	10.48195600	-1.74255000	1.89772000
6	0	9.36793600	-4.26920500	1.51278100
6	0	6.63891100	4.62488600	-0.36285800
6	0	8.88671900	3.45644700	0.80132400
6	0	4.63784500	-6.18021600	-0.66683200
6	0	2.39003700	-5.01177700	-1.83101400
6	0	0.79479900	0.18722000	-2.92740900
6	0	1.90882000	2.71387500	-2.54247100
6	0	11.06290900	-2.85266700	2.48770400
6	0	10.50225300	-4.12426300	2.29397500
6	0	7.57497200	5.41596000	0.28207600
6	0	8.70623200	4.82791700	0.86797600
6	0	3.51439300	-6.94743800	-0.92601100
6	0	2.38313300	-6.35939500	-1.51191200
6	0	0.02645600	1.32118900	-3.13164000

6	0	0.58711200	2.59278500	-2.93791100
1	0	11.95322800	-2.73890300	3.10085900
1	0	10.95824000	-4.99558800	2.75705000
1	0	10.91688900	-0.75610100	2.04800600
1	0	8.93300400	-5.25565300	1.36249500
1	0	5.76133000	5.08106400	-0.81737400
1	0	9.76430000	3.00027000	1.25584000
1	0	7.43330900	6.49241900	0.33439100
1	0	9.44094000	5.44882700	1.37418100
1	0	5.51542600	-6.63639400	-0.21231600
1	0	1.51245600	-4.55559900	-2.28553000
1	0	3.50897400	-8.00517600	-0.67555000
1	0	1.50134300	-6.96158400	-1.71534100
1	0	0.35986700	-0.79922800	-3.07769600
1	0	2.34375200	3.70032400	-2.39218400
1	0	-1.01094500	1.22614600	-3.44201800
1	0	-0.01595700	3.48283100	-3.09821000