Structure, Stability and Electronic Properties of One-Dimensional Tetrathia- and Tetraselena[8]circulene-based Materials: A Comparative DFT Study

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Electronic Supplementary Information

List of Content

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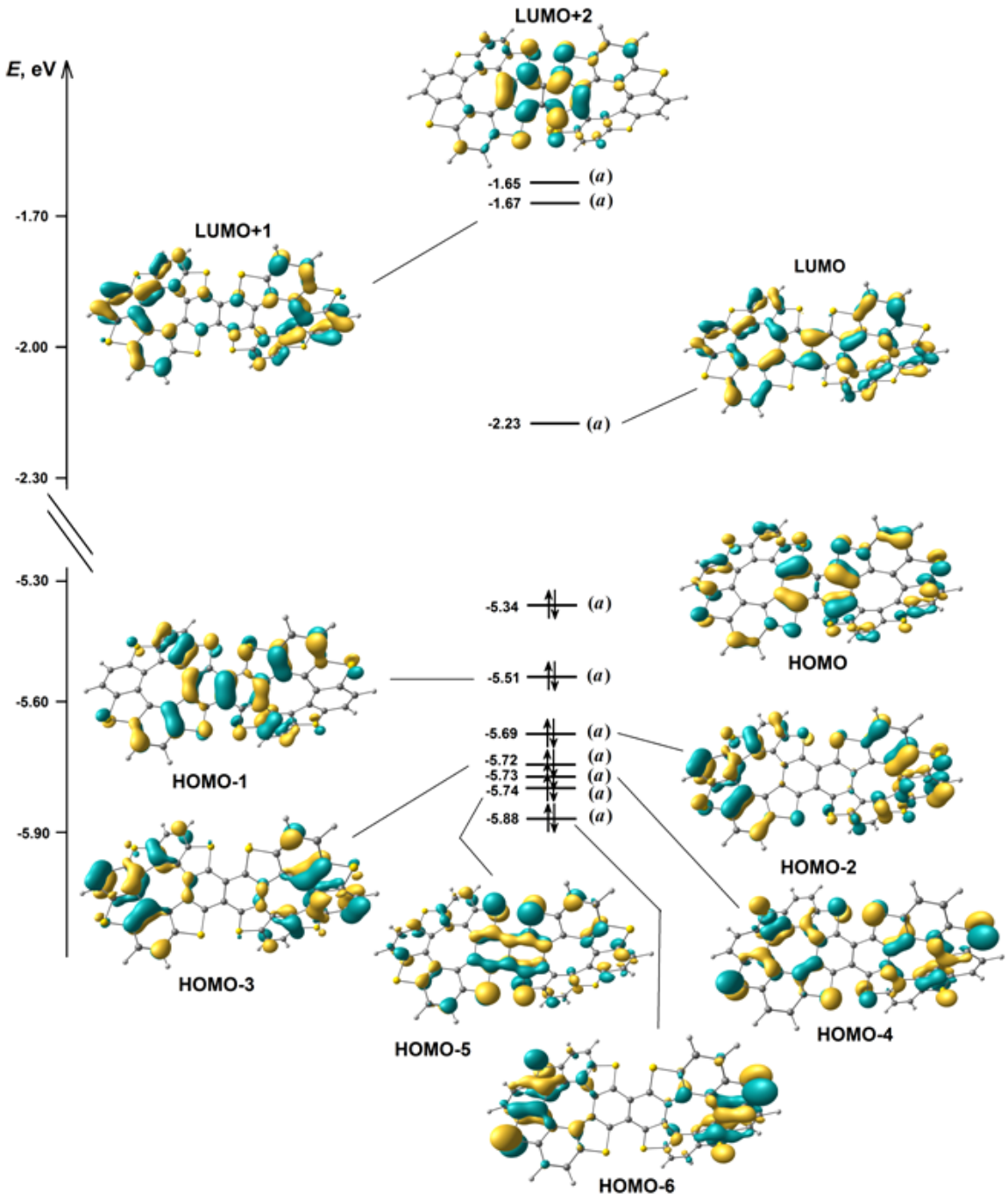

Figure S1. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=2 (type **I**) calculated at the B3LYP/6-31G(d) level of theory.

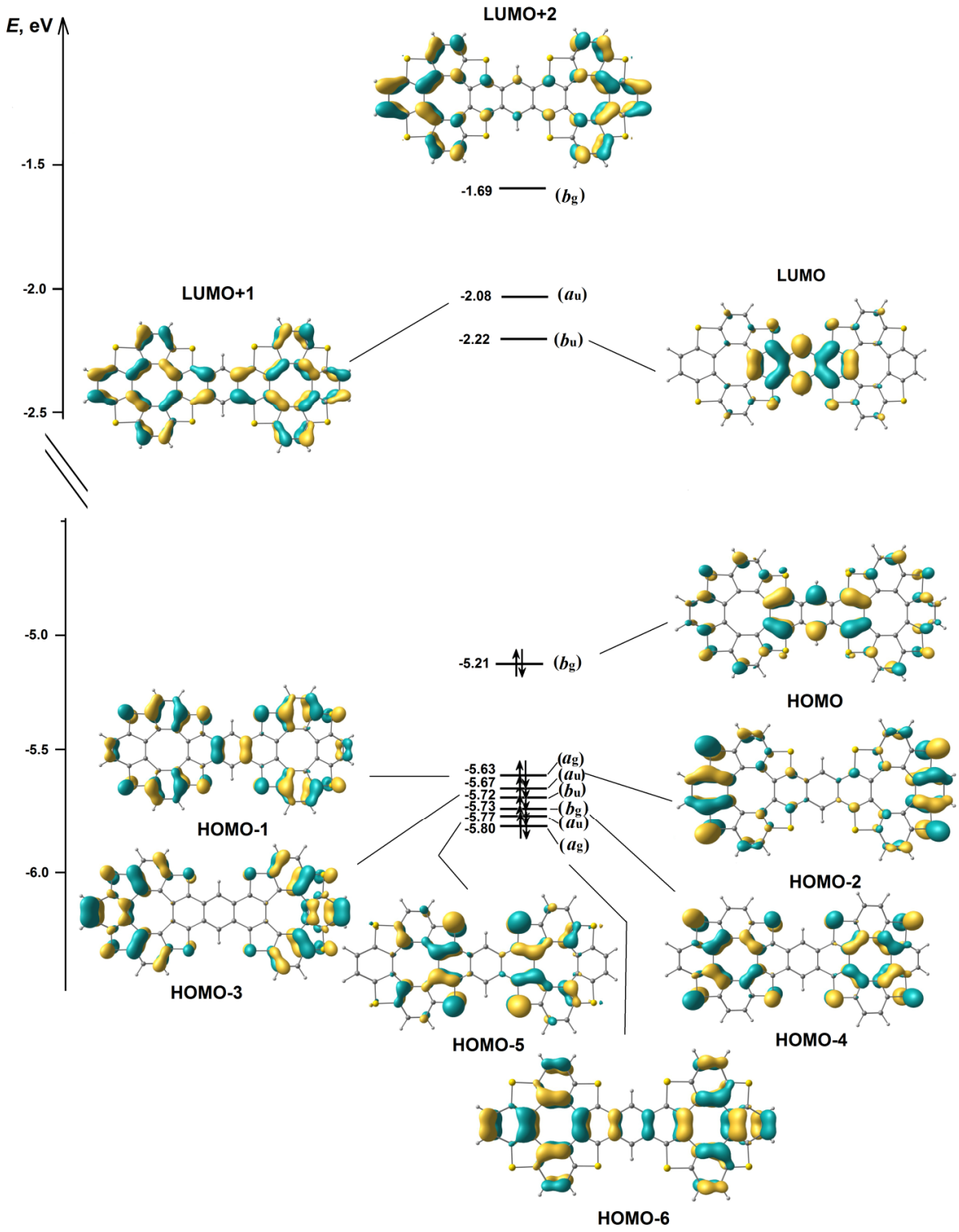

Figure S2. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=2 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.

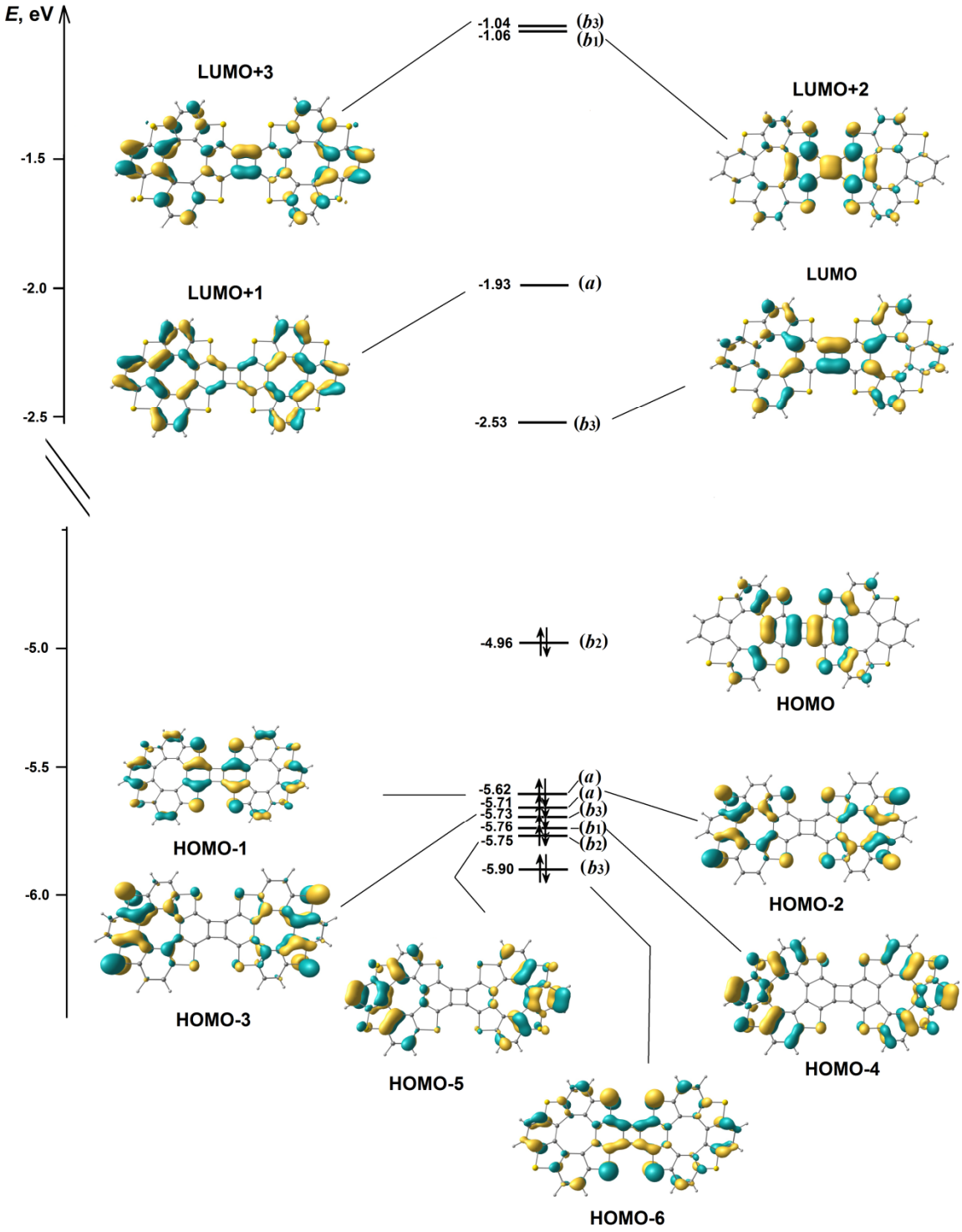

Figure S3. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=2 (type **III**) calculated at the B3LYP/6-31G(d) level of theory.

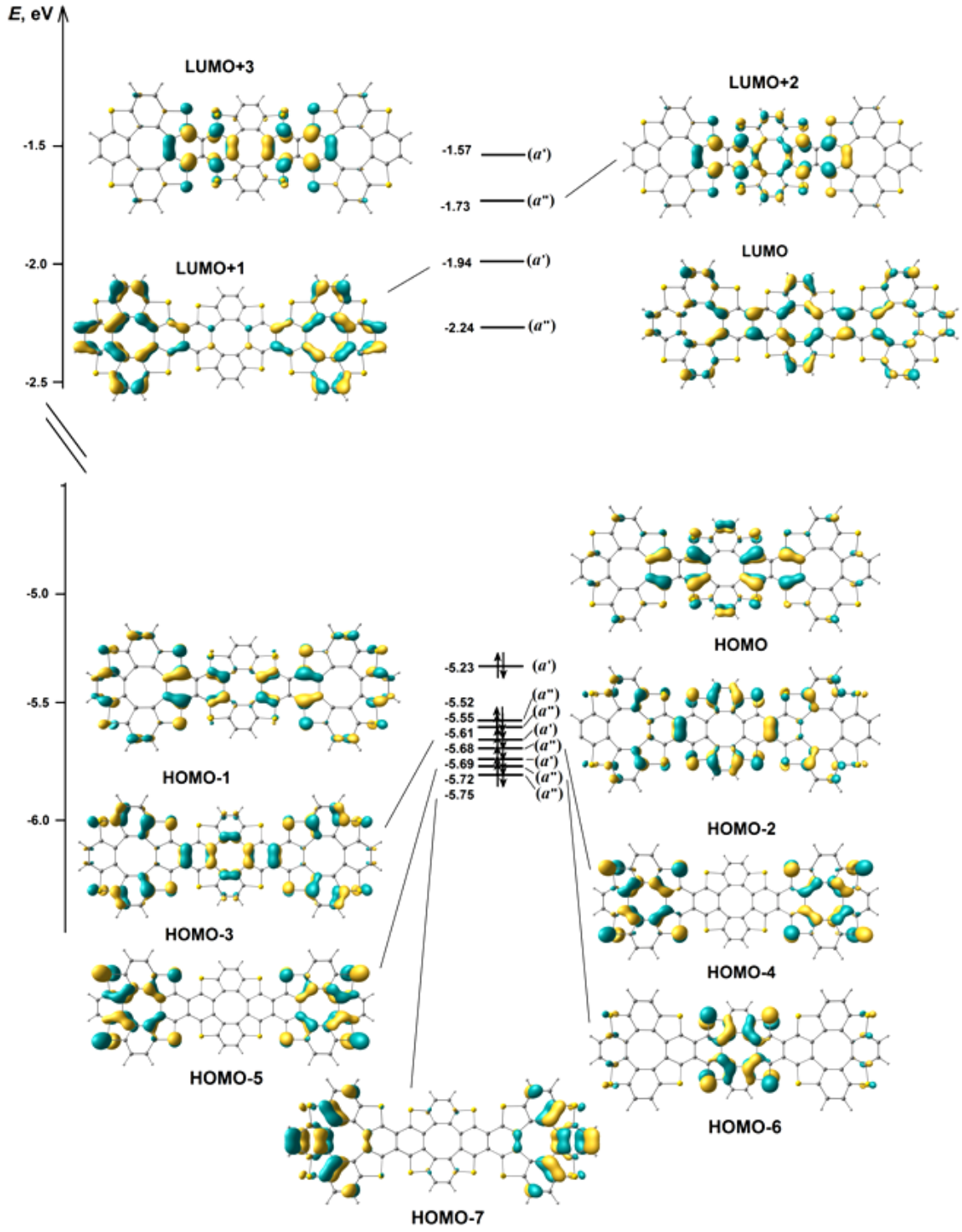

Figure S4. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=3 (type **I**) calculated at the B3LYP/6-31G(d) level of theory.

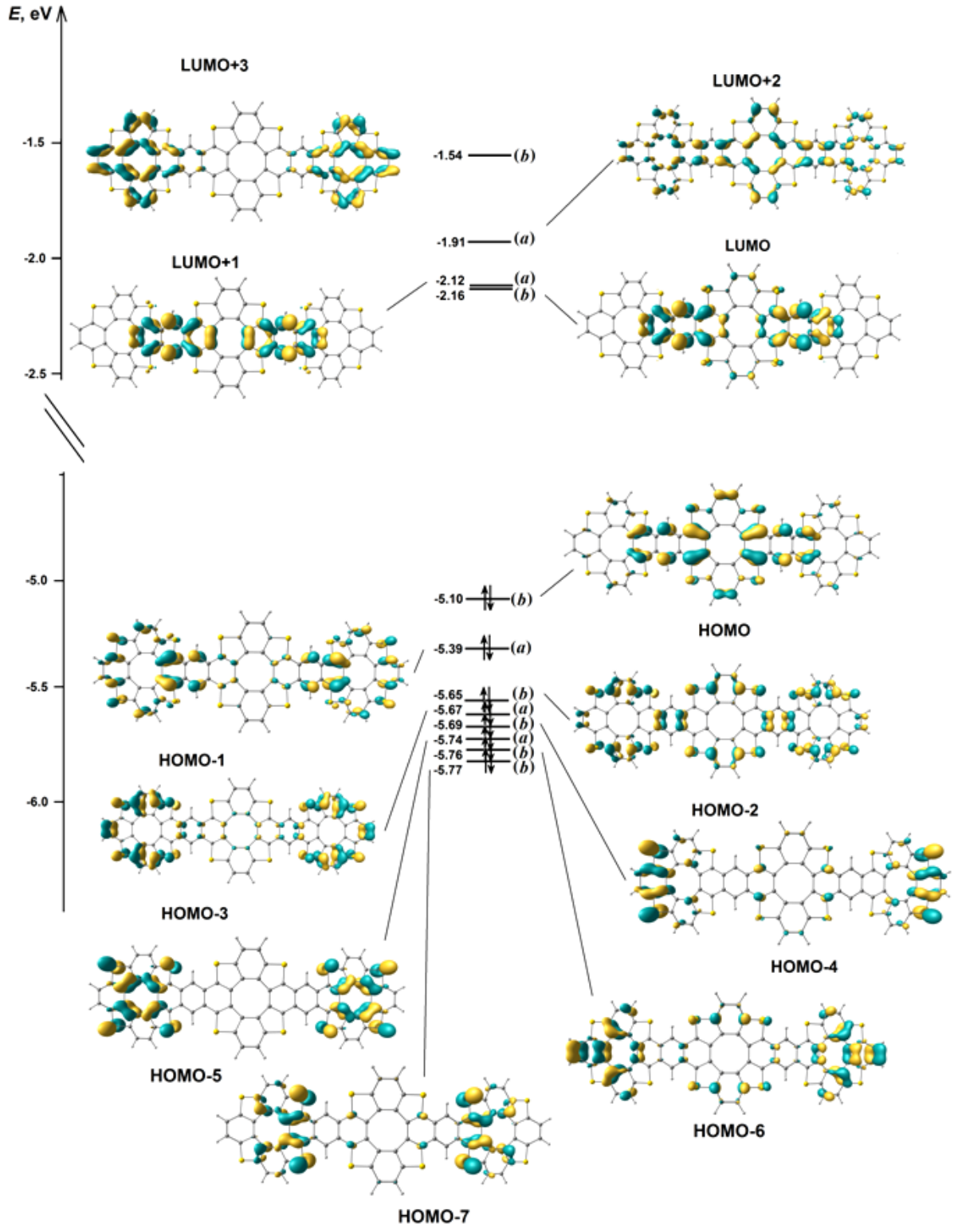

Figure S5. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=3 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.

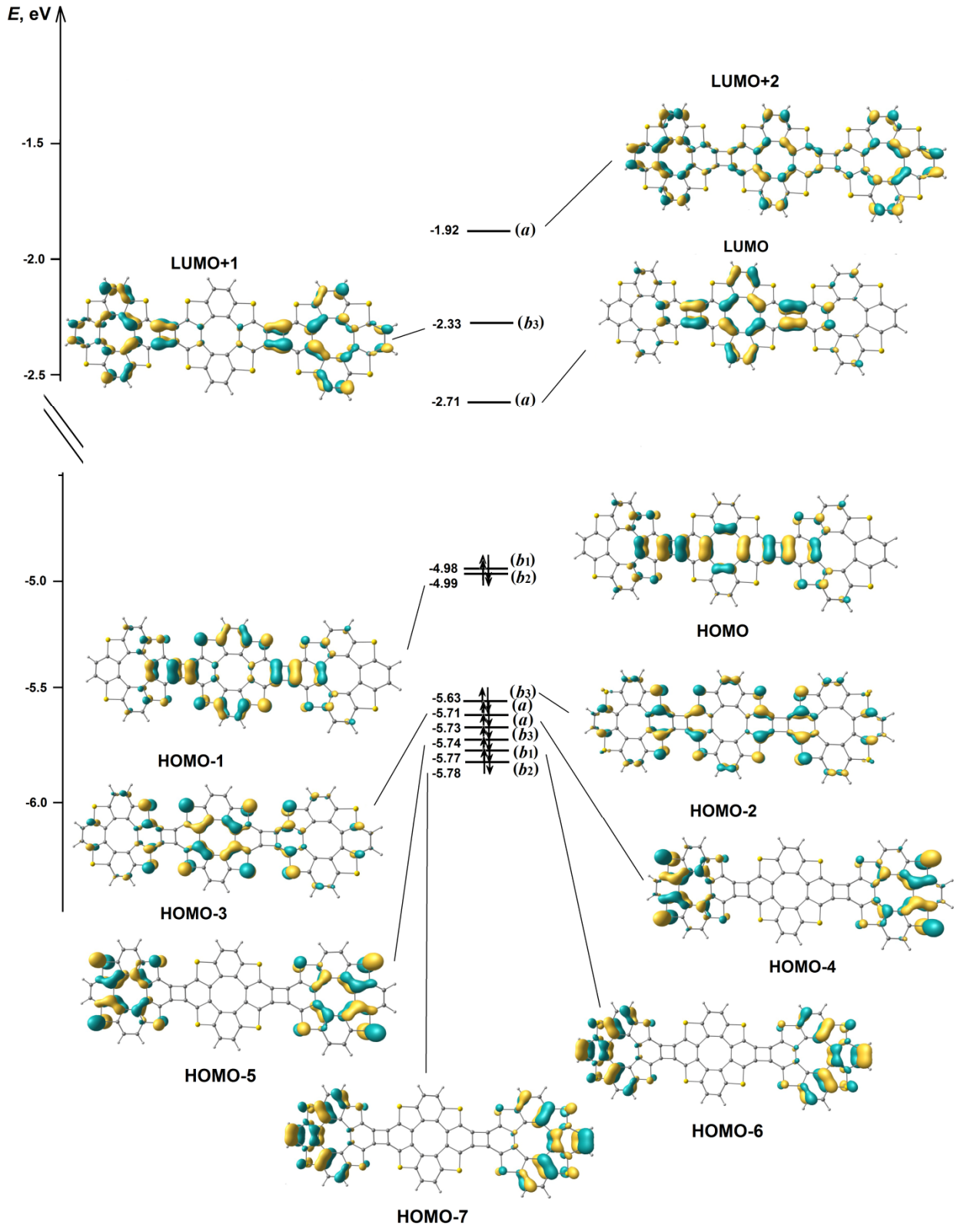

Figure S6. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=3 (type **III**) calculated at the B3LYP/6-31G(d) level of theory.

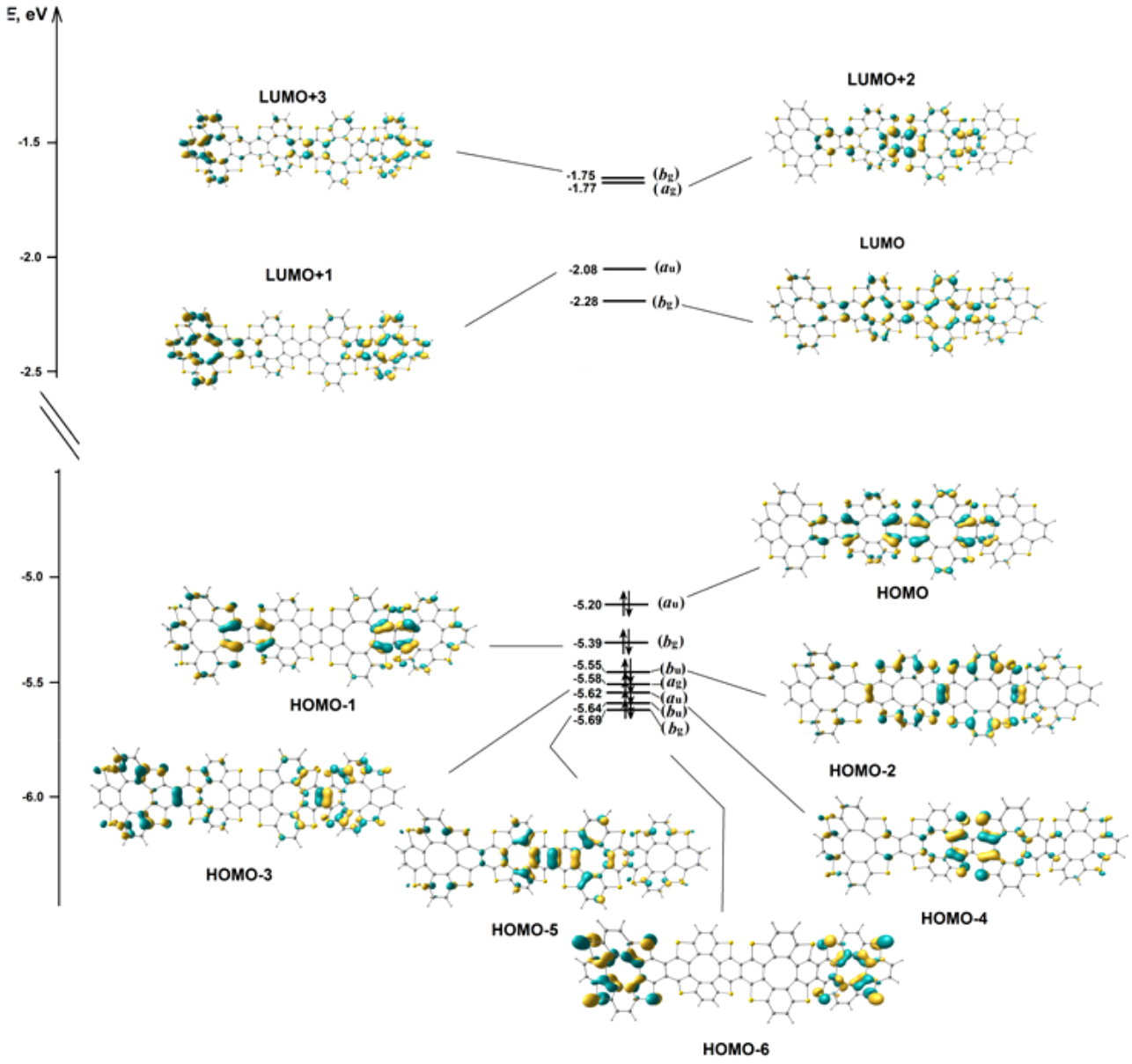

Figure S7. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=4 (type **I**) calculated at the B3LYP/6-31G(d) level of theory.

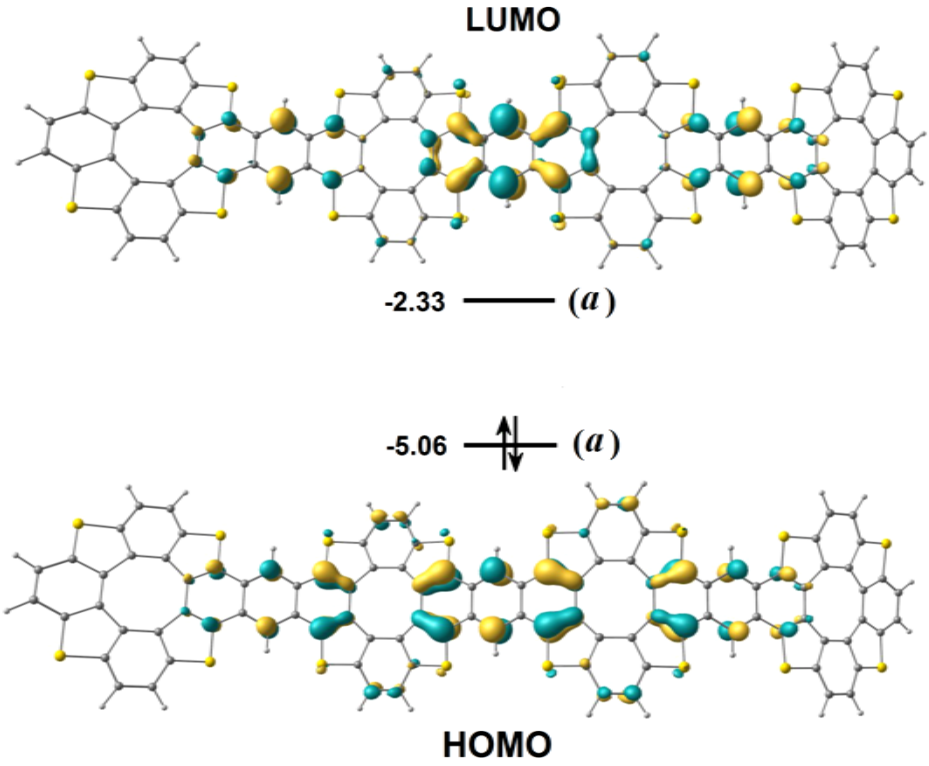

Figure S8. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=4 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.

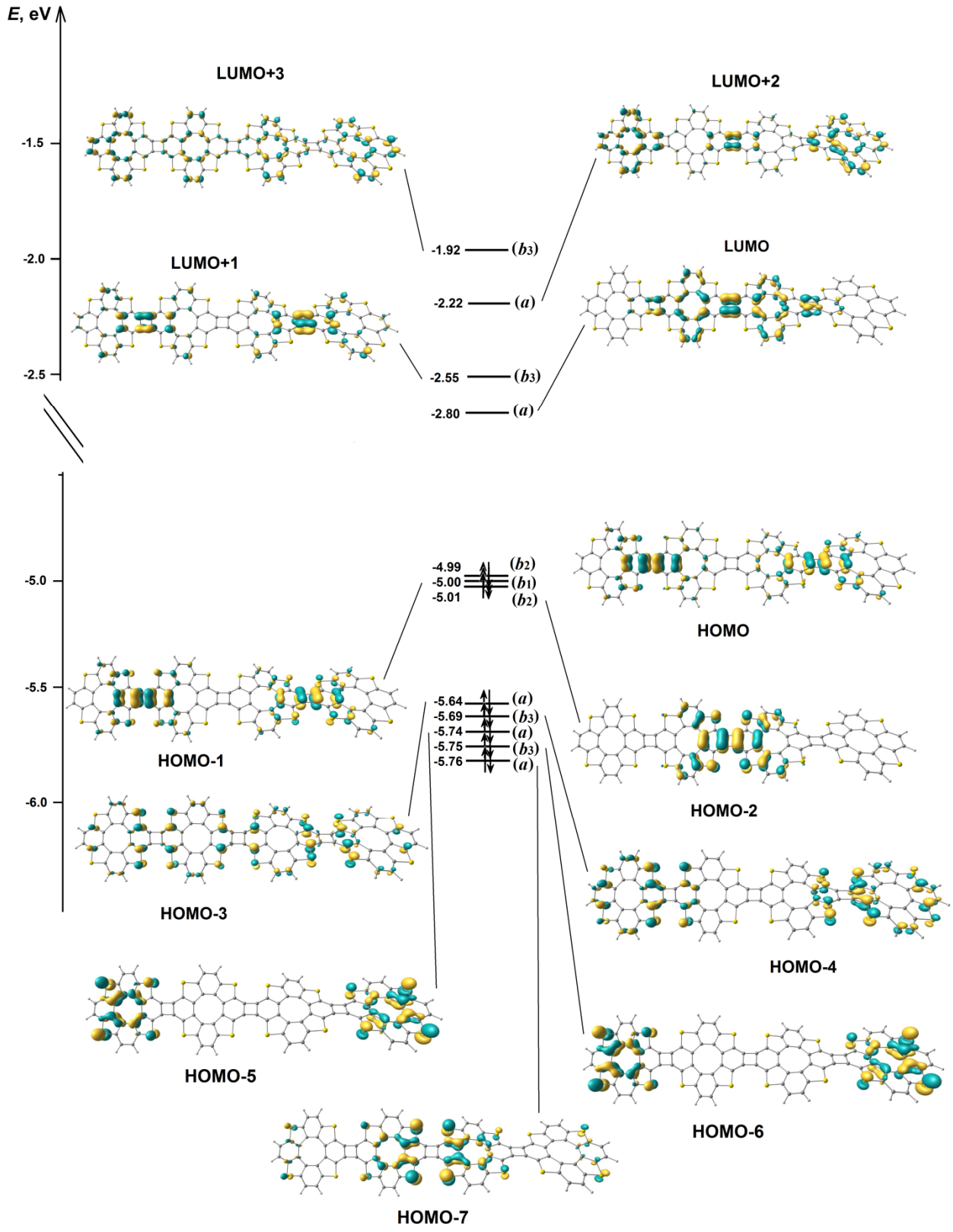

Figure S9. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=4 (type **III**) calculated at the B3LYP/6-31G(d) level of theory.

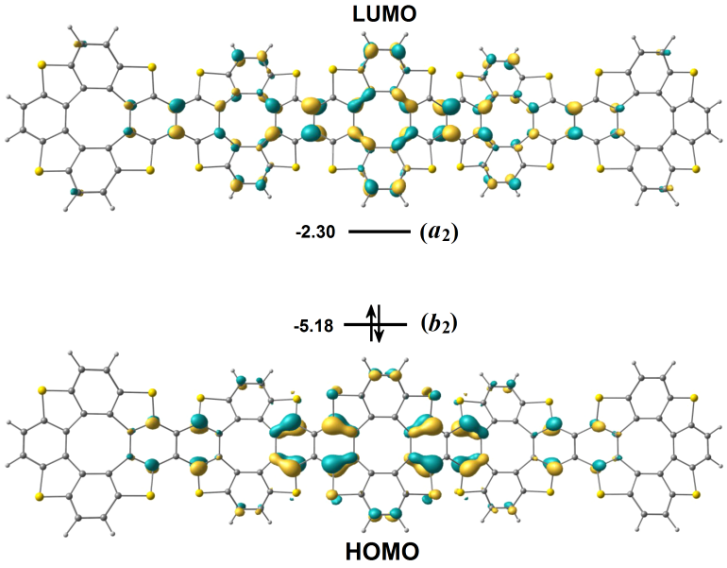

Figure S10. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=5 (type **I**) calculated at the B3LYP/6-31G(d) level of theory.

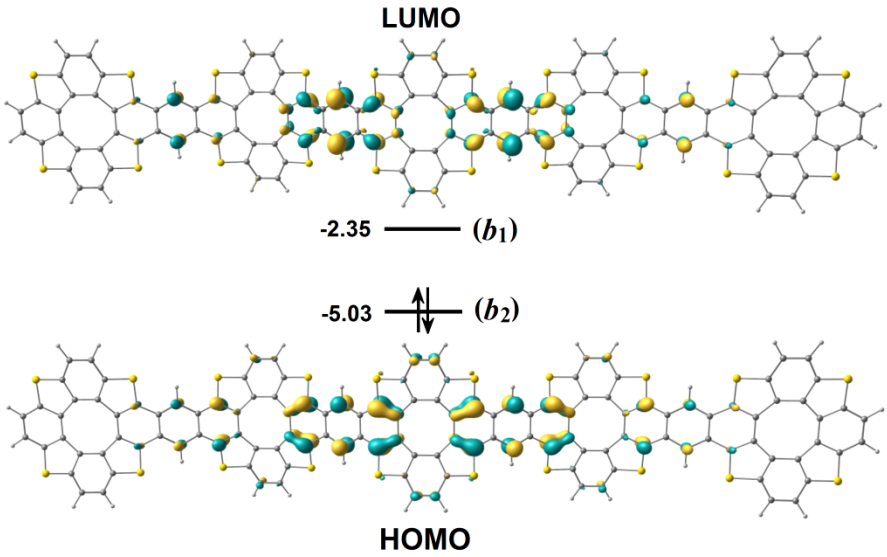

Figure S11. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=5 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.

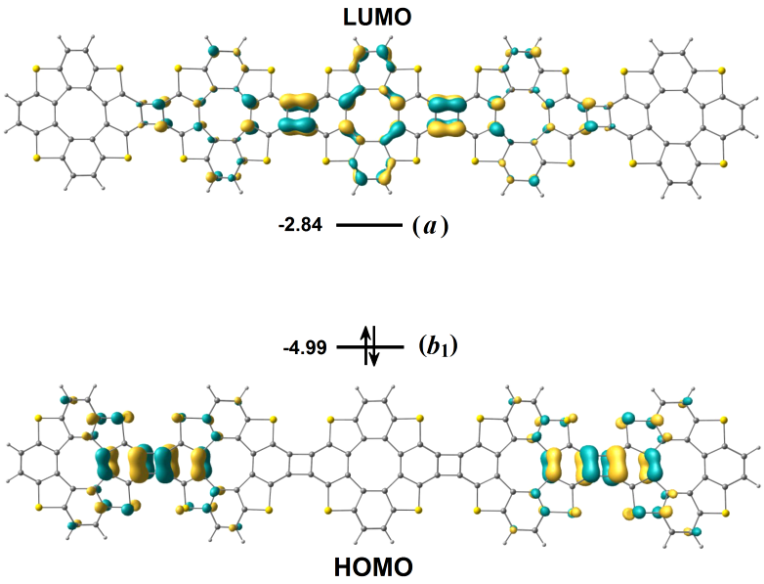

Figure S12. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=5 (type **III**) calculated at the B3LYP/6-31G(d) level of theory.

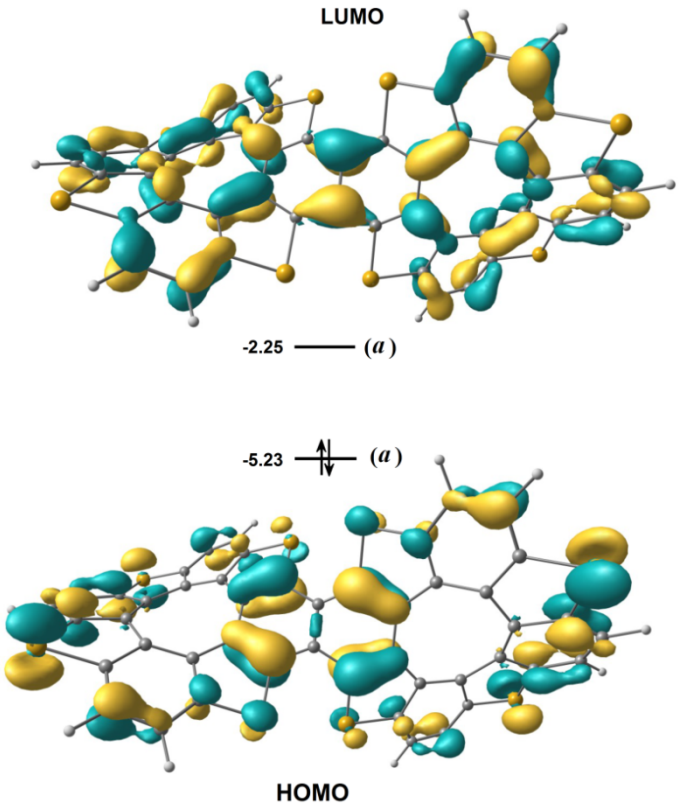

Figure S13. Molecular orbital diagram of the tetraselena[8]circulene-based compound with n=2 (type **I**) calculated at the B3LYP/6-31G(d) level of theory.

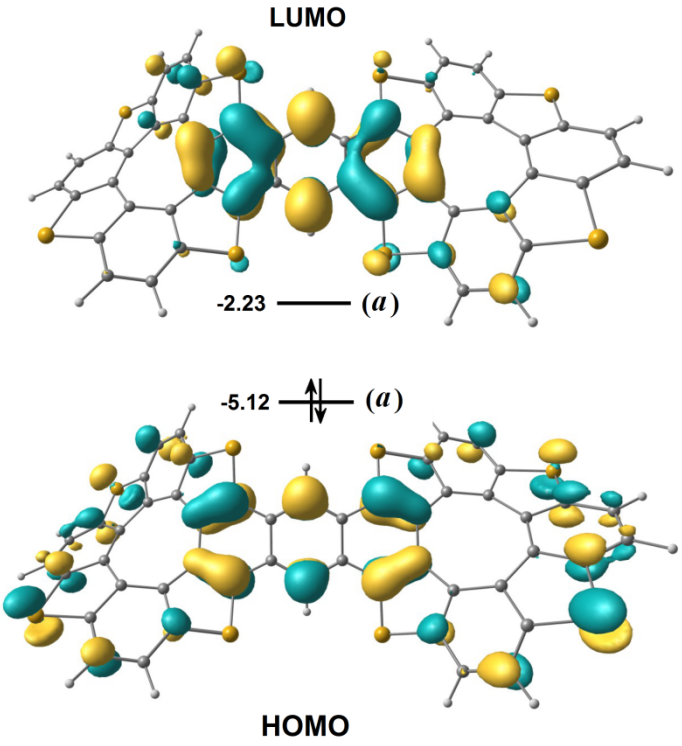

Figure S14. Molecular orbital diagram of the tetraselena[8]circulene-based compound with n=2 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.

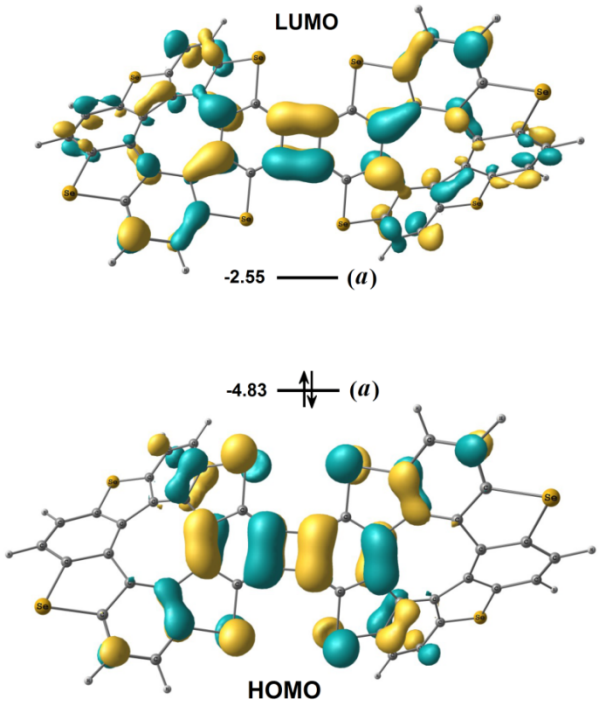

Figure S15. Molecular orbital diagram of the tetraselena[8]circulene-based compound with n=2 (type **III**) calculated at the B3LYP/6-31G(d) level of theory.

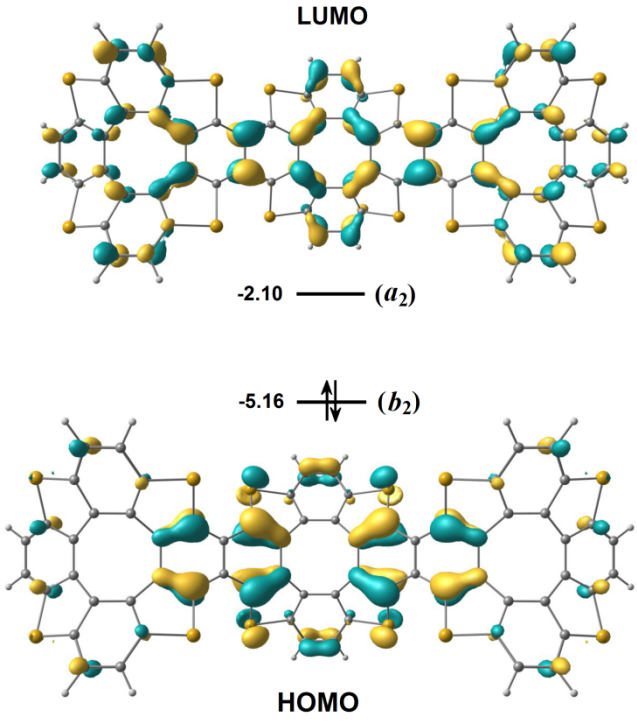

Figure S16. Molecular orbital diagram of the tetraselena[8]circulene-based compound with n=3 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.

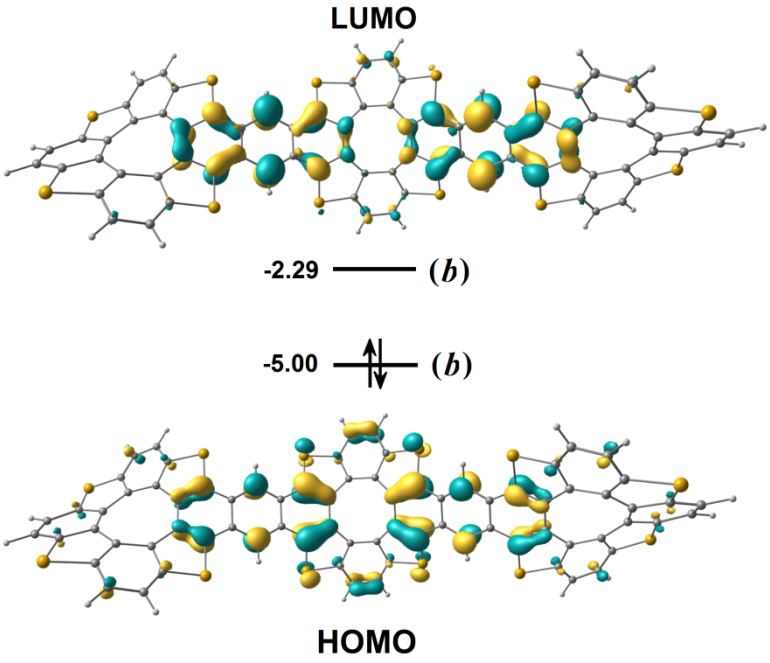

Figure S17. Molecular orbital diagram of the tetraselena[8]circulene-based compound with n=3 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.

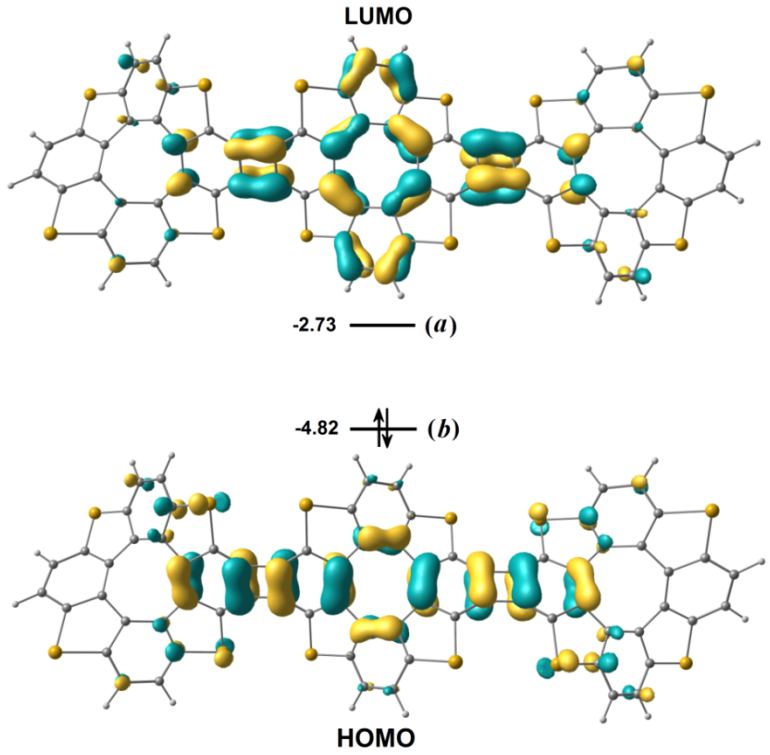

Figure S18. Molecular orbital diagram of the tetraselena[8]circulene-based compound with n=3 (type **III**) calculated at the B3LYP/6-31G(d) level of theory.

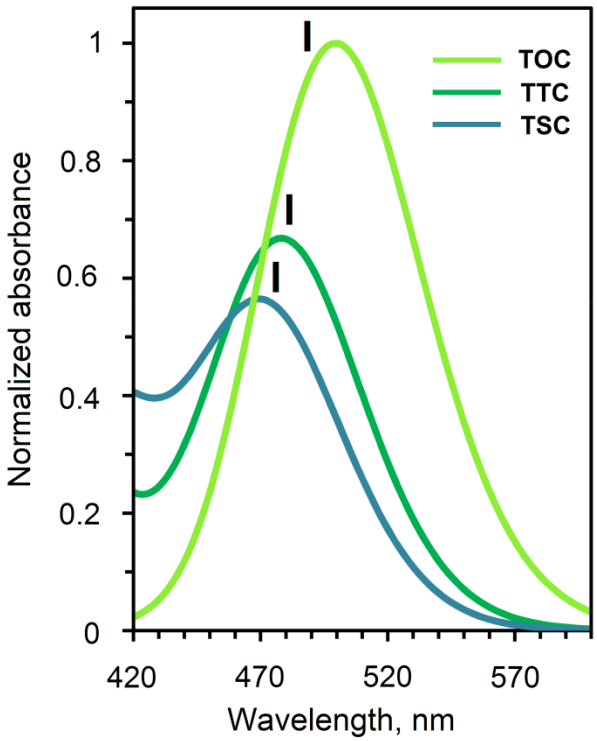

Figure S19. Electronic absorption spectra of the **TOC**-, **TTC**- and **TSC**-based ribbons (type **I**) with n=3 calculated by the TD DFT/B3LYP/6-31G(d) method; **I** denotes the first absorption band (band half-width 3000 cm^{-1}, Gaussian distribution function).

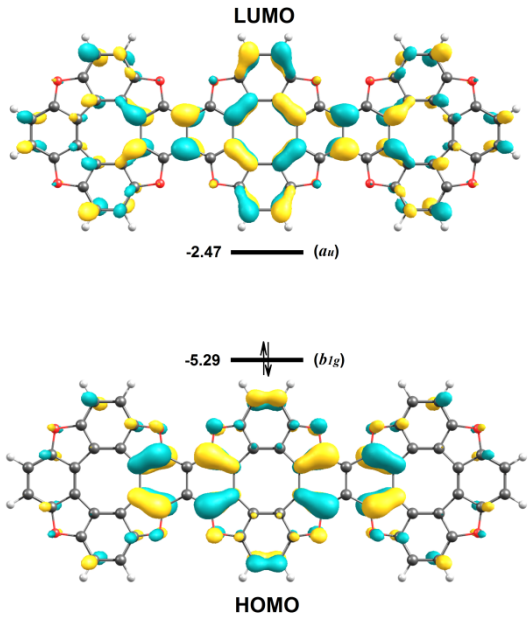

Figure S20. Molecular orbital diagram of the tetraoxa[8]circulene(TOC)-based compound with n=3 (type **I**) calculated at the B3LYP/6-31G(d) level of theory.

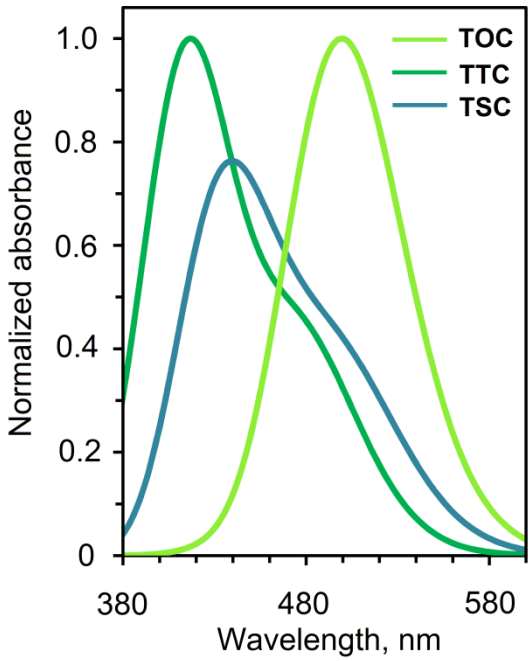

Figure S21. Electronic absorption spectra of the **TOC**-, **TTC**- and **TSC**-based ribbons (type **II**) with n=3 calculated by the TD DFT/B3LYP/6-31G(d) method (band half-width 3000 cm^{-1}, Gaussian distribution function).

Table S1. Wavelengths (λ), oscillator strengths (*f*) and orbital assignment of the selected electronic transitions in the calculated absorption spectra of the **TTC**-based oligomers

Compound	State	Transition	λ, nm	*f*	Assignment
TTC (D_{2d} symmetry point group)	S_1	$X^1A \rightarrow 1^1A_2$	394	0	HOMO-3→LUMO (99%)
	S_2	$X^1A \rightarrow 1^1A_1$	389	0	HOMO-2→LUMO (98%)
	$S_{3(4)}$	$X^1A \rightarrow 1^1E$	382	0.2000	HOMO→LUMO (95%) (HOMO-1→LUMO (95%))
TTCs (type **I**)					
n=2 (C_1 symmetry point group)	S_1	$X^1A \rightarrow 1^1A$	460	0.4840	HOMO→LUMO (92%)
	S_2	$X^1A \rightarrow 2^1A$	442	0.0352	HOMO-1→LUMO (77%)
	S_3	$X^1A \rightarrow 3^1A$	413	0.0198	HOMO-2→LUMO (92%)
	S_4	$X^1A \rightarrow 4^1A$	407	0.0894	HOMO-4→LUMO (92%)
	S_5	$X^1A \rightarrow 5^1A$	406	0.0993	HOMO-3→LUMO (78%)
	S_8	$X^1A \rightarrow 8^1A$	378	0.0293	HOMO→LUMO+2 (92%)
	S_{10}	$X^1A \rightarrow 10^1A$	373	0.0199	HOMO-1→LUMO+1 (83%) HOMO-7→LUMO (7%) HOMO-3→LUMO+1 (5%)
	S_{11}	$X^1A \rightarrow 11^1A$	369	0.6995	HOMO-1→LUMO+2 (86%)
	S_{12}	$X^1A \rightarrow 12^1A$	346	0.0161	HOMO-4→LUMO+2 (88%) HOMO-2→LUMO+1 (8%)
	S_{15}	$X^1A \rightarrow 15^1A$	343	0.0100	HOMO-5→LUMO+2 (62%) HOMO-7→LUMO (14%) HOMO-6→LUMO+2 (11%) HOMO-3→LUMO+1 (10%)
	S_{16}	$X^1A \rightarrow 16^1A$	342	0.1768	HOMO-3→LUMO+2 (93%)
	S_{18}	$X^1A \rightarrow 18^1A$	339	0.1444	HOMO-2→LUMO+1 (85%) HOMO-4→LUMO+2 (7%)
	S_{19}	$X^1A \rightarrow 19^1A$	337	0.0217	HOMO-5→LUMO+1 (84%)
	S_{20}	$X^1A \rightarrow 20^1A$	333	0.0385	HOMO-3→LUMO+1 (50%) HOMO-7→LUMO (45%)
n=3 (C_s symmetry point group)	S_1	$X^1A' \rightarrow 1^1A''$	479	1.0199	HOMO→LUMO (95%)
	S_2	$X^1A' \rightarrow 1^1A'$	433	0.0094	HOMO-1→LUMO (60%) HOMO→LUMO+1 (23%)
	S_4	$X^1A' \rightarrow 2^1A'$	424	0.0967	HOMO-2→LUMO (81%) HOMO-7→LUMO (6%)
	S_5	$X^1A' \rightarrow 3^1A'$	415	0.0023	HOMO→LUMO+1 (67%) HOMO-1→LUMO (22%) HOMO-6→LUMO (7%)
	S_7	$X^1A' \rightarrow 3^1A''$	407	0.0616	HOMO-5→LUMO (82%) HOMO-4→LUMO+1 (13%)
	S_8	$X^1A' \rightarrow 5^1A'$	404	0.0061	HOMO-6→LUMO (53%) HOMO-4→LUMO (27%) HOMO-5→LUMO+1 (9%) HOMO-1→LUMO (8%)
	S_{10}	$X^1A' \rightarrow 6^1A'$	402	0.0586	HOMO-7→LUMO (74%) HOMO-8→LUMO+1 (14%) HOMO-2→LUMO (7%)
	S_{12}	$X^1A' \rightarrow 6^1A''$	382	0.0774	HOMO-1→LUMO+1 (85%) HOMO-9→LUMO (5%)
	S_{13}	$X^1A' \rightarrow 7^1A'$	381	0.0021	HOMO→LUMO+3 (56%) HOMO-3→LUMO+1 (28%) HOMO-2→LUMO (7%)
	S_{15}	$X^1A' \rightarrow 8^1A''$	378	0.2423	HOMO-9→LUMO (+61%)

					HOMO-6→LUMO+1 (18%)
	S_{16}	$X^1A'\rightarrow 8^1A'$	374	0.0744	HOMO-3→LUMO+1 (45%) HOMO→LUMO+3 (33%)
	S_{17}	$X^1A'\rightarrow 9^1A''$	372	0.7048	HOMO-3→LUMO+2 (38%) HOMO-2→LUMO+3 (23%) HOMO→LUMO+4 (11%)
	S_{18}	$X^1A'\rightarrow 9^1A'$	370	0.0513	HOMO-2→LUMO+2 (73%) HOMO-3→LUMO+3 (7%)
	S_{19}	$X^1A'\rightarrow 10^1A'$	365	0.0393	HOMO-1→LUMO+2 (78%) HOMO-6→LUMO+2 (12%)
	S_{20}	$X^1A'\rightarrow 10^1A''$	363	0.0162	HOMO-4→LUMO+1 (47%) HOMO→LUMO+4 (20%) HOMO-6→LUMO+1 (17%) HOMO-9→LUMO (7%)
n=4 (C_{2h} symmetry point group)	S_1	$X^1A_g\rightarrow 1^1B_u$	492	1.6221	HOMO→LUMO (92%)
	S_2	$X^1A_g\rightarrow 1^1A_g$	454	0	HOMO-1→LUMO (54%) HOMO→LUMO+2 (37%)
	S_5	$X^1A_g\rightarrow 1^1B_u$	426	0.0732	HOMO-4→LUMO (53%) HOMO-1→LUMO+1 (24%)
	S_7	$X^1A_g\rightarrow 2^1A_u$	424	0.1335	HOMO-2→LUMO (77%) HOMO-3→LUMO+1 (7%)
	S_9	$X^1A_g\rightarrow 2^1B_u$	410	0.0075	HOMO-1→LUMO+1 (21%) HOMO-7→LUMO (20%) HOMO-10→LUMO (19%) HOMO-4→LUMO (18%) HOMO-6→LUMO+1 (13%)
	S_{11}	$X^1A_g\rightarrow 3^1B_u$	407	0.1953	HOMO-7→LUMO (44%) HOMO-1→LUMO+1 (28%) HOMO-6→LUMO+1 (11%)
	S_{13}	$X^1A_g\rightarrow 3^1A_u$	403	0.0492	HOMO-11→LUMO (51%) HOMO-9→LUMO+1 (28%) HOMO-5→LUMO (10%)
	S_{15}	$X^1A_g\rightarrow 4^1B_u$	397	0.0300	HOMO-10→LUMO (58%) HOMO-4→LUMO (15%) HOMO-8→LUMO+1 (11%) HOMO→LUMO+3 (8%)
	S_{16}	$X^1A_g\rightarrow 5^1B_u$	394	0.0130	HOMO→LUMO+3 (67%) HOMO-1→LUMO+1 (15%)
	S_{19}	$X^1A_g\rightarrow 5^1A_u$	386	0.0126	HOMO-3→LUMO+1 (54%) HOMO→LUMO+5 (13%) HOMO-2→LUMO (9%)
n=5 (C_{2v} symmetry point group)	S_1	$X^1A_1\rightarrow 1^1B_1$	499	2.2636	HOMO→LUMO (88%)
	S_2	$X^1A_1\rightarrow 1^1A_1$	468	0.0046	HOMO-1→LUMO (53%) HOMO→LUMO+1 (38%)
	S_4	$X^1A_1\rightarrow 2^1B_1$	441	0.1664	HOMO-1→LUMO+1 (39%) HOMO-2→LUMO (35%) HOMO→LUMO+2 (11%)
	S_8	$X^1A_1\rightarrow 2^1B_2$	425	0.1683	HOMO-3→LUMO (72%) HOMO-4→LUMO+1 (13%)
	S_9	$X^1A_1\rightarrow 2^1A_1$	424	0.0029	HOMO-6→LUMO (51%) HOMO-2→LUMO+1 (19%)
	S_{10}	$X^1A_1\rightarrow 3^1B_1$	420	0.0586	HOMO-2→LUMO (46%) HOMO-1→LUMO+1 (27%) HOMO→LUMO+2 (10%)
	S_{12}	$X^1A_1\rightarrow 4^1B_1$	413	0.0783	HOMO→LUMO+2 (69%) HOMO-1→LUMO+1 (16%)
	S_{13}	$X^1A_1\rightarrow 5^1B_1$	410	0.0499	HOMO-11→LUMO (35%)

					HOMO-8→LUMO (28%) HOMO-9→LUMO+1 (14%)
	S_{15}	$X^1A_1 \rightarrow 6^1B_1$	406	0.0518	HOMO-11→LUMO (31%) HOMO-8→LUMO (25%) HOMO-9→LUMO+1 (16%) HOMO-10→LUMO+1 (12%)
	S_{18}	$X^1A_1 \rightarrow 3^1B_2$	403	0.0450	HOMO-12→LUMO (41%) HOMO-13→LUMO+1 (32%) HOMO-12→LUMO+2 (9%) HOMO-5→LUMO (8%)
	S_{19}	$X^1A_1 \rightarrow 5^1A_1$	403	0.0107	HOMO-1→LUMO+2 (25%) HOMO-2→LUMO+1 (22%) HOMO-9→LUMO (13%) HOMO-6→LUMO (10%)
TTCs (type **II**)					
n=2 (C_{2h} symmetry point group)	S_1	$X^1A_g \rightarrow 1^1A_u$	478	0.0013	HOMO→LUMO (97%)
	S_2	$X^1A_g \rightarrow 1^1B_u$	460	0.3193	HOMO→LUMO+1 (79%) HOMO-1→LUMO (11%)
	S_3	$X^1A_g \rightarrow 2^1B_u$	416	0.7932	HOMO-1→LUMO (85%) HOMO→LUMO+1 (11%)
	S_6	$X^1A_g \rightarrow 2^1A_u$	408	0.0053	HOMO-4→LUMO (93%)
	S_8	$X^1A_g \rightarrow 3^1B_u$	396	0.6420	HOMO-6→LUMO (60%) HOMO-4→LUMO+1 (28%)
	S_{10}	$X^1A \rightarrow 3^1A_u$	390	0.0235	HOMO-6→LUMO+1 (65%) HOMO-1→LUMO+1 (26%)
	S_{13}	$X^1A_g \rightarrow 4^1A_u$	383	0.2424	HOMO-1→LUMO+1 (64%) HOMO-6→LUMO+1 (23%) HOMO-4→LUMO (6%)
	S_{15}	$X^1A_g \rightarrow 4^1B_u$	378	0.4004	HOMO-4→LUMO+1 (63%) HOMO-6→LUMO (30%)
	S_{18}	$X^1A_g \rightarrow 5^1B_u$	341	0.0161	HOMO-2→LUMO+2 (91%)
	S_{20}	$X^1A_g \rightarrow 6^1B_u$	336	0.0304	HOMO-5→LUMO+2 (93%)
n=3 (C_2 symmetry point group)	S_1	$X^1A \rightarrow 1^1A$	507	0	HOMO→LUMO (97%)
	S_2	$X^1A \rightarrow 1^1B$	483	0.0052	HOMO→LUMO+1 (92%)
	S_3	$X^1A \rightarrow 2^1B$	479	1.0651	HOMO→LUMO+2 (89%)
	S_5	$X^1A \rightarrow 2^1A$	447	0.0008	HOMO→LUMO+3 (36%) HOMO-1→LUMO+2 (24%) HOMO-2→LUMO (19%) HOMO-9→LUMO+1 (6%)
	S_7	$X^1A \rightarrow 4^1B$	422	1.9992	HOMO-3→LUMO (56%) HOMO-2→LUMO+1 (28%)
	S_8	$X^1A \rightarrow 4^1A$	417	0.0076	HOMO→LUMO+3 (56%) HOMO-1→LUMO+2 (23%) HOMO-2→LUMO (15%)
	S_9	$X^1A \rightarrow 5^1A$	412	0.0220	HOMO-2→LUMO (48%) HOMO-1→LUMO+2 (30%) HOMO-6→LUMO (6%) HOMO-9→LUMO+1 (6%) HOMO-3→LUMO+1 (6%)
	S_{10}	$X^1A \rightarrow 5^1B$	411	0.0020	HOMO-5→LUMO (53%) HOMO-7→LUMO+1 (18%) HOMO-8→LUMO (17%) HOMO-4→LUMO+1 (6%)
	S_{12}	$X^1A \rightarrow 6^1B$	409	0.0126	HOMO-8→LUMO (73%) HOMO-5→LUMO (14%) HOMO-4→LUMO+1 (8%)
	S_{14}	$X^1A \rightarrow 7^1B$	403	0.6169	HOMO-9→LUMO (43%)

					HOMO-6→LUMO+1 (27%) HOMO-3→LUMO (16%)
	S_{15}	$X^1A \rightarrow 8^1A$	400	0.0184	HOMO-6→LUMO (59%) HOMO-3→LUMO+1 (18%) HOMO-1→LUMO+2 (8%)
	S_{16}	$X^1A \rightarrow 8^1B$	394	0.0801	HOMO-2→LUMO+1 (47%) HOMO-9→LUMO (20%) HOMO-3→LUMO (10%) HOMO-1→LUMO+3 (9%)
	S_{17}	$X^1A \rightarrow 9^1B$	392	0.2060	HOMO-1→LUMO+3 (54%) HOMO→LUMO+4 (10%) HOMO-2→LUMO+1 (9%) HOMO-4→LUMO+3 (9%)
	S_{19}	$X^1A \rightarrow 10^1A$	388	0.0122	HOMO-5→LUMO+2 (27%) HOMO-3→LUMO+1 (22%) HOMO-8→LUMO+2 (12%) HOMO-9→LUMO+1 (11%)
n=4 (C_1 symmetry point group)	S_1	$X^1A \rightarrow 1^1A$	518	0	HOMO→LUMO (94%)
	S_2	$X^1A \rightarrow 2^1A$	498	0.0019	HOMO→LUMO+1 (76%) HOMO-1→LUMO (19%)
	S_3	$X^1A \rightarrow 3^1A$	489	1.9529	HOMO→LUMO+2 (86%)
	S_4	$X^1A \rightarrow 4^1A$	484	0.0094	HOMO→LUMO+3 (77%) HOMO-1→LUMO+1 (18%)
	S_9	$X^1A \rightarrow 9^1A$	441	0.0241	HOMO-1→LUMO+4 (22%) HOMO-3→LUMO (20%) HOMO-2→LUMO+2 (13%) HOMO→LUMO+5 (12%)
	S_{12}	$X^1A \rightarrow 12^1A$	425	3.2847	HOMO-6→LUMO (30%) HOMO-4→LUMO+1 (23%) HOMO-3→LUMO+3 (15%)
	S_{15}	$X^1A \rightarrow 15^1A$	413	0.0065	HOMO-10→LUMO (46%) HOMO-2→LUMO+3 (24%) HOMO-8→LUMO+1 (13%)
	S_{16}	$X^1A \rightarrow 16^1A$	411	0.0930	HOMO-3→LUMO (38%) HOMO-1→LUMO+4 (34%) HOMO-4→LUMO+1 (6%)
	S_{17}	$X^1A \rightarrow 17^1A$	410.6	0.0012	HOMO-7→LUMO+1 (31%) HOMO-5→LUMO (20%) HOMO-8→LUMO (16%) HOMO-12→LUMO (6%) HOMO-8→LUMO+3 (6%)
	S_{18}	$X^1A \rightarrow 18^1A$	410.4	0.0104	HOMO-7→LUMO (42%) HOMO-5→LUMO+1 (24%) HOMO-8→LUMO+1 (16%) HOMO-7→LUMO+3 (10%)
	S_{20}	$X^1A_1 \rightarrow 20^1A$	406	0.4042	HOMO→LUMO+5 (75%) HOMO-2→LUMO+2 (8%)
n=5 (C_{2v} symmetry point group)	S_1	$X^1A_1 \rightarrow 1^1A_2$	523	0	HOMO→LUMO (90%)
	S_2	$X^1A_1 \rightarrow 1^1B_2$	509	0.0001	HOMO→LUMO+1 (65%) HOMO-1→LUMO (28%)
	S_3	$X^1A_1 \rightarrow 1^1B_1$	495	3.0042	HOMO→LUMO+3 (81%) HOMO-1→LUMO+5 (11%)
	S_5	$X^1A_1 \rightarrow 2^1B_2$	484	0.0131	HOMO→LUMO+4 (61%) HOMO-1→LUMO+2 (29%)
	S_7	$X^1A_1 \rightarrow 1^1A_1$	472	0.0032	HOMO-1→LUMO+3 (42%) HOMO→LUMO+5 (39%)
	S_9	$X^1A_1 \rightarrow 2^1B_1$	453	0.0878	HOMO-1→LUMO+5 (28%)

					HOMO-2→LUMO+3 (20%) HOMO→LUMO+6 (18%)
	S_{15}	$X^1A_1 \rightarrow 3^1A_1$	438	0.0015	HOMO-2→LUMO+5 (15%) HOMO-4→LUMO (14%) HOMO→LUMO+5 (12%) HOMO-6→LUMO (10%) HOMO-3→LUMO+3 (7%) HOMO-5→LUMO+1 (7%)
	S_{16}	$X^1A_1 \rightarrow 3^1B_1$	427	3.8679	HOMO-9→LUMO (21%) HOMO-6→LUMO+1 (16%) HOMO-13→LUMO (16%) HOMO-5→LUMO+2 (11%)
	S_{19}	$X^1A_1 \rightarrow 4^1B_1$	421	1.2655	HOMO→LUMO+6 (52%) HOMO-1→LUMO+5 (19%) HOMO→LUMO+3 (8%) HOMO-2→LUMO+3 (7%)
	S_{20}	$X^1A_1 \rightarrow 7^1B_2$	420	0.0035	HOMO-3→LUMO (50%) HOMO-2→LUMO+4 (11%) HOMO-3→LUMO+2 (9%) HOMO-2→LUMO+1 (8%) HOMO-12→LUMO (7%)
TTCs (type **III**)					
n=2 (D_2 symmetry point group)	S_1	$X^1A \rightarrow 1^1B_1$	639	0.0012	HOMO→LUMO (98%)
	S_2	$X^1A \rightarrow 1^1B_2$	480	0.0427	HOMO→LUMO+1 (89%)
	S_3	$X^1A \rightarrow 1^1B_3$	470	0.3011	HOMO-1→LUMO (79%) HOMO-2→LUMO (15%)
	S_4	$X^1A \rightarrow 2^1B_1$	450	0.0011	HOMO-5→LUMO (95%)
	S_5	$X^1A \rightarrow 2^1B_3$	447	0.2182	HOMO-2→LUMO (81%) HOMO-1→LUMO (15%)
	S_7	$X^1A \rightarrow 2^1B_2$	444	0.0918	HOMO-4→LUMO (82%) HOMO→LUMO+1 (9%)
	S_9	$X^1A \rightarrow 3^1B_2$	406	0.0586	HOMO-7→LUMO (85%) HOMO-4→LUMO (7%)
	S_{11}	$X^1A \rightarrow 3^1B_3$	367	0.6961	HOMO→LUMO+2 (47%) HOMO-3→LUMO+1 (45%)
	S_{14}	$X^1A \rightarrow 4^1B_3$	359	0.4338	HOMO-3→LUMO+1 (47%) HOMO→LUMO+2 (40%)
	S_{15}	$X^1A \rightarrow 4^1B_1$	358.7	0.0023	HOMO-4→LUMO+1 (88%)
	S_{16}	$X^1A \rightarrow 4^1B_2$	358.3	0.1153	HOMO-5→LUMO+1 (87%) HOMO-7→LUMO (6%)
	S_{17}	$X^1A \rightarrow 5^1B_3$	346	0.0219	HOMO-6→LUMO+1 (91%)
	S_{18}	$X^1A \rightarrow 5^1B_1$	337	0.0015	HOMO-7→LUMO+1 (82%) HOMO→LUMO+3 (9%)
	S_{19}	$X^1A \rightarrow 6^1B_3$	317	0.2646	HOMO-8→LUMO (71%) HOMO→LUMO+6 (17%)
n=3 (D_2 symmetry point group)	S_1	$X^1A \rightarrow 1^1B_1$	700	0.0001	HOMO→LUMO (95%)
	S_2	$X^1A \rightarrow 1^1B_2$	660	0.0008	HOMO-1→LUMO (95%)
	S_3	$X^1A \rightarrow 2^1B_2$	543	0.0382	HOMO→LUMO+1 (91%)
	S_5	$X^1A \rightarrow 1^1B_3$	495	0.8767	HOMO-2→LUMO (89%)
	S_8	$X^1A \rightarrow 2^1B_3$	462	0.1297	HOMO-5→LUMO (84%) HOMO-4→LUMO+1 (8%)
	S_{10}	$X^1A \rightarrow 3^1B_2$	461	0.0101	HOMO-7→LUMO (74%) HOMO-1→LUMO+2 (11%) HOMO-6→LUMO+1 (11%)
	S_{11}	$X^1A \rightarrow 4^1B_1$	458	0.0011	HOMO-6→LUMO (54%) HOMO→LUMO+2 (38%)
	S_{13}	$X^1A \rightarrow 4^1B_2$	449	0.0894	HOMO-1→LUMO+2 (81%)

					HOMO-7→LUMO (10%)
	S_{16}	$X^1A \rightarrow 5^1B_2$	421	0.0718	HOMO-10→LUMO (81%) HOMO-6→LUMO+1 (5%)
	S_{20}	$X^1A \rightarrow 5^1B_3$	400	0.1106	HOMO-4→LUMO+1 (69%) HOMO-3→LUMO+1 (11%) HOMO-5→LUMO (7%)
n=4 (D_2 symmetry point group)	S_1	$X^1A \rightarrow 1^1B_1$	723	0.0008	HOMO→LUMO (50%)
	S_2	$X^1A \rightarrow 1^1B_2$	689	0.0006	HOMO-1→LUMO (80%) HOMO→LUMO+1 (18%)
	S_3	$X^1A \rightarrow 2^1B_1$	670	0.0007	HOMO-2→LUMO (56%) HOMO→LUMO (34%) HOMO-1→LUMO+1 (9%)
	S_4	$X^1A \rightarrow 2^1B_2$	587	0.0229	HOMO-2→LUMO+1 (65%) HOMO→LUMO+1 (24%) HOMO-1→LUMO (8%)
	S_5	$X^1A \rightarrow 3^1B_1$	577	0.0013	HOMO-1→LUMO+1 (74%) HOMO→LUMO (15%) HOMO→LUMO+2 (9%)
	S_6	$X^1A \rightarrow 3^1B_2$	576	0.0016	HOMO→LUMO+1 (49%) HOMO-2→LUMO+1 (30%) HOMO-1→LUMO (11%)
	S_7	$X^1A \rightarrow 1^1B_3$	506	1.4637	HOMO-3→LUMO (81%) HOMO-7→LUMO (7%) HOMO-4→LUMO+1 (7%)
	S_8	$X^1A \rightarrow 4^1B_1$	506	0.0042	HOMO→LUMO+2 (73%) HOMO-1→LUMO+3 (8%) HOMO-2→LUMO+2 (7%) HOMO-1→LUMO+1 (6%)
	S_9	$X^1A \rightarrow 4^1B_2$	504	0.0471	HOMO-1→LUMO+2 (76%) HOMO→LUMO+3 (11%) HOMO→LUMO+1 (7%)
	S_{10}	$X^1A \rightarrow 5^1B_1$	497	0.0023	HOMO-2→LUMO+2 (87%)
	S_{11}	$X^1A \rightarrow 2^1B_3$	490	0.0229	HOMO-7→LUMO (59%) HOMO-5→LUMO (25%) HOMO-4→LUMO+1 (5%)
	S_{14}	$X^1A \rightarrow 3^1B_3$	465	0.0877	HOMO-5→LUMO (50%) HOMO-7→LUMO (19%) HOMO-6→LUMO+1 (16%) HOMO-11→LUMO (7%)
	S_{16}	$X^1A \rightarrow 6^1B_1$	463.8	0.0040	HOMO-8→LUMO (71%) HOMO-9→LUMO+1 (21%)
	S_{17}	$X^1A \rightarrow 5^1B_2$	463.8	0.0285	HOMO-9→LUMO (71%) HOMO-8→LUMO+1 (21%)
	S_{20}	$X^1A \rightarrow 7^1B_1$	441	0.0059	HOMO-1→LUMO+3 (84%) HOMO→LUMO+2 (9%)
n=5 (D_2 symmetry point group)	S_1	$X^1A \rightarrow 1^1B_1$	730	0	HOMO-2→LUMO (65%) HOMO→LUMO (18%) HOMO-3→LUMO+1 (6%) HOMO-1→LUMO+1 (5%)
	S_2	$X^1A \rightarrow 1^1B_2$	707	0.0002	HOMO-3→LUMO (43%) HOMO-1→LUMO (27%) HOMO→LUMO+1 (20%)
	S_3	$X^1A \rightarrow 3^1B_1$	683	0.0001	HOMO→LUMO (45%) HOMO-1→LUMO+1 (25%) HOMO-2→LUMO (24%)
	S_4	$X^1A \rightarrow 2^1B_2$	674	0.0003	HOMO-3→LUMO (45%) HOMO-1→LUMO (36%) HOMO→LUMO+1 (12%)
	S_6	$X^1A \rightarrow 3^1B_2$	602	0.0251	HOMO-2→LUMO+1 (63%)

					HOMO→LUMO+1 (11%) HOMO-1→LUMO (9%)
	S_7	$X^1A \rightarrow 4^1B_1$	593	0.0002	HOMO-1→LUMO+1 (48%) HOMO→LUMO (26%) HOMO→LUMO+2 (12%) HOMO-3→LUMO+1 (9%)
	S_{10}	$X^1A \rightarrow 5^1B_2$	536	0.0264	HOMO-1→LUMO+2 (65%) HOMO→LUMO+1 (17%) HOMO→LUMO+3 (13%)
	S_{12}	$X^1A \rightarrow 6^1B_2$	531	0.0160	HOMO-3→LUMO+2 (90%)
	S_{13}	$X^1A \rightarrow 1^1B_3$	512	2.0862	HOMO-4→LUMO (73%) HOMO-5→LUMO+1 (9%) HOMO-8→LUMO (7%)
	S_{16}	$X^1A \rightarrow 2^1B_3$	490	0.0554	HOMO-6→LUMO (51%) HOMO-8→LUMO (11%) HOMO-5→LUMO+1 (11%) HOMO-7→LUMO+1 (6%)
	S_{17}	$X^1A \rightarrow 7^1B_2$	484	0.0155	HOMO→LUMO+3 (56%) HOMO-1→LUMO+4 (12%) HOMO-1→LUMO+2 (12%) HOMO-2→LUMO+3 (10%)
	S_{19}	$X^1A \rightarrow 8^1B_2$	475	0.0271	HOMO-2→LUMO+3 (78%) HOMO→LUMO+3 (6%)

Table S2. Wavelengths (λ), oscillator strengths (*f*) and orbital assignment of the selected electronic transitions in the calculated absorption spectra of the **TSC**-based oligomers

Compound	State	Transition	λ, nm	*f*	Assignment
TSC (D_{2d} symmetry point group)	S_1	$X^1A \rightarrow 1^1A_2$	429	0	HOMO-3→LUMO (99%)
	S_2	$X^1A \rightarrow 1^1A_1$	420	0	HOMO-2→LUMO (98%)
	$S_{3(4)}$	$X^1A \rightarrow 1^1E$	415	0.1749	HOMO→LUMO (95%) (HOMO-1→LUMO (95%))
TSCs (Type **I**)					
n=2 (C_1 symmetry point group)	S_1	$X^1A \rightarrow 1^1A$	485	0.4157	HOMO→LUMO (91%)
	S_2	$X^1A \rightarrow 2^1A$	476	0.0238	HOMO-1→LUMO (80%) HOMO-5→LUMO (14%)
	S_3	$X^1A \rightarrow 3^1A$	441	0.0354	HOMO-2→LUMO (91%)
	S_4	$X^1A \rightarrow 4^1A$	437	0.0642	HOMO-5→LUMO (80%) HOMO-1→LUMO (14%)
	S_5	$X^1A \rightarrow 5^1A$	431	0.0750	HOMO-4→LUMO (80%) HOMO-6→LUMO (16%)
	S_{10}	$X^1A \rightarrow 19^1A$	399	0.5084	HOMO-1→LUMO+2 (86%)
n=3 (C_{2v} symmetry point group)	S_1	$X^1A_1 \rightarrow 1^1B_1$	473	0.8103	HOMO→LUMO (93%)
	S_2	$X^1A_1 \rightarrow 1^1A_1$	445	0.0004	HOMO-2→LUMO (93%)
	S_3	$X^1A_1 \rightarrow 1^1B_2$	439	0.0905	HOMO-1→LUMO (84%)
	S_4	$X^1A_1 \rightarrow 2^1A_1$	436	0.0036	HOMO-3→LUMO (45%) HOMO→LUMO+1 (26%) HOMO-6→LUMO (10%)
	S_6	$X^1A_1 \rightarrow 2^1B_1$	430	0.0119	HOMO-4→LUMO (76%) HOMO-2→LUMO+1 (15%)
	S_7	$X^1A_1 \rightarrow 3^1A_1$	418	0.0121	HOMO-6→LUMO (62%) HOMO-4→LUMO+1 (13%) HOMO→LUMO+1 (9%)

	S_{10}	$X^1A_1 \rightarrow 2^1B_2$	410	0.0038	HOMO-2→LUMO+2 (81%) HOMO-4→LUMO+3 (9%)
	S_{11}	$X^1A_1 \rightarrow 5^1A_1$	407	0.0487	HOMO-1→LUMO+3 (56%) HOMO-5→LUMO+2 (30%)
	S_{12}	$X^1A_1 \rightarrow 3^1B_1$	406	0.3572	HOMO-3→LUMO+1 (45%) HOMO→LUMO+3 (33%)
	S_{13}	$X^1A_1 \rightarrow 3^1B_2$	403	0.0440	HOMO→LUMO+3 (79%) HOMO-1→LUMO (8%)
	S_{15}	$X^1A_1 \rightarrow 4^1B_1$	400	0.0730	HOMO-7→LUMO (49%) HOMO-2→LUMO+1 (18%)
	S_{20}	$X^1A_1 \rightarrow 6^1B_1$	384	0.0780	HOMO-3→LUMO+1 (57%) HOMO-7→LUMO (16%)
n=4 (C_s symmetry point group)	S_1	$X^1A' \rightarrow 1^1A'$	483	1.3109	HOMO→LUMO (90%)
	S_2	$X^1A' \rightarrow 2^1A'$	453	0	HOMO-1→LUMO (56%) HOMO→LUMO+1 (32%)
	S_4	$X^1A' \rightarrow 1^1A''$	441	0.1013	HOMO-2→LUMO (81%)
	S_8	$X^1A' \rightarrow 5^1A'$	430	0.0422	HOMO-7→LUMO (27%) HOMO-1→LUMO+1 (21%) HOMO-8→LUMO (15%)
	S_{11}	$X^1A' \rightarrow 8^1A'$	416	0.1884	HOMO-8→LUMO (45%) HOMO-1→LUMO+1 (18%) HOMO-6→LUMO+1 (18%)
	S_{12}	$X^1A' \rightarrow 4^1A''$	412	0.0136	HOMO-9→LUMO (39%) HOMO→LUMO+2 (32%)
	S_{15}	$X^1A' \rightarrow 9^1A'$	408	0.1520	HOMO-2→LUMO+2 (54%) HOMO-5→LUMO+3 (15%)
n=5 (C_{2v} symmetry point group)	S_1	$X^1A_1 \rightarrow 1^1B_1$	488	1.8603	HOMO→LUMO (88%)
	S_2	$X^1A_1 \rightarrow 1^1A_1$	464	0.0034	HOMO-1→LUMO (53%) HOMO→LUMO+1 (38%)
	S_5	$X^1A_1 \rightarrow 1^1B_2$	442	0.1200	HOMO-2→LUMO (76%) HOMO-5→LUMO+1 (8%)
	S_6	$X^1A_1 \rightarrow 3^1B_1$	441	0.0349	HOMO-6→LUMO (76%) HOMO-3→LUMO+1 (20%)
TSCs (Type **II**)					
n=2 (C_1 symmetry point group)	S_1	$X^1A \rightarrow 1^1A$	497	0.0437	HOMO→LUMO (96%)
	S_2	$X^1A \rightarrow 2^1A$	486	0.2867	HOMO→LUMO+1 (81%) HOMO-1→LUMO (9%)
	S_3	$X^1A \rightarrow 3^1A$	443	0.6007	HOMO-1→LUMO (85%) HOMO→LUMO+1 (9%)
	S_6	$X^1A \rightarrow 6^1A$	433	0.0151	HOMO-4→LUMO (79%) HOMO-1→LUMO+1 (8%) HOMO-6→LUMO (7%)
	S_8	$X^1A \rightarrow 8^1A$	426	0.0563	HOMO-4→LUMO+1 (52%) HOMO-6→LUMO+1 (18%) HOMO-1→LUMO+1 (17%)
	S_9	$X^1A \rightarrow 9^1A$	420	0.3575	HOMO-6→LUMO (53%) HOMO-6→LUMO+1 (29%)
	S_{12}	$X^1A \rightarrow 12^1A$	413	0.2573	HOMO-1→LUMO+1 (67%) HOMO-4→LUMO+1 (13%) HOMO-4→LUMO (12%)
	S_{15}	$X^1A \rightarrow 15^1A$	401	0.5448	HOMO-6→LUMO+1 (41%) HOMO-6→LUMO (29%) HOMO-4→LUMO+1 (17%)
n=3 (C_2 symmetry	S_1	$X^1A \rightarrow 1^1A$	527	0	HOMO→LUMO (97%)

point group)					
	S_2	$X^1A \rightarrow 1^1B$	502	0.1407	HOMO→LUMO+1 (91%)
	S_3	$X^1A \rightarrow 2^1B$	500	0.7857	HOMO→LUMO+2 (88%)
	S_4	$X^1A \rightarrow 2^1A$	471	0.0063	HOMO→LUMO+3 (48%) HOMO-1→LUMO+2 (16%) HOMO-2→LUMO (14%)
	S_7	$X^1A \rightarrow 4^1B$	446	0.9895	HOMO-3→LUMO (52%) HOMO-5→LUMO (17%) HOMO-2→LUMO+1 (17%)
	S_8	$X^1A \rightarrow 4^1A$	441	0.0572	HOMO-2→LUMO (53%) HOMO→LUMO+3 (30%) HOMO-3→LUMO+1 (8%)
	S_9	$X^1A \rightarrow 5^1B$	440	0.2555	HOMO-5→LUMO (69%) HOMO-2→LUMO+1 (13%) HOMO-9→LUMO (6%)
	S_{11}	$X^1A \rightarrow 6^1B$	434	0.0852	HOMO-7→LUMO (58%) HOMO-6→LUMO+2 (8%) HOMO-4→LUMO+1 (7%) HOMO-6→LUMO+1 (7%)
	S_{12}	$X^1A \rightarrow 6^1A$	433	0.0210	HOMO-8→LUMO (21%) HOMO-1→LUMO+2 (21%) HOMO-4→LUMO (18%) HOMO-7→LUMO+1 (12%) HOMO-6→LUMO (6%)
	S_{14}	$X^1A \rightarrow 7^1B$	426	0.4466	HOMO-9→LUMO (31%) HOMO-8→LUMO+1 (23%) HOMO-3→LUMO (11%) HOMO-6→LUMO+2 (6%) HOMO-6→LUMO+1 (6%)
	S_{15}	$X^1A \rightarrow 8^1A$	424	0.0422	HOMO-6→LUMO (27%) HOMO-8→LUMO (22%) HOMO-3→LUMO+1 (11%) HOMO-1→LUMO+2 (10%) HOMO-7→LUMO+2 (6%) HOMO-7→LUMO+1 (6%)
	S_{16}	$X^1A \rightarrow 8^1B$	419	0.0568	HOMO-1→LUMO+3 (37%) HOMO-4→LUMO+2 (23%) HOMO-6→LUMO+2 (9%) HOMO-7→LUMO+3 (7%) HOMO-4→LUMO+1 (6%)
	S_{18}	$X^1A \rightarrow 9^1B$	417	0.1874	HOMO-6→LUMO+2 (27%) HOMO-1→LUMO+3 (18%) HOMO-9→LUMO+3 (12%) HOMO-6→LUMO+1 (11%) HOMO-8→LUMO+2 (6%)
n=4 (C_1 symmetry point group)	S_1	$X^1A \rightarrow 1^1A$	535	0.0001	HOMO→LUMO (93%)
	S_2	$X^1A \rightarrow 2^1A$	518	0.0083	HOMO→LUMO+1 (78%) HOMO-1→LUMO (17%)
	S_3	$X^1A \rightarrow 3^1A$	503	0.0173	HOMO→LUMO+3 (78%) HOMO-1→LUMO+1 (17%)
	S_4	$X^1A \rightarrow 4^1A$	502	1.6174	HOMO→LUMO+2 (81%) HOMO-1→LUMO+4 (11%)
	S_9	$X^1A \rightarrow 9^1A$	458	0.0453	HOMO-1→LUMO+4 (21%) HOMO→LUMO+5 (15%) HOMO-2→LUMO+2 (11%) HOMO-8→LUMO (9%)
	S_{12}	$X^1A \rightarrow 12^1A$	444	0.2378	HOMO-5→LUMO (37%) HOMO-7→LUMO (26%) HOMO-6→LUMO+1 (13%) HOMO-4→LUMO+1 (6%)

	S_{14}	$X^1A \rightarrow 14^1A$	442	1.4065	HOMO-4→LUMO+1 (25%) HOMO-3→LUMO+3 (15%) HOMO-8→LUMO (10%) HOMO-3→LUMO (9%) HOMO-12→LUMO (9%)
	S_{19}	$X^1A \rightarrow 19^1A$	432	0.5003	HOMO-9→LUMO+1 (24%) HOMO-10→LUMO (20%) HOMO-7→LUMO+3 (8%) HOMO-5→LUMO (6%)
n=5 (C_2 symmetry point group)	S_1	$X^1A \rightarrow 1^1A$	540	0	HOMO→LUMO (88%) HOMO-1→LUMO+1 (7%)
	S_2	$X^1A \rightarrow 1^1B$	528	0.0088	HOMO→LUMO+1 (65%) HOMO-1→LUMO (27%)
	S_4	$X^1A \rightarrow 2^1B$	505	2.5225	HOMO→LUMO+3 (70%) HOMO-1→LUMO+5 (15%) HOMO→LUMO+6 (7%)
	S_5	$X^1A \rightarrow 3^1B$	503	0.0526	HOMO→LUMO+4 (63%) HOMO-1→LUMO+2 (27%) HOMO-2→LUMO+1 (6%)
	S_6	$X^1A \rightarrow 4^1B$	496	0.0103	HOMO-1→LUMO (61%) HOMO→LUMO+1 (21%) HOMO-2→LUMO+1 (6%)
	S_7	$X^1A \rightarrow 3^1A$	490	0.0102	HOMO→LUMO+5 (44%) HOMO-1→LUMO+3 (38%) HOMO-2→LUMO+5 (5%)
	S_9	$X^1A \rightarrow 5^1B$	470	0.0084	HOMO→LUMO+6 (23%) HOMO-1→LUMO+5 (21%) HOMO-2→LUMO+3 (16%)
	S_{10}	$X^1A \rightarrow 6^1B$	469	0.0034	HOMO-1→LUMO+2 (26%) HOMO→LUMO+4 (23%) HOMO-2→LUMO+1 (16%) HOMO-3→LUMO (8%)
	S_{13}	$X^1A \rightarrow 7^1B$	456	0.0048	HOMO-2→LUMO+1 (39%) HOMO-1→LUMO+2 (22%) HOMO-3→LUMO (13%) HOMO→LUMO+1 (6%)
	S_{14}	$X^1A \rightarrow 7^1A$	456	0.0038	HOMO→LUMO+5 (31%) HOMO-2→LUMO+5 (14%) HOMO-1→LUMO+3 (13%) HOMO-4→LUMO (9%)
	S_{15}	$X^1A \rightarrow 8^1A$	452	0.0071	HOMO-1→LUMO+3 (24%) HOMO→LUMO+5 (20%) HOMO-1→LUMO+6 (16%) HOMO-4→LUMO (7%)
	S_{16}	$X^1A \rightarrow 8^1B$	445	0.0310	HOMO-7→LUMO (50%) HOMO-3→LUMO+2 (12%) HOMO-7→LUMO+2 (7%) HOMO-2→LUMO+4 (7%)
	S_{17}	$X^1A \rightarrow 9^1B$	445	1.0553	HOMO-8→LUMO (26%) HOMO-6→LUMO+1 (11%) HOMO-9→LUMO+1 (9%) HOMO-5→LUMO+2 (7%) HOMO-4→LUMO+1 (6%) HOMO→LUMO+6 (6%)
	S_{20}	$X^1A \rightarrow 10^1B$	443	0.1826	HOMO→LUMO+6 (37%) HOMO→LUMO+3 (20%) HOMO-1→LUMO+5 (17%) HOMO-8→LUMO (7%)
TSCs (Type **III**)					
n=2 (C_1 symmetry	S_1	$X^1A \rightarrow 1^1A$	695	0.0079	HOMO→LUMO (98%)

point group)					
	S_2	$X^1A \rightarrow 2^1A$	528	0.0343	HOMO→LUMO+1 (89%) HOMO-5→LUMO (6%)
	S_3	$X^1A \rightarrow 3^1A$	508	0.2631	HOMO-1→LUMO (79%) HOMO-2→LUMO (16%)
	S_4	$X^1A \rightarrow 4^1A$	487	0.0090	HOMO-4→LUMO (94%)
	S_5	$X^1A \rightarrow 5^1A$	482	0.2060	HOMO-2→LUMO (80%) HOMO-1→LUMO (16%)
	S_7	$X^1A \rightarrow 7^1A$	479	0.0732	HOMO-5→LUMO (79%) HOMO→LUMO+1 (9%)
	S_9	$X^1A \rightarrow 9^1A$	441	0.0401	HOMO-7→LUMO (82%) HOMO-5→LUMO (10%)
	S_{11}	$X^1A \rightarrow 11^1A$	395	0.3739	HOMO-3→LUMO+1 (61%) HOMO→LUMO+2 (33%)
	S_{13}	$X^1A \rightarrow 13^1A$	388	0.0220	HOMO-5→LUMO+1 (74%) HOMO→LUMO+3 (20%)
	S_{14}	$X^1A \rightarrow 14^1A$	388	0.0676	HOMO-4→LUMO+1 (84%) HOMO-7→LUMO (6%)
	S_{15}	$X^1A \rightarrow 15^1A$	387	0.5168	HOMO→LUMO+2 (54%) HOMO-3→LUMO+1 (30%) HOMO-6→LUMO+1 (9%)
	S_{17}	$X^1A \rightarrow 17^1A$	383	0.0109	HOMO→LUMO+4 (91%)
	S_{18}	$X^1A \rightarrow 18^1A$	374	0.0020	HOMO-6→LUMO+1 (87%)
	S_{19}	$X^1A \rightarrow 19^1A$	365	0.0107	HOMO-7→LUMO+1 (64%) HOMO→LUMO+3 (25%)
n=3 (C_2 symmetry point group)	S_1	$X^1A \rightarrow 1^1B$	779	0	HOMO→LUMO (95%)
	S_2	$X^1A \rightarrow 1^1A$	718	0.0004	HOMO-1→LUMO (94%)
	S_3	$X^1A \rightarrow 2^1A$	595	0.0359	HOMO→LUMO+1 (89%)
	S_4	$X^1A \rightarrow 2^1B$	586	0.0003	HOMO-1→LUMO+1 (88%) HOMO→LUMO+2 (8%)
	S_5	$X^1A \rightarrow 3^1B$	540	0.7386	HOMO-2→LUMO (91%)
	S_8	$X^1A \rightarrow 4^1A$	499	0.0056	HOMO-7→LUMO (67%) HOMO-1→LUMO+2 (14%) HOMO-6→LUMO+1 (12%)
	S_{10}	$X^1A \rightarrow 6^1B$	497	0.1529	HOMO-5→LUMO (84%) HOMO-4→LUMO+1 (7%)
	S_{12}	$X^1A \rightarrow 6^1A$	486	0.0821	HOMO-1→LUMO+2 (78%) HOMO-7→LUMO (13%)
	S_{15}	$X^1A \rightarrow 8^1A$	454	0.0703	HOMO-10→LUMO (83%) HOMO-7→LUMO (6%)
	S_{20}	$X^1A \rightarrow 10^1B$	429	0.1344	HOMO-4→LUMO+1 (80%) HOMO-5→LUMO+2 (7%) HOMO-5→LUMO (7%)
n=4 (C_1 symmetry point group)	S_1	$X^1A \rightarrow 1^1A$	805	0.0008	HOMO→LUMO (80%) HOMO-2→LUMO (10%) HOMO-1→LUMO+1 (7%)
	S_2	$X^1A \rightarrow 2^1A$	759	0.0001	HOMO-1→LUMO (77%) HOMO→LUMO+1 (20%)
	S_3	$X^1A \rightarrow 3^1A$	721	0.0037	HOMO-2→LUMO (84%) HOMO-1→LUMO+1 (9%)
	S_4	$X^1A \rightarrow 4^1A$	641	0.0188	HOMO→LUMO+1 (63%) HOMO-2→LUMO+1 (17%) HOMO-1→LUMO (15%)
	S_5	$X^1A \rightarrow 5^1A$	625	0.0026	HOMO-1→LUMO+1 (72%) HOMO→LUMO (11%) HOMO→LUMO+2 (8%)
	S_7	$X^1A \rightarrow 7^1A$	553	0.0095	HOMO→LUMO+2 (75%) HOMO-1→LUMO+3 (11%) HOMO-1→LUMO+1 (8%)

	S_8	$X^1A \rightarrow 8^1A$	551	1.2660	HOMO-3→LUMO (83%) HOMO-4→LUMO+1 (9%)
	S_9	$X^1A \rightarrow 9^1A$	548	0.0381	HOMO-1→LUMO+2 (66%) HOMO→LUMO+3 (15%) HOMO-2→LUMO+1 (8%)
	S_{11}	$X^1A \rightarrow 11^1A$	535	0.0108	HOMO-5→LUMO (62%) HOMO-7→LUMO (26%)
	S_{12}	$X^1A \rightarrow 12^1A$	527	0.0066	HOMO-2→LUMO+2 (90%)
	S_{14}	$X^1A \rightarrow 14^1A$	501	0.0237	HOMO-8→LUMO (68%) HOMO-9→LUMO+1 (22%)
	S_{16}	$X^1A \rightarrow 16^1A$	500	0.1045	HOMO-7→LUMO (49%) HOMO-5→LUMO (19%) HOMO-6→LUMO+1 (16%)
	S_{18}	$X^1A \rightarrow 18^1A$	492	0.0014	HOMO→LUMO+3 (65%) HOMO-1→LUMO+2 (13%) HOMO-2→LUMO+3 (11%)
	S_{19}	$X^1A \rightarrow 19^1A$	478	0.0111	HOMO-1→LUMO+3 (81%) HOMO→LUMO+2 (10%)
n=5 (D_2 symmetry point group)	S_1	$X^1A \rightarrow 1^1B_1$	818	0	HOMO→LUMO (68%) HOMO-2→LUMO (15%) HOMO-1→LUMO+1 (9%)
	S_2	$X^1A \rightarrow 1^1B_2$	784	0.0001	HOMO-1→LUMO (52%) HOMO→LUMO+1 (28%) HOMO-3→LUMO (15%)
	S_5	$X^1A \rightarrow 3^1B_2$	661	0.0208	HOMO→LUMO+1 (53%) HOMO-1→LUMO (21%) HOMO-2→LUMO+1 (16%)
	S_{10}	$X^1A \rightarrow 5^1B_2$	582	0.0374	HOMO-1→LUMO+2 (62%) HOMO→LUMO+3 (11%) HOMO-2→LUMO+1 (9%) HOMO→LUMO+1 (9%)
	S_{12}	$X^1A \rightarrow 6^1B_2$	568	0.0051	HOMO-3→LUMO+2 (86%)
	S_{13}	$X^1A \rightarrow 1^1B_3$	560	1.7869	HOMO-4→LUMO (73%) HOMO-5→LUMO+1 (9%) HOMO-6→LUMO (9%)
	S_{16}	$X^1A \rightarrow 2^1B_3$	537	0.0480	HOMO-6→LUMO (61%) HOMO-5→LUMO+1 (14%) HOMO-7→LUMO+1 (11%)
	S_{17}	$X^1A \rightarrow 7^1B_2$	529	0.0098	HOMO→LUMO+3 (60%) HOMO-1→LUMO+4 (16%) HOMO-1→LUMO+2 (14%)
	S_{19}	$X^1A \rightarrow 8^1B_2$	511	0.0270	HOMO-2→LUMO+3 (72%) HOMO→LUMO+3 (7%) HOMO-3→LUMO+4 (5%)

Table S3. Wavelengths (λ), oscillator strengths (*f*) and orbital assignment of the selected electronic transitions in the calculated absorption spectra of the **TOC**-based oligomers (n=3)

Compound	State	Transition	λ, nm	f	Assignment
TOC (type **I**)					
n=3 (D_{2h} symmetry point group)	S_1	$X^1A_g \rightarrow 1^1B_{1u}$	499	1.5459	HOMO→LUMO (97%)
	S_2	$X^1A_g \rightarrow 1^1B_{3g}$	466	0.0000	HOMO-1→LUMO (94%)
	S_3	$X^1A_g \rightarrow 1^1B_{2u}$	438	0.0224	HOMO-3→LUMO (84%) HOMO-1→LUMO+1 (8%)
	S_4	$X^1A_g \rightarrow 1^1A_g$	423	0.0000	HOMO-2→LUMO (94%)
	S_5	$X^1A_g \rightarrow 2^1A_g$	420	0.0000	HOMO→LUMO+1 (95%)
TOC (type **II**)					
n=3 (D_{2h} symmetry point group)	S_1	$X^1A_g \rightarrow 1^1B_{1u}$	502	1.7004	HOMO→LUMO (94%)
	S_2	$X^1A_g \rightarrow 1^1B_{3g}$	463	0.0000	HOMO→LUMO+1 (95%)
	S_3	$X^1A_g \rightarrow 1^1A_g$	446	0.0000	HOMO→LUMO+2 (62%) HOMO-1→LUMO (23%)
	S_4	$X^1A_g \rightarrow 1^1B_{2u}$	433	0.0005	HOMO→LUMO+3 (90%)
	S_5	$X^1A_g \rightarrow 2^1A_g$	428	0.0000	HOMO-1→LUMO (64%) HOMO→LUMO+2 (31%)
TOC (type **III**)					
n=3 (D_{2h} symmetry point group)	S_1	$X^1A_g \rightarrow 1^1B_{3g}$	766	0.0000	HOMO→LUMO (96%)
	S_2	$X^1A_g \rightarrow 1^1B_{2u}$	667	0.0001	HOMO-1→LUMO+1 (91%)
	S_3	$X^1A_g \rightarrow 2^1B_{2u}$	574	0.0202	HOMO→LUMO+1 (88%) HOMO-1→LUMO (8%)
	S_4	$X^1A_g \rightarrow 2^1B_{3g}$	544	0.0000	HOMO-1→LUMO+1 (87%)
	S_5	$X^1A_g \rightarrow 3^1B_{3g}$	475	0.0000	HOMO→LUMO+2 (66%) HOMO-2→LUMO (17%)

Table S4. The optimized Cartesian coordinates of the tetrathia[8]circulene (**TTC**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.822081	3.319165	0.002767
2	6	2.822081	-3.319165	0.002767
3	6	-3.319165	-2.822081	-0.002767
4	6	3.319165	2.822081	-0.002767
5	6	3.711728	-2.281243	-0.002767
6	6	-3.711728	2.281243	-0.002767
7	6	-2.281243	-3.711728	0.002767
8	6	2.281243	3.711728	0.002767
9	6	-1.703121	-0.874946	-0.001869
10	6	1.703121	0.874946	-0.001869
11	6	0.874946	-1.703121	0.001869
12	6	-0.874946	1.703121	0.001869
13	6	-0.604176	-1.816900	0.001869
14	6	0.604176	1.816900	0.001869
15	6	-1.816900	0.604176	-0.001869
16	6	1.816900	-0.604176	-0.001869
17	6	-3.006375	-1.459836	-0.004716
18	6	3.006375	1.459836	-0.004716
19	6	1.459836	-3.006375	0.004716
20	6	-1.459836	3.006375	0.004716
21	6	-0.982863	-3.194275	0.004716
22	6	0.982863	3.194275	0.004716
23	6	-3.194275	0.982863	-0.004716
24	6	3.194275	-0.982863	-0.004716
25	16	-0.332423	4.321495	0.009293
26	16	0.332423	-4.321495	0.009293
27	16	-4.321495	-0.332423	-0.009293
28	16	4.321495	0.332423	-0.009293
29	1	2.444215	4.784938	0.005381
30	1	4.354824	3.147274	-0.005381
31	1	4.784938	-2.444215	-0.005381
32	1	3.147274	-4.354824	0.005381
33	1	-2.444215	-4.784938	0.005381
34	1	-4.354824	-3.147274	-0.005381
35	1	-4.784938	2.444215	-0.005381
36	1	-3.147274	4.354824	0.005381

Table S5. The optimized Cartesian coordinates of the directly fused **TTC**-based ribbon with n=2 (type **I**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.998721	1.486051	-0.933322
2	6	6.047209	0.573384	0.436926
3	6	4.998560	1.485709	0.933864
4	6	-6.047339	0.573611	-0.436450
5	6	4.998494	-1.485702	-0.934115
6	6	-6.047273	-0.573956	0.436638
7	6	-4.998482	-1.486192	0.933562
8	6	6.047233	-0.573633	-0.436854
9	6	-3.573408	-1.596938	0.718858
10	6	2.525832	-0.699347	-0.200681
11	6	3.573531	-1.596799	-0.718974
12	6	-2.525706	-0.699363	0.200652
13	6	3.573659	1.597099	0.718423
14	6	-2.525792	0.699609	-0.200601
15	6	-3.573666	1.597075	-0.718589
16	6	2.525859	0.699752	0.200164
17	6	-5.585975	-2.532656	1.703056
18	6	1.259957	1.334642	0.211393
19	6	5.585973	-2.531824	-1.704048

20	6	-1.259815	1.334449	-0.212269
21	6	5.586062	2.531666	1.704020
22	6	-1.259668	-1.334012	0.212290
23	6	-5.586392	2.532419	-1.702816
24	6	1.259892	-1.334129	-0.211924
25	6	-2.987638	2.819691	-1.151519
26	6	7.330964	-1.016672	-0.871410
27	6	2.987657	2.819789	1.151127
28	6	-7.331008	-1.017394	0.870806
29	6	2.987379	-2.819418	-1.151736
30	6	-7.331148	1.016799	-0.870694
31	6	-2.987114	-2.819401	1.151918
32	6	7.330942	1.016261	0.871682
33	6	4.937919	-3.673225	-2.189545
34	6	-4.937852	-3.673956	2.188677
35	6	0.000078	0.697931	-0.000321
36	6	-4.938487	3.673881	-2.188344
37	6	4.938118	3.673167	2.189418
38	6	0.000102	-0.697392	0.000066
39	6	-3.619398	3.844746	-1.863763
40	6	3.619303	3.844529	1.863932
41	6	8.566486	-0.505759	-0.462273
42	6	-8.566587	-0.506266	0.462108
43	6	3.618981	-3.844287	-1.864395
44	6	-3.618694	-3.844525	1.864223
45	6	8.566463	0.505185	0.462758
46	6	-8.566650	0.505437	-0.462070
47	16	-7.303894	2.395930	-1.926545
48	16	7.303479	2.394781	1.928366
49	16	7.303480	-2.395290	-1.927988
50	16	-7.303534	-2.396580	1.926592
51	16	-1.296461	-2.965273	0.819206
52	16	1.296839	-2.965584	-0.818423
53	16	1.297177	2.966235	0.817568
54	16	-1.297004	2.965857	-0.818785
55	1	-3.064304	4.727208	-2.166197
56	1	-3.063427	-4.726843	2.166760
57	1	3.063888	-4.726783	-2.166733
58	1	5.486660	-4.415045	-2.761208
59	1	5.486864	4.414826	2.761287
60	1	3.064315	4.727123	2.166177
61	1	-5.487438	4.415826	-2.759645
62	1	-5.486676	-4.416014	2.759953
63	1	-9.489979	0.928734	-0.844984
64	1	-9.489859	-0.929743	0.844957
65	1	9.489779	0.928150	0.846067
66	1	9.489815	-0.928860	-0.845396

Table S6. The optimized Cartesian coordinates of the directly fused **TTC**-based ribbon with n=3 (type **I**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.711862	1.731540	-7.626656
2	6	0.789719	1.739663	9.069606
3	6	-1.070628	0.722692	-1.748682
4	6	-1.478948	1.694391	-0.721260
5	6	0.342734	0.725765	-6.606348
6	6	0.607929	0.719699	10.120248
7	6	-1.478949	-1.694392	-0.721260
8	6	0.342734	-0.725765	-6.606348
9	6	0.607929	-0.719698	10.120248
10	6	0.711862	-1.731540	-7.626656
11	6	0.789719	-1.739663	9.069607
12	6	-1.070629	-0.722693	-1.748681
13	6	0.789719	-1.739663	-9.069607
14	6	0.711862	-1.731540	7.626656
15	6	-1.070629	-0.722693	1.748681
16	6	-1.478949	-1.694392	0.721260
17	6	0.607929	-0.719698	-10.120248

18	6	0.342734	-0.725765	6.606348
19	6	-1.478948	1.694391	0.721260
20	6	0.607929	0.719699	-10.120248
21	6	0.342734	0.725765	6.606348
22	6	0.789719	1.739663	-9.069606
23	6	0.711862	1.731540	7.626656
24	6	-1.070628	0.722692	1.748682
25	6	0.906515	-2.994390	-7.002432
26	6	1.001031	-3.016848	9.668268
27	6	-0.863102	1.352820	2.998900
28	6	-1.790211	-2.935875	-1.336015
29	6	0.537974	1.337739	-11.402939
30	6	0.093878	1.347375	5.354860
31	6	-1.790209	2.935874	-1.336015
32	6	0.537974	-1.337738	-11.402940
33	6	0.093878	-1.347377	5.354861
34	6	0.906514	2.994391	-7.002431
35	6	1.001030	3.016849	9.668266
36	6	-0.863103	-1.352821	2.998901
37	6	1.001030	3.016849	-9.668266
38	6	0.906514	2.994391	7.002431
39	6	-0.863103	-1.352821	-2.998901
40	6	-1.790209	2.935874	1.336015
41	6	0.093878	-1.347377	-5.354861
42	6	0.537974	-1.337738	11.402940
43	6	-1.790211	-2.935875	1.336015
44	6	0.093878	1.347375	-5.354860
45	6	0.537974	1.337739	11.402939
46	6	1.001031	-3.016848	-9.668268
47	6	0.906515	-2.994390	7.002432
48	6	-0.863102	1.352820	-2.998900
49	6	-2.232517	-4.094236	-0.685327
50	6	1.244286	-4.198229	-7.630082
51	6	1.281032	-4.212346	8.998410
52	6	0.353780	0.685333	-12.625581
53	6	-0.381773	0.702016	4.175426
54	6	1.244285	4.198230	-7.630081
55	6	1.281031	4.212347	8.998407
56	6	-2.232514	4.094235	-0.685328
57	6	0.353780	-0.685331	-12.625582
58	6	-0.381773	-0.702017	4.175427
59	6	1.281031	4.212347	-8.998407
60	6	1.244285	4.198230	7.630081
61	6	-2.232514	4.094235	0.685328
62	6	-0.381773	-0.702017	-4.175427
63	6	0.353780	-0.685331	12.625582
64	6	-2.232517	-4.094236	0.685327
65	6	1.281032	-4.212346	-8.998410
66	6	1.244286	-4.198229	7.630082
67	6	-0.381773	0.702016	-4.175426
68	6	0.353780	0.685333	12.625581
69	16	0.548330	3.027227	-5.311695
70	16	0.817540	3.051926	11.395463
71	16	-1.426939	3.005055	-3.029268
72	16	-1.426941	-3.005057	-3.029268
73	16	0.548331	-3.027227	-5.311695
74	16	0.817541	-3.051924	11.395465
75	16	0.817541	-3.051924	-11.395465
76	16	0.548331	-3.027227	5.311695
77	16	-1.426941	-3.005057	3.029268
78	16	-1.426939	3.005055	3.029268
79	16	0.817540	3.051926	-11.395463
80	16	0.548330	3.027227	5.311695
81	1	1.476313	5.122864	-9.556240
82	1	1.405904	5.097152	7.043333
83	1	1.476315	-5.122862	-9.556243
84	1	1.405905	-5.097153	7.043335
85	1	-2.495828	-4.979583	1.255665
86	1	-2.495828	-4.979583	-1.255665
87	1	-2.495824	4.979583	-1.255666
88	1	-2.495824	4.979583	1.255666
89	1	1.405904	5.097152	-7.043333
90	1	1.476313	5.122864	9.556240
91	1	1.405905	-5.097153	-7.043335
92	1	1.476315	-5.122862	9.556243
93	1	0.269349	1.255532	13.545507
94	1	0.269349	-1.255529	13.545508
95	1	0.269349	1.255532	-13.545507
96	1	0.269349	-1.255529	-13.545508

Table S7. The optimized Cartesian coordinates of the directly fused **TTC**-based ribbon with n=4 (type **I**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.240201	3.402509	1.699228
2	6	0.484450	-13.304316	1.739361
3	6	-0.243449	14.343136	0.719651
4	6	-0.791505	-2.396373	0.722901
5	6	-0.484450	13.304316	1.739361
6	6	-1.240201	-3.402509	1.699228
7	6	0.791505	2.396373	0.722901
8	6	0.243449	-14.343136	0.719651
9	6	-0.484450	13.304316	-1.739361
10	6	-1.240201	-3.402509	-1.699228
11	6	0.791505	2.396373	-0.722901
12	6	0.243449	-14.343136	-0.719651
13	6	1.240201	3.402509	-1.699228
14	6	0.484450	-13.304316	-1.739361
15	6	-0.243449	14.343136	-0.719651
16	6	-0.791505	-2.396373	-0.722901
17	6	1.317466	4.843194	-1.697788
18	6	0.487369	-11.859295	-1.731125
19	6	-0.174342	10.820008	-0.725748
20	6	-0.970965	-5.891121	-0.722972
21	6	-0.487369	11.859295	-1.731125
22	6	-1.317466	-4.843194	-1.697788
23	6	0.970965	5.891121	-0.722972
24	6	0.174342	-10.820008	-0.725748
25	6	-0.487369	11.859295	1.731125
26	6	-1.317466	-4.843194	1.697788
27	6	0.970965	5.891121	0.722972
28	6	0.174342	-10.820008	0.725748
29	6	1.317466	4.843194	1.697788
30	6	0.487369	-11.859295	1.731125
31	6	-0.174342	10.820008	0.725748
32	6	-0.970965	-5.891121	0.722972
33	6	1.506285	2.773709	-2.945071
34	6	0.662791	-13.913808	-3.016421
35	6	0.004771	9.556719	1.347494
36	6	-0.831011	-7.151511	1.352313
37	6	-0.662791	13.913808	-3.016421
38	6	-1.506285	-2.773709	-2.945071
39	6	0.831011	7.151511	1.352313
40	6	-0.004771	-9.556719	1.347494
41	6	-0.662791	13.913808	3.016421
42	6	-1.506285	-2.773709	2.945071
43	6	0.831011	7.151511	-1.352313
44	6	-0.004771	-9.556719	-1.347494
45	6	1.506285	2.773709	2.945071
46	6	0.662791	-13.913808	3.016421
47	6	0.004771	9.556719	-1.347494
48	6	-0.831011	-7.151511	-1.352313
49	6	1.654645	5.441090	2.940921
50	6	0.717818	-11.246875	2.993650
51	6	-0.101738	15.619823	-1.337765
52	6	-0.522757	-1.157255	-1.351916
53	6	-0.717818	11.246875	2.993650
54	6	-1.654645	-5.441090	2.940921
55	6	0.522757	1.157255	-1.351916
56	6	0.101738	-15.619823	-1.337765
57	6	-0.717818	11.246875	-2.993650
58	6	-1.654645	-5.441090	-2.940921
59	6	0.522757	1.157255	1.351916
60	6	0.101738	-15.619823	1.337765
61	6	1.654645	5.441090	-2.940921
62	6	0.717818	-11.246875	-2.993650
63	6	-0.101738	15.619823	1.337765
64	6	-0.522757	-1.157255	1.351916
65	6	-0.981158	13.260601	-4.211540
66	6	-1.972798	-3.400975	-4.106602

67	6	1.972798	3.400975	-4.106602
68	6	0.981158	-13.260601	-4.211540
69	6	0.415406	8.353028	0.701930
70	6	-0.415406	-8.353028	0.701930
71	6	1.972798	3.400975	4.106602
72	6	0.981158	-13.260601	4.211540
73	6	-0.981158	13.260601	4.211540
74	6	-1.972798	-3.400975	4.106602
75	6	0.415406	8.353028	-0.701930
76	6	-0.415406	-8.353028	-0.701930
77	6	2.050238	4.769304	4.103998
78	6	1.021265	-11.892354	4.197226
79	6	-1.021265	11.892354	4.197226
80	6	-2.050238	-4.769304	4.103998
81	6	0.150971	16.830167	-0.685357
82	6	0.000000	0.000000	-0.702979
83	6	-0.150971	-16.830167	-0.685357
84	6	-1.021265	11.892354	-4.197226
85	6	-2.050238	-4.769304	-4.103998
86	6	2.050238	4.769304	-4.103998
87	6	1.021265	-11.892354	-4.197226
88	6	0.150971	16.830167	0.685357
89	6	0.000000	0.000000	0.702979
90	6	-0.150971	-16.830167	0.685357
91	16	1.061053	1.099711	3.010435
92	16	0.382261	-15.627953	3.051831
93	16	-0.382261	15.627953	3.051831
94	16	-1.061053	-1.099711	3.010435
95	16	-0.382261	15.627953	-3.051831
96	16	-1.061053	-1.099711	-3.010435
97	16	1.061053	1.099711	-3.010435
98	16	0.382261	-15.627953	-3.051831
99	16	1.388808	7.152019	-3.006478
100	16	0.453531	-9.538973	-3.026903
101	16	-0.453531	9.538973	-3.026903
102	16	-1.388808	-7.152019	-3.006478
103	16	-0.453531	9.538973	3.026903
104	16	-1.388808	-7.152019	3.006478
105	16	1.388808	7.152019	3.006478
106	16	0.453531	-9.538973	3.026903
107	1	2.338239	5.326104	4.990268
108	1	1.216397	-11.315513	5.095912
109	1	2.338239	5.326104	-4.990268
110	1	1.216397	-11.315513	-5.095912
111	1	-1.216397	11.315513	-5.095912
112	1	-2.338239	-5.326104	-4.990268
113	1	-1.145708	13.828401	-5.121966
114	1	-2.196684	-2.818507	-4.994878
115	1	-1.145708	13.828401	5.121966
116	1	-2.196684	-2.818507	4.994878
117	1	-1.216397	11.315513	5.095912
118	1	-2.338239	-5.326104	4.990268
119	1	2.196684	2.818507	4.994878
120	1	1.145708	-13.828401	5.121966
121	1	2.196684	2.818507	-4.994878
122	1	1.145708	-13.828401	-5.121966
123	1	-0.286881	-17.743930	1.255498
124	1	-0.286881	-17.743930	-1.255498
125	1	0.286881	17.743930	1.255498
126	1	0.286881	17.743930	-1.255498

Table S8. The optimized Cartesian coordinates of the directly fused **TTC**-based ribbon with n=5 (type **I**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-16.002580	1.731110	-0.881047
2	6	0.721493	1.702609	-0.789603
3	6	17.445612	1.739352	-0.956291
4	6	-10.123428	0.722955	0.902190

5	6	6.624095	0.722895	0.916276
6	6	-9.096319	1.697519	1.306694
7	6	7.653579	1.698857	1.309433
8	6	-14.981884	0.725740	-0.511938
9	6	1.750654	0.723185	-0.401812
10	6	18.495933	0.719643	-0.771702
11	6	-9.096319	-1.697519	1.306694
12	6	7.653579	-1.698857	1.309433
13	6	-14.981884	-0.725740	-0.511938
14	6	1.750654	-0.723185	-0.401812
15	6	18.495933	-0.719643	-0.771702
16	6	-16.002580	-1.731110	-0.881047
17	6	0.721493	-1.702609	-0.789603
18	6	17.445612	-1.739352	-0.956291
19	6	-10.123428	-0.722955	0.902190
20	6	6.624095	-0.722895	0.916276
21	6	-17.445612	-1.739352	-0.956291
22	6	-0.721493	-1.702609	-0.789603
23	6	16.002580	-1.731110	-0.881047
24	6	-6.624095	-0.722895	0.916276
25	6	10.123428	-0.722955	0.902190
26	6	-7.653579	-1.698857	1.309433
27	6	9.096319	-1.697519	1.306694
28	6	-18.495933	-0.719643	-0.771702
29	6	-1.750654	-0.723185	-0.401812
30	6	14.981884	-0.725740	-0.511938
31	6	-7.653579	1.698857	1.309433
32	6	9.096319	1.697519	1.306694
33	6	-18.495933	0.719643	-0.771702
34	6	-1.750654	0.723185	-0.401812
35	6	14.981884	0.725740	-0.511938
36	6	-17.445612	1.739352	-0.956291
37	6	-0.721493	1.702609	-0.789603
38	6	16.002580	1.731110	-0.881047
39	6	-6.624095	0.722895	0.916276
40	6	10.123428	0.722955	0.902190
41	6	-15.378499	-2.993593	-1.078065
42	6	1.335499	-2.950053	-1.082301
43	6	18.044545	-3.016409	-1.167326
44	6	-5.372048	1.352015	0.716488
45	6	11.374087	1.352350	0.692767
46	6	-9.711973	-2.940515	1.610789
47	6	7.040478	-2.944377	1.610947
48	6	-19.778384	1.337776	-0.699060
49	6	-3.003288	1.351398	-0.200258
50	6	13.730224	1.347472	-0.264396
51	6	-9.711973	2.940515	1.610789
52	6	7.040478	2.944377	1.610947
53	6	-19.778384	-1.337776	-0.699060
54	6	-3.003288	-1.351398	-0.200258
55	6	13.730224	-1.347472	-0.264396
56	6	-15.378499	2.993593	-1.078065
57	6	1.335499	2.950053	-1.082301
58	6	18.044545	3.016409	-1.167326
59	6	-5.372048	-1.352015	0.716488
60	6	11.374087	-1.352350	0.692767
61	6	-18.044545	3.016409	-1.167326
62	6	-1.335499	2.950053	-1.082301
63	6	15.378499	2.993593	-1.078065
64	6	-11.374087	-1.352350	0.692767
65	6	5.372048	-1.352015	0.716488
66	6	-7.040478	2.944377	1.610947
67	6	9.711973	2.940515	1.610789
68	6	-13.730224	-1.347472	-0.264396
69	6	3.003288	-1.351398	-0.200258
70	6	19.778384	-1.337776	-0.699060
71	6	-7.040478	-2.944377	1.610947
72	6	9.711973	-2.940515	1.610789
73	6	-13.730224	1.347472	-0.264396
74	6	3.003288	1.351398	-0.200258
75	6	19.778384	1.337776	-0.699060
76	6	-18.044545	-3.016409	-1.167326
77	6	-1.335499	-2.950053	-1.082301
78	6	15.378499	-2.993593	-1.078065
79	6	-11.374087	1.352350	0.692767
80	6	5.372048	1.352015	0.716488
81	6	-9.063099	-4.103264	2.043851
82	6	7.692579	-4.105697	2.042681
83	6	-16.006604	-4.197137	-1.416122

84	6	0.685192	-4.116272	-1.503011
85	6	17.375038	-4.211483	-1.450022
86	6	-21.000605	0.685375	-0.512009
87	6	-4.187898	0.702882	0.257680
88	6	12.550843	0.701940	0.211558
89	6	-16.006604	4.197137	-1.416122
90	6	0.685192	4.116272	-1.503011
91	6	17.375038	4.211483	-1.450022
92	6	-9.063099	4.103264	2.043851
93	6	7.692579	4.105697	2.042681
94	6	-21.000605	-0.685375	-0.512009
95	6	-4.187898	-0.702882	0.257680
96	6	12.550843	-0.701940	0.211558
97	6	-17.375038	4.211483	-1.450022
98	6	-0.685192	4.116272	-1.503011
99	6	16.006604	4.197137	-1.416122
100	6	-7.692579	4.105697	2.042681
101	6	9.063099	4.103264	2.043851
102	6	-12.550843	-0.701940	0.211558
103	6	4.187898	-0.702882	0.257680
104	6	21.000605	-0.685375	-0.512009
105	6	-7.692579	-4.105697	2.042681
106	6	9.063099	-4.103264	2.043851
107	6	-17.375038	-4.211483	-1.450022
108	6	-0.685192	-4.116272	-1.503011
109	6	16.006604	-4.197137	-1.416122
110	6	-12.550843	0.701940	0.211558
111	6	4.187898	0.702882	0.257680
112	6	21.000605	0.685375	-0.512009
113	16	-13.687439	3.026782	-0.721409
114	16	3.031926	3.011798	-0.733824
115	16	19.771332	3.051858	-0.979677
116	16	-11.405470	3.006375	1.250152
117	16	5.344523	3.010133	1.258771
118	16	-11.405470	-3.006375	1.250152
119	16	5.344523	-3.010133	1.258771
120	16	-13.687439	-3.026782	-0.721409
121	16	3.031926	-3.011798	-0.733824
122	16	19.771332	-3.051858	-0.979677
123	16	-19.771332	-3.051858	-0.979677
124	16	-3.031926	-3.011798	-0.733824
125	16	13.687439	-3.026782	-0.721409
126	16	-5.344523	-3.010133	1.258771
127	16	11.405470	-3.006375	1.250152
128	16	-5.344523	3.010133	1.258771
129	16	11.405470	3.006375	1.250152
130	16	-19.771332	3.051858	-0.979677
131	16	-3.031926	3.011798	-0.733824
132	16	13.687439	3.026782	-0.721409
133	1	-17.933083	5.121907	-1.645110
134	1	-1.255928	5.005454	-1.752078
135	1	15.420055	5.095811	-1.579842
136	1	-17.933083	-5.121907	-1.645110
137	1	-1.255928	-5.005454	-1.752078
138	1	15.420055	-5.095811	-1.579842
139	1	-7.123356	-4.993760	2.299118
140	1	9.634955	-4.989454	2.300945
141	1	-9.634955	-4.989454	2.300945
142	1	7.123356	-4.993760	2.299118
143	1	-9.634955	4.989454	2.300945
144	1	7.123356	4.993760	2.299118
145	1	-7.123356	4.993760	2.299118
146	1	9.634955	4.989454	2.300945
147	1	-15.420055	5.095811	-1.579842
148	1	1.255928	5.005454	-1.752078
149	1	17.933083	5.121907	-1.645110
150	1	-15.420055	-5.095811	-1.579842
151	1	1.255928	-5.005454	-1.752078
152	1	17.933083	-5.121907	-1.645110
153	1	-21.920386	1.255472	-0.425597
154	1	-21.920386	-1.255472	-0.425597
155	1	21.920386	1.255472	-0.425597
156	1	21.920386	-1.255472	-0.425597

Table S9. The optimized Cartesian coordinates of the **TTC** ribbon linked via benzene-core linker with n=2 (type **II**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.772856	-4.067690	4.282218
2	6	3.312561	5.323628	4.280977
3	6	-3.312561	-5.323628	-4.280977
4	6	2.772856	4.067690	-4.282218
5	6	-4.214038	-8.857509	0.684004
6	6	0.659085	1.027008	0.708936
7	6	-0.659085	-1.027008	-0.708936
8	6	4.214038	8.857509	-0.684004
9	6	-2.772856	-4.067690	-4.282218
10	6	3.312561	5.323628	-4.280977
11	6	-3.312561	-5.323628	4.280977
12	6	2.772856	4.067690	4.282218
13	6	-4.214038	-8.857509	-0.684004
14	6	0.659085	1.027008	-0.708936
15	6	-0.659085	-1.027008	0.708936
16	6	4.214038	8.857509	0.684004
17	6	-3.404383	-6.463395	0.722524
18	6	1.954698	3.221721	0.735289
19	6	-1.954698	-3.221721	-0.735289
20	6	3.404383	6.463395	-0.722524
21	6	-3.098327	-5.455533	-1.763088
22	6	2.515806	4.128880	-1.763646
23	6	-2.515806	-4.128880	1.763646
24	6	3.098327	5.455533	1.763088
25	6	-3.404383	-6.463395	-0.722524
26	6	1.954698	3.221721	-0.735289
27	6	-1.954698	-3.221721	0.735289
28	6	3.404383	6.463395	0.722524
29	6	-3.098327	-5.455533	1.763088
30	6	2.515806	4.128880	1.763646
31	6	-2.515806	-4.128880	-1.763646
32	6	3.098327	5.455533	-1.763088
33	6	-3.849107	-7.675513	1.333268
34	6	1.362448	2.095114	1.347246
35	6	-1.362448	-2.095114	-1.347246
36	6	3.849107	7.675513	-1.333268
37	6	-3.425962	-5.978710	-3.051408
38	6	2.369009	3.536428	-3.054647
39	6	-2.369009	-3.536428	3.054647
40	6	3.425962	5.978710	3.051408
41	6	-3.849107	-7.675513	-1.333268
42	6	1.362448	2.095114	-1.347246
43	6	-1.362448	-2.095114	1.347246
44	6	3.849107	7.675513	1.333268
45	6	-3.425962	-5.978710	3.051408
46	6	2.369009	3.536428	3.054647
47	6	-2.369009	-3.536428	-3.054647
48	6	3.425962	5.978710	-3.051408
49	6	-0.000000	0.000000	-1.393824
50	6	-0.000000	0.000000	1.393824
51	16	-1.548427	-2.016611	3.065786
52	16	3.984946	7.619509	3.060165
53	16	-3.984946	-7.619509	-3.060165
54	16	1.548427	2.016611	-3.065786
55	16	-3.984946	-7.619509	3.060165
56	16	1.548427	2.016611	3.065786
57	16	-1.548427	-2.016611	-3.065786
58	16	3.984946	7.619509	-3.060165
59	1	-0.000000	0.000000	-2.479440
60	1	0.000000	0.000000	2.479440
61	1	-2.627640	-3.504646	5.198907
62	1	3.622149	5.817028	5.196938
63	1	-3.622149	-5.817028	5.196938
64	1	2.627640	3.504646	5.198907
65	1	-3.622149	-5.817028	-5.196938
66	1	2.627640	3.504646	-5.198907
67	1	-2.627640	-3.504646	-5.198907
68	1	3.622149	5.817028	-5.196938

69	1	4.512795	9.729332	1.257682
70	1	4.512795	9.729332	-1.257682
71	1	-4.512795	-9.729332	1.257682
72	1	-4.512795	-9.729332	-1.257682

Table S10. The optimized Cartesian coordinates of the **TTC** ribbon linked via benzene-core linker with n=3 (type **II**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.283867	-10.196208	-0.910743
2	6	-4.237870	0.684127	1.835438
3	6	-4.283003	11.560392	-1.015548
4	6	4.283003	-11.560392	-1.015548
5	6	4.237870	-0.684127	1.835438
6	6	4.283867	10.196208	-0.910743
7	6	-0.685028	-15.195779	-0.790867
8	6	-0.710096	-4.267652	0.685540
9	6	-0.709025	6.638609	0.108489
10	6	0.709025	-6.638609	0.108489
11	6	0.710096	4.267652	0.685540
12	6	0.685028	15.195779	-0.790867
13	6	4.284467	-10.198325	-0.900935
14	6	4.237870	0.684112	1.835447
15	6	4.282542	11.558008	-1.028480
16	6	-4.282542	-11.558008	-1.028480
17	6	-4.237870	-0.684112	1.835447
18	6	-4.284467	10.198325	-0.900935
19	6	0.682875	-15.196174	-0.787510
20	6	0.710094	-4.267651	0.685515
21	6	0.709023	6.638585	0.108427
22	6	-0.709023	-6.638585	0.108427
23	6	-0.710094	4.267651	0.685515
24	6	-0.682875	15.196174	-0.787510
25	6	-0.723005	-12.668288	-0.767593
26	6	-0.733336	-1.769001	1.147840
27	6	-0.735293	9.133682	-0.413717
28	6	0.735293	-9.133682	-0.413717
29	6	0.733336	1.769001	1.147840
30	6	0.723005	12.668288	-0.767593
31	6	1.763416	-11.616149	-0.785106
32	6	1.748474	-0.724039	1.391832
33	6	1.764162	10.172431	-0.655632
34	6	-1.764162	-10.172431	-0.655632
35	6	-1.748474	0.724039	1.391832
36	6	-1.763416	11.616149	-0.785106
37	6	0.722155	-12.668694	-0.764666
38	6	0.733336	-1.769001	1.147817
39	6	0.735361	9.133487	-0.414625
40	6	-0.735361	-9.133487	-0.414625
41	6	-0.733336	1.769001	1.147817
42	6	-0.722155	12.668694	-0.764666
43	6	-1.763650	-11.615189	-0.790834
44	6	-1.748475	-0.724034	1.391840
45	6	-1.764172	10.173205	-0.651889
46	6	1.764172	-10.173205	-0.651889
47	6	1.748475	0.724034	1.391840
48	6	1.763650	11.615189	-0.790834
49	6	-1.333811	-13.958683	-0.812452
50	6	-1.348158	-3.030954	1.009388
51	6	-1.347175	7.876839	-0.211541
52	6	1.347175	-7.876839	-0.211541
53	6	1.348158	3.030954	1.009388
54	6	1.333811	13.958683	-0.812452
55	6	3.052236	-12.216657	-0.924435
56	6	3.028563	-1.331097	1.564705
57	6	3.055594	9.564496	-0.699796
58	6	-3.055594	-9.564496	-0.699796
59	6	-3.028563	1.331097	1.564705
60	6	-3.052236	12.216657	-0.924435

61	6	1.332440	-13.959438	-0.806325
62	6	1.348158	-3.030950	1.009346
63	6	1.347165	7.876631	-0.212313
64	6	-1.347165	-7.876631	-0.212313
65	6	-1.348158	3.030950	1.009346
66	6	-1.332440	13.959438	-0.806325
67	6	-3.052286	-12.214921	-0.935155
68	6	-3.028564	-1.331090	1.564725
69	6	-3.055894	9.565777	-0.694272
70	6	3.055894	-9.565777	-0.694272
71	6	3.028564	1.331090	1.564725
72	6	3.052286	12.214921	-0.935155
73	6	1.394745	-5.452891	0.397026
74	6	1.394746	5.452883	0.397000
75	6	-1.394746	-5.452883	0.397000
76	6	-1.394745	5.452891	0.397026
77	16	-3.066605	-7.862771	-0.405375
78	16	-3.050693	3.044962	1.328085
79	16	-3.060036	13.949835	-0.942658
80	16	3.060036	-13.949835	-0.942658
81	16	3.050693	-3.044962	1.328085
82	16	3.066605	7.862771	-0.405375
83	16	-3.060823	-13.948064	-0.955837
84	16	-3.050690	-3.044960	1.328152
85	16	-3.066876	7.863613	-0.402340
86	16	3.066876	-7.863613	-0.402340
87	16	3.050690	3.044960	1.328152
88	16	3.060823	13.948064	-0.955837
89	1	2.480507	-5.448714	0.390666
90	1	2.480509	5.448692	0.390575
91	1	-2.480509	-5.448692	0.390575
92	1	-2.480507	5.448714	0.390666
93	1	-5.200758	-9.616209	-0.947262
94	1	-5.146009	1.258113	1.990743
95	1	-5.199274	12.127086	-1.148117
96	1	-5.198647	-12.124096	-1.164743
97	1	-5.146004	-1.258103	1.990750
98	1	-5.201639	9.618702	-0.936332
99	1	5.199274	-12.127086	-1.148117
100	1	5.146009	-1.258113	1.990743
101	1	5.200758	9.616209	-0.947262
102	1	5.201639	-9.618702	-0.936332
103	1	5.146004	1.258103	1.990750
104	1	5.198647	12.124096	-1.164743
105	1	-1.256424	16.117781	-0.798119
106	1	1.259048	16.117059	-0.804264
107	1	-1.259048	-16.117059	-0.804264
108	1	1.256424	-16.117781	-0.798119

Table S11. The optimized Cartesian coordinates of the **TTC** ribbon linked via benzene-core linker with n=4 (type **II**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	15.775857	-4.281259	-0.515320
2	6	4.627086	-4.176727	-1.855720
3	6	-5.988619	-4.176226	1.986703
4	6	-17.085090	-4.300227	0.124900
5	6	16.990690	4.222179	0.718172
6	6	6.031271	4.299144	-1.809010
7	6	-4.665797	4.302112	1.717758
8	6	-15.720122	4.252958	-0.214209
9	6	20.285015	-0.845137	1.891885
10	6	9.671477	-0.683712	-1.073955
11	6	-1.160587	-0.654880	0.374535
12	6	-12.079361	-0.704147	0.681779
13	6	12.083286	0.712742	-0.622947
14	6	1.161436	0.765230	-0.374565
15	6	-9.676048	0.735771	1.021010
16	6	-20.251704	0.510420	-2.067086

17	6	15.719011	4.253305	0.217459
18	6	4.665780	4.300762	-1.723228
19	6	-6.031212	4.300345	1.804746
20	6	-16.992237	4.221832	-0.713797
21	6	17.086432	-4.299059	-0.127083
22	6	5.989180	-4.177561	-1.984631
23	6	-4.626451	-4.175235	1.858600
24	6	-15.774545	-4.282227	0.513213
25	6	20.250276	0.510667	2.070968
26	6	9.676108	0.735378	-1.021475
27	6	-1.161421	0.765547	0.371828
28	6	-12.083320	0.712776	0.623055
29	6	12.079565	-0.704183	-0.681849
30	6	1.160959	-0.655203	-0.374939
31	6	-9.671210	-0.683319	1.073469
32	6	-20.285746	-0.845599	-1.889519
33	6	17.962112	-0.812117	0.896301
34	6	7.142411	-0.689248	-1.325115
35	6	-3.615462	-0.678631	1.032030
36	6	-14.576430	-0.759103	0.173047
37	6	14.573113	0.708558	-0.077624
38	6	3.619377	0.787221	-1.020532
39	6	-7.148220	0.777523	1.282125
40	6	-17.935450	0.622533	-1.061443
41	6	16.972026	1.692054	0.714326
42	6	6.092521	1.800353	-1.423974
43	6	-4.647760	1.804371	1.320824
44	6	-15.611803	1.722969	-0.216148
45	6	15.633229	-1.792392	-0.070953
46	6	4.633895	-1.693977	-1.373964
47	6	-6.076038	-1.695617	1.501442
48	6	-17.017972	-1.816281	-0.353636
49	6	17.934576	0.622906	1.064098
50	6	7.148361	0.776815	-1.283364
51	6	-3.619287	0.788000	1.018125
52	6	-14.573355	0.708295	0.078589
53	6	14.576545	-0.758794	-0.172715
54	6	3.615804	-0.679426	-1.032507
55	6	-7.142118	-0.688525	1.324423
56	6	-17.962354	-0.812669	-0.895041
57	6	17.018318	-1.815563	0.353582
58	6	6.076420	-1.696553	-1.501413
59	6	-4.633471	-1.692953	1.374432
60	6	-15.632822	-1.792955	0.070726
61	6	15.611190	1.723310	0.218110
62	6	4.647822	1.803389	-1.323990
63	6	-6.092404	1.801242	1.421652
64	6	-16.972989	1.691693	-0.711443
65	6	19.176100	-1.450135	1.295116
66	6	8.409255	-1.309577	-1.311078
67	6	-2.367372	-1.292483	0.796811
68	6	-13.342048	-1.352908	0.516128
69	6	13.344601	1.338097	-0.376206
70	6	2.371948	1.402960	-0.786062
71	6	-8.419496	1.385585	1.221217
72	6	-19.116116	1.194481	-1.626131
73	6	17.556199	2.969654	0.973540
74	6	6.690844	3.083147	-1.607626
75	6	-4.034465	3.088515	1.429840
76	6	-15.072479	3.030376	-0.018817
77	6	15.097377	-3.061765	-0.446231
78	6	4.010675	-2.970870	-1.509013
79	6	-6.660947	-2.972725	1.754657
80	6	-17.645239	-3.099334	-0.320133
81	6	19.114677	1.194746	1.630063
82	6	8.419547	1.385025	-1.222159
83	6	-2.372025	1.403641	0.782494
84	6	-13.344818	1.337961	0.376836
85	6	13.342361	-1.352745	-0.516226
86	6	2.367862	-1.293191	-0.796309
87	6	-8.408891	-1.308994	1.310578
88	6	-19.176252	-1.450774	-1.294007
89	6	17.646096	-3.098337	0.319025
90	6	6.661422	-2.973755	-1.753928
91	6	-4.010085	-2.969599	1.511065
92	6	-15.096536	-3.062415	0.445091
93	6	15.071756	3.030695	0.020949
94	6	4.034407	3.087329	-1.434680
95	6	-6.690760	3.084091	1.604825

96	6	-17.557674	2.969319	-0.969381
97	6	10.880206	1.408760	-0.789684
98	6	-0.000078	1.450869	-0.001927
99	6	-10.880309	1.408978	0.789557
100	6	10.872659	-1.379117	-0.898455
101	6	0.000276	-1.340597	0.000363
102	6	-10.872306	-1.378904	0.898132
103	16	13.411079	-3.054893	-0.819784
104	16	2.323942	-2.993362	-1.124798
105	16	-8.389073	-3.002295	1.674373
106	16	-19.255168	-3.149710	-0.960900
107	16	19.129603	2.926568	1.699692
108	16	8.417122	3.095835	-1.492557
109	16	-2.340636	3.110197	1.077550
110	16	-13.409502	3.065745	0.447436
111	16	19.255864	-3.148686	0.960215
112	16	8.389582	-3.003038	-1.674142
113	16	-2.323215	-2.992228	1.127470
114	16	-13.410253	-3.055252	0.818677
115	16	13.409042	3.065918	-0.446301
116	16	2.340377	3.109128	-1.083344
117	16	-8.417109	3.096518	1.490838
118	16	-19.131669	2.926349	-1.694243
119	1	10.872766	2.491097	-0.702882
120	1	-0.000203	2.536814	-0.002783
121	1	-10.873075	2.491318	0.702841
122	1	10.860897	-2.464911	-0.896826
123	1	0.000418	-2.426585	0.001251
124	1	-10.860360	-2.464693	0.896459
125	1	15.260813	-5.178532	-0.844040
126	1	4.038944	-5.081718	-1.971346
127	1	-6.543483	-5.081929	2.210574
128	1	-17.672308	-5.213163	0.126099
129	1	17.673998	-5.211770	-0.129023
130	1	6.544078	-5.083365	-2.208027
131	1	-4.038195	-5.080012	1.975376
132	1	-15.259160	-5.179561	0.841228
133	1	17.546755	5.129722	0.931288
134	1	6.596691	5.209511	-1.981716
135	1	-4.085448	5.214059	1.816950
136	1	-15.205708	5.186324	-0.007757
137	1	15.204585	5.186672	0.011054
138	1	4.085368	5.212529	-1.823692
139	1	-6.596637	5.210762	1.977167
140	1	-17.548688	5.129369	-0.925932
141	1	-21.147187	-1.440362	-2.176932
142	1	-21.085033	1.053039	-2.502465
143	1	21.146563	-1.439840	2.179098
144	1	21.083136	1.053156	2.507408

Table S12. The optimized Cartesian coordinates of the **TTC** ribbon linked via benzene-core linker with n=5 (type **II**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	21.104712	4.283928	-1.096744
2	6	10.232820	4.238249	1.682070
3	6	-0.684081	4.238956	-1.148489
4	6	-11.601026	4.238242	1.676503
5	6	-22.466379	4.282551	-1.216161
6	6	22.466379	-4.282551	-1.216161
7	6	11.601026	-4.238242	1.676503
8	6	0.684081	-4.238956	-1.148489
9	6	-10.232820	-4.238249	1.682070
10	6	-21.104712	-4.283928	-1.096744
11	6	26.103862	0.683962	-0.988881
12	6	15.180309	0.710082	0.515242
13	6	4.269681	0.710210	-0.010473
14	6	-6.644066	0.710240	0.550124
15	6	-17.549292	0.709034	-0.069801

16	6	17.549292	-0.709034	-0.069801
17	6	6.644066	-0.710240	0.550124
18	6	-4.269681	-0.710210	-0.010473
19	6	-15.180309	-0.710082	0.515242
20	6	-26.103862	-0.683962	-0.988881
21	6	21.104712	-4.283928	-1.096744
22	6	10.232820	-4.238249	1.682070
23	6	-0.684081	-4.238956	-1.148489
24	6	-11.601026	-4.238242	1.676503
25	6	-22.466379	-4.282551	-1.216161
26	6	22.466379	4.282551	-1.216161
27	6	11.601026	4.238242	1.676503
28	6	0.684081	4.238956	-1.148489
29	6	-10.232820	4.238249	1.682070
30	6	-21.104712	4.283928	-1.096744
31	6	26.103862	-0.683962	-0.988881
32	6	15.180309	-0.710082	0.515242
33	6	4.269681	-0.710210	-0.010473
34	6	-6.644066	-0.710240	0.550124
35	6	-17.549292	-0.709034	-0.069801
36	6	17.549292	0.709034	-0.069801
37	6	6.644066	0.710240	0.550124
38	6	-4.269681	0.710210	-0.010473
39	6	-15.180309	0.710082	0.515242
40	6	-26.103862	0.683962	-0.988881
41	6	23.576451	0.722573	-0.960898
42	6	12.683249	0.733344	0.986487
43	6	1.769562	0.733328	-0.466896
44	6	-9.144948	0.733308	1.001062
45	6	-20.042586	0.735316	-0.600195
46	6	20.042586	-0.735316	-0.600195
47	6	9.144948	-0.733308	1.001062
48	6	-1.769562	-0.733328	-0.466896
49	6	-12.683249	-0.733344	0.986487
50	6	-23.576451	-0.722573	-0.960898
51	6	22.523568	-1.763473	-0.980863
52	6	11.639162	-1.748555	1.234015
53	6	0.724096	-1.748727	-0.708427
54	6	-10.191065	-1.748555	1.239928
55	6	-21.081069	-1.764104	-0.843150
56	6	21.081069	1.764104	-0.843150
57	6	10.191065	1.748555	1.239928
58	6	-0.724096	1.748727	-0.708427
59	6	-11.639162	1.748555	1.234015
60	6	-22.523568	1.763473	-0.980863
61	6	23.576451	-0.722573	-0.960898
62	6	12.683249	-0.733344	0.986487
63	6	1.769562	-0.733328	-0.466896
64	6	-9.144948	-0.733308	1.001062
65	6	-20.042586	-0.735316	-0.600195
66	6	20.042586	0.735316	-0.600195
67	6	9.144948	0.733308	1.001062
68	6	-1.769562	0.733328	-0.466896
69	6	-12.683249	0.733344	0.986487
70	6	-23.576451	0.722573	-0.960898
71	6	22.523568	1.763473	-0.980863
72	6	11.639162	1.748555	1.234015
73	6	0.724096	1.748727	-0.708427
74	6	-10.191065	1.748555	1.239928
75	6	-21.081069	1.764104	-0.843150
76	6	21.081069	-1.764104	-0.843150
77	6	10.191065	-1.748555	1.239928
78	6	-0.724096	-1.748727	-0.708427
79	6	-11.639162	-1.748555	1.234015
80	6	-22.523568	-1.763473	-0.980863
81	6	24.866910	1.333145	-1.006840
82	6	13.944703	1.348138	0.843273
83	6	3.031900	1.348065	-0.330301
84	6	-7.882282	1.348097	0.868276
85	6	-18.786339	1.347175	-0.394382
86	6	18.786339	-1.347175	-0.394382
87	6	7.882282	-1.348097	0.868276
88	6	-3.031900	-1.348065	-0.330301
89	6	-13.944703	-1.348138	0.843273
90	6	-24.866910	-1.333145	-1.006840
91	6	23.123304	-3.052159	-1.124646
92	6	12.246866	-3.028754	1.403920
93	6	1.330957	-3.029127	-0.879978
94	6	-9.584792	-3.028747	1.414771

95	6	-20.473177	-3.055599	-0.885523
96	6	20.473177	3.055599	-0.885523
97	6	9.584792	3.028747	1.414771
98	6	-1.330957	3.029127	-0.879978
99	6	-12.246866	3.028754	1.403920
100	6	-23.123304	3.052159	-1.124646
101	6	24.866910	-1.333145	-1.006840
102	6	13.944703	-1.348138	0.843273
103	6	3.031900	-1.348065	-0.330301
104	6	-7.882282	-1.348097	0.868276
105	6	-18.786339	-1.347175	-0.394382
106	6	18.786339	1.347175	-0.394382
107	6	7.882282	1.348097	0.868276
108	6	-3.031900	1.348065	-0.330301
109	6	-13.944703	1.348138	0.843273
110	6	-24.866910	1.333145	-1.006840
111	6	23.123304	3.052159	-1.124646
112	6	12.246866	3.028754	1.403920
113	6	1.330957	3.029127	-0.879978
114	6	-9.584792	3.028747	1.414771
115	6	-20.473177	3.055599	-0.885523
116	6	20.473177	-3.055599	-0.885523
117	6	9.584792	-3.028747	1.414771
118	6	-1.330957	-3.029127	-0.879978
119	6	-12.246866	-3.028754	1.403920
120	6	-23.123304	-3.052159	-1.124646
121	6	16.364568	-1.394750	0.222757
122	6	5.456831	-1.395748	0.270060
123	6	-5.456831	-1.395748	0.270060
124	6	-16.364568	-1.394750	0.222757
125	6	16.364568	1.394750	0.222757
126	6	5.456831	1.395748	0.270060
127	6	-5.456831	1.395748	0.270060
128	6	-16.364568	1.394750	0.222757
129	16	18.772077	3.066635	-0.587376
130	16	7.869941	3.050918	1.185657
131	16	-3.045005	3.051217	-0.645637
132	16	-13.959820	3.050806	1.161084
133	16	-24.856429	3.060398	-1.147476
134	16	24.856429	-3.060398	-1.147476
135	16	13.959820	-3.050806	1.161084
136	16	3.045005	-3.051217	-0.645637
137	16	-7.869941	-3.050918	1.185657
138	16	-18.772077	-3.066635	-0.587376
139	16	24.856429	3.060398	-1.147476
140	16	13.959820	3.050806	1.161084
141	16	3.045005	3.051217	-0.645637
142	16	-7.869941	3.050918	1.185657
143	16	-18.772077	3.066635	-0.587376
144	16	18.772077	-3.066635	-0.587376
145	16	7.869941	-3.050918	1.185657
146	16	-3.045005	-3.051217	-0.645637
147	16	-13.959820	-3.050806	1.161084
148	16	-24.856429	-3.060398	-1.147476
149	1	16.360430	-2.480512	0.216500
150	1	5.456944	-2.481719	0.269874
151	1	-5.456944	-2.481719	0.269874
152	1	-16.360430	-2.480512	0.216500
153	1	16.360430	2.480512	0.216500
154	1	5.456944	2.481719	0.269874
155	1	-5.456944	2.481719	0.269874
156	1	-16.360430	2.480512	0.216500
157	1	20.524765	5.200906	-1.131860
158	1	9.659436	5.146438	1.839281
159	1	-1.258162	5.147217	-1.302715
160	1	-12.175671	5.146436	1.829017
161	1	-23.032378	5.198709	-1.352441
162	1	23.032378	5.198709	-1.352441
163	1	12.175671	5.146436	1.829017
164	1	1.258162	5.147217	-1.302715
165	1	-9.659436	5.146438	1.839281
166	1	-20.524765	5.200906	-1.131860
167	1	23.032378	-5.198709	-1.352441
168	1	12.175671	-5.146436	1.829017
169	1	1.258162	-5.147217	-1.302715
170	1	-9.659436	-5.146438	1.839281
171	1	-20.524765	-5.200906	-1.131860
172	1	20.524765	-5.200906	-1.131860
173	1	9.659436	-5.146438	1.839281

174	1	-1.258162	-5.147217	-1.302715
175	1	-12.175671	-5.146436	1.829017
176	1	-23.032378	-5.198709	-1.352441
177	1	27.025290	1.257732	-1.002701
178	1	27.025290	-1.257732	-1.002701
179	1	-27.025290	1.257732	-1.002701
180	1	-27.025290	-1.257732	-1.002701

Table S13. The optimized Cartesian coordinates of the **TTC** ribbon linked through four-membered ring with n=2 (type **III**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.347580	4.266703	0.527431
2	6	-5.700263	4.235249	-0.722005
3	6	5.700263	-4.235249	-0.722005
4	6	-4.347580	-4.266703	0.527431
5	6	9.309723	0.655513	0.193026
6	6	-0.753813	0.695769	-0.000490
7	6	0.753813	-0.695769	-0.000490
8	6	-9.309723	-0.655513	0.193026
9	6	4.347580	-4.266703	-0.527431
10	6	-5.700263	-4.235249	0.722005
11	6	5.700263	4.235249	0.722005
12	6	-4.347580	4.266703	-0.527431
13	6	9.309723	-0.655513	-0.193026
14	6	-0.753813	-0.695769	0.000490
15	6	0.753813	0.695769	0.000490
16	6	-9.309723	0.655513	-0.193026
17	6	6.781271	0.703381	0.165613
18	6	-3.234393	0.720482	-0.040153
19	6	3.234393	-0.720482	-0.040153
20	6	-6.781271	-0.703381	0.165613
21	6	5.732212	-1.739113	-0.317820
22	6	-4.289204	-1.757986	0.192602
23	6	4.289204	1.757986	0.192602
24	6	-5.732212	1.739113	-0.317820
25	6	6.781271	-0.703381	-0.165613
26	6	-3.234393	-0.720482	0.040153
27	6	3.234393	0.720482	0.040153
28	6	-6.781271	0.703381	-0.165613
29	6	5.732212	1.739113	0.317820
30	6	-4.289204	1.757986	-0.192602
31	6	4.289204	-1.757986	-0.192602
32	6	-5.732212	-1.739113	0.317820
33	6	8.071382	1.285742	0.350823
34	6	-1.937475	1.381392	-0.027078
35	6	1.937475	-1.381392	-0.027078
36	6	-8.071382	-1.285742	0.350823
37	6	6.340615	-2.999342	-0.604786
38	6	-3.696787	-3.055325	0.279551
39	6	3.696787	3.055325	0.279551
40	6	-6.340615	2.999342	-0.604786
41	6	8.071382	-1.285742	-0.350823
42	6	-1.937475	-1.381392	0.027078
43	6	1.937475	1.381392	0.027078
44	6	-8.071382	1.285742	-0.350823
45	6	6.340615	2.999342	0.604786
46	6	-3.696787	3.055325	-0.279551
47	6	3.696787	-3.055325	-0.279551
48	6	-6.340615	-2.999342	0.604786
49	16	1.968770	3.109497	0.112723
50	16	-8.067003	2.970468	-0.753782
51	16	8.067003	-2.970468	-0.753782
52	16	-1.968770	-3.109497	0.112723
53	16	8.067003	2.970468	0.753782
54	16	-1.968770	3.109497	-0.112723
55	16	1.968770	-3.109497	-0.112723
56	16	-8.067003	-2.970468	0.753782
57	1	3.781076	5.191050	0.582043

58	1	-6.271377	5.132978	-0.936921
59	1	6.271377	5.132978	0.936921
60	1	-3.781076	5.191050	-0.582043
61	1	3.781076	-5.191050	-0.582043
62	1	-6.271377	-5.132978	0.936921
63	1	6.271377	-5.132978	-0.936921
64	1	-3.781076	-5.191050	0.582043
65	1	-10.230652	1.207210	-0.353855
66	1	-10.230652	-1.207210	0.353855
67	1	10.230652	1.207210	0.353855
68	1	10.230652	-1.207210	-0.353855

Table S14. The optimized Cartesian coordinates of the **TTC** ribbon linked through four-membered ring with n=3 (type **III**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-9.351163	4.264683	0.561432
2	6	0.664959	4.285345	-0.159682
3	6	10.708164	4.279765	-0.400233
4	6	-10.708164	-4.279765	-0.400233
5	6	-0.664959	-4.285345	-0.159682
6	6	9.351163	-4.264683	0.561432
7	6	-14.317393	0.683170	-0.002763
8	6	-4.248575	0.678670	0.155576
9	6	5.756277	0.677794	-0.155888
10	6	-5.756277	-0.677794	-0.155888
11	6	4.248575	-0.678670	0.155576
12	6	14.317393	-0.683170	-0.002763
13	6	-9.351163	-4.264683	-0.561432
14	6	0.664959	-4.285345	0.159682
15	6	10.708164	-4.279765	0.400233
16	6	-10.708164	4.279765	0.400233
17	6	-0.664959	4.285345	0.159682
18	6	9.351163	4.264683	-0.561432
19	6	-14.317393	-0.683170	0.002763
20	6	-4.248575	-0.678670	-0.155576
21	6	5.756277	-0.677794	0.155888
22	6	-5.756277	0.677794	0.155888
23	6	4.248575	0.678670	-0.155576
24	6	14.317393	0.683170	0.002763
25	6	-11.787922	0.722186	0.030136
26	6	-1.771625	0.712647	0.102732
27	6	8.237928	0.709561	-0.132373
28	6	-8.237928	-0.709561	-0.132373
29	6	1.771625	-0.712647	0.102732
30	6	11.787922	-0.722186	0.030136
31	6	-10.738587	-1.762850	-0.147137
32	6	-0.716995	-1.758095	-0.103291
33	6	9.293284	-1.751929	0.250060
34	6	-9.293284	1.751929	0.250060
35	6	0.716995	1.758095	-0.103291
36	6	10.738587	1.762850	-0.147137
37	6	-11.787922	-0.722186	-0.030136
38	6	-1.771625	-0.712647	-0.102732
39	6	8.237928	-0.709561	0.132373
40	6	-8.237928	0.709561	0.132373
41	6	1.771625	0.712647	-0.102732
42	6	11.787922	0.722186	-0.030136
43	6	-10.738587	1.762850	0.147137
44	6	-0.716995	1.758095	0.103291
45	6	9.293284	1.751929	-0.250060
46	6	-9.293284	-1.751929	-0.250060
47	6	0.716995	-1.758095	0.103291
48	6	10.738587	-1.762850	0.147137
49	6	-13.078855	1.332045	0.016751
50	6	-3.064694	1.355987	0.272072
51	6	6.939981	1.349991	-0.291575
52	6	-6.939981	-1.349991	-0.291575
53	6	3.064694	-1.355987	0.272072

54	6	13.078855	-1.332045	0.016751
55	6	-11.348756	-3.053365	-0.208990
56	6	-1.305651	-3.048931	-0.268341
57	6	8.699441	-3.031527	0.478727
58	6	-8.699441	3.031527	0.478727
59	6	1.305651	3.048931	-0.268341
60	6	11.348756	3.053365	-0.208990
61	6	-13.078855	-1.332045	-0.016751
62	6	-3.064694	-1.355987	-0.272072
63	6	6.939981	-1.349991	0.291575
64	6	-6.939981	1.349991	0.291575
65	6	3.064694	1.355987	-0.272072
66	6	13.078855	1.332045	-0.016751
67	6	-11.348756	3.053365	0.208990
68	6	-1.305651	3.048931	0.268341
69	6	8.699441	3.031527	-0.478727
70	6	-8.699441	-3.031527	-0.478727
71	6	1.305651	-3.048931	0.268341
72	6	11.348756	-3.053365	0.208990
73	16	-6.968755	3.048478	0.618221
74	16	3.023367	3.066857	-0.535374
75	16	13.076689	3.062440	-0.083967
76	16	-13.076689	-3.062440	-0.083967
77	16	-3.023367	-3.066857	-0.535374
78	16	6.968755	-3.048478	0.618221
79	16	-13.076689	3.062440	0.083967
80	16	-3.023367	3.066857	0.535374
81	16	6.968755	3.048478	-0.618221
82	16	-6.968755	-3.048478	-0.618221
83	16	3.023367	-3.066857	0.535374
84	16	13.076689	-3.062440	0.083967
85	1	-8.782633	5.173832	0.730391
86	1	1.223628	5.206612	-0.291247
87	1	11.281691	5.200671	-0.436246
88	1	-11.281691	5.200671	0.436246
89	1	-1.223628	5.206612	0.291247
90	1	8.782633	5.173832	-0.730391
91	1	-8.782633	-5.173832	-0.730391
92	1	1.223628	-5.206612	0.291247
93	1	11.281691	-5.200671	0.436246
94	1	-11.281691	-5.200671	-0.436246
95	1	-1.223628	-5.206612	-0.291247
96	1	8.782633	-5.173832	0.730391
97	1	15.238129	1.258147	0.003759
98	1	15.238129	-1.258147	-0.003759
99	1	-15.238129	1.258147	-0.003759
100	1	-15.238129	-1.258147	0.003759

Table S15. The optimized Cartesian coordinates of the **TTC** ribbon linked through four-membered ring with n=4 (type **III**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-14.350667	4.013615	1.546632
2	6	-4.335569	4.204265	0.841074
3	6	5.664095	4.128338	-1.157831
4	6	15.707285	4.067179	-1.390286
5	6	-15.707285	-4.067179	-1.390286
6	6	-5.664095	-4.128338	-1.157831
7	6	4.335569	-4.204265	0.841074
8	6	14.350667	-4.013615	1.546632
9	6	-19.316489	0.665204	0.155727
10	6	-9.248158	0.622604	0.311842
11	6	0.753611	0.696350	-0.000726
12	6	10.755838	0.621652	-0.311878
13	6	-10.755838	-0.621652	-0.311878
14	6	-0.753611	-0.696350	-0.000726
15	6	9.248158	-0.622604	0.311842
16	6	19.316489	-0.665204	0.155727
17	6	-14.350667	-4.013615	-1.546632

18	6	-4.335569	-4.204265	-0.841074
19	6	5.664095	-4.128338	1.157831
20	6	15.707285	-4.067179	1.390286
21	6	-15.707285	4.067179	1.390286
22	6	-5.664095	4.128338	1.157831
23	6	4.335569	4.204265	-0.841074
24	6	14.350667	4.013615	-1.546632
25	6	-19.316489	-0.665204	-0.155727
26	6	-9.248158	-0.622604	-0.311842
27	6	0.753611	-0.696350	0.000726
28	6	10.755838	-0.621652	0.311878
29	6	-10.755838	0.621652	0.311878
30	6	-0.753611	0.696350	0.000726
31	6	9.248158	0.622604	-0.311842
32	6	19.316489	0.665204	-0.155727
33	6	-16.787109	0.695302	0.197439
34	6	-6.771536	0.668338	0.267706
35	6	3.229836	0.717125	-0.063094
36	6	13.237385	0.658353	-0.295896
37	6	-13.237385	-0.658353	-0.295896
38	6	-3.229836	-0.717125	-0.063094
39	6	6.771536	-0.668338	0.267706
40	6	16.787109	-0.695302	0.197439
41	6	-15.737818	-1.679543	-0.554964
42	6	-5.717062	-1.684765	-0.511871
43	6	4.283969	-1.733943	0.306535
44	6	14.292700	-1.644107	0.654492
45	6	-14.292700	1.644107	0.654492
46	6	-4.283969	1.733943	0.306535
47	6	5.717062	1.684765	-0.511871
48	6	15.737818	1.679543	-0.554964
49	6	-16.787109	-0.695302	-0.197439
50	6	-6.771536	-0.668338	-0.267706
51	6	3.229836	-0.717125	0.063094
52	6	13.237385	-0.658353	0.295896
53	6	-13.237385	0.658353	0.295896
54	6	-3.229836	0.717125	0.063094
55	6	6.771536	0.668338	-0.267706
56	6	16.787109	0.695302	-0.197439
57	6	-15.737818	1.679543	0.554964
58	6	-5.717062	1.684765	0.511871
59	6	4.283969	1.733943	-0.306535
60	6	14.292700	1.644107	-0.654492
61	6	-14.292700	-1.644107	-0.654492
62	6	-4.283969	-1.733943	-0.306535
63	6	5.717062	-1.684765	0.511871
64	6	15.737818	-1.679543	0.554964
65	6	-18.077971	1.291798	0.325639
66	6	-8.064304	1.253420	0.585047
67	6	1.937137	1.382670	-0.042364
68	6	11.939514	1.242898	-0.602400
69	6	-11.939514	-1.242898	-0.602400
70	6	-1.937137	-1.382670	-0.042364
71	6	8.064304	-1.253420	0.585047
72	6	18.077971	-1.291798	0.325639
73	6	-16.347837	-2.920151	-0.915884
74	6	-6.305012	-2.900536	-0.976560
75	6	3.695497	-3.028037	0.443858
76	6	13.699010	-2.833816	1.178273
77	6	-13.699010	2.833816	1.178273
78	6	-3.695497	3.028037	0.443858
79	6	6.305012	2.900536	-0.976560
80	6	16.347837	2.920151	-0.915884
81	6	-18.077971	-1.291798	-0.325639
82	6	-8.064304	-1.253420	-0.585047
83	6	1.937137	-1.382670	0.042364
84	6	11.939514	-1.242898	0.602400
85	6	-11.939514	1.242898	0.602400
86	6	-1.937137	1.382670	0.042364
87	6	8.064304	1.253420	-0.585047
88	6	18.077971	1.291798	-0.325639
89	6	-16.347837	2.920151	0.915884
90	6	-6.305012	2.900536	0.976560
91	6	3.695497	3.028037	-0.443858
92	6	13.699010	2.833816	-1.178273
93	6	-13.699010	-2.833816	-1.178273
94	6	-3.695497	-3.028037	-0.443858
95	6	6.305012	-2.900536	0.976560
96	6	16.347837	-2.920151	0.915884

97	16	-11.968482	2.816493	1.320344
98	16	-1.979039	3.108498	0.177725
99	16	8.022169	2.854071	-1.244526
100	16	18.075609	2.958998	-0.793985
101	16	-18.075609	-2.958998	-0.793985
102	16	-8.022169	-2.854071	-1.244526
103	16	1.979039	-3.108498	0.177725
104	16	11.968482	-2.816493	1.320344
105	16	-18.075609	2.958998	0.793985
106	16	-8.022169	2.854071	1.244526
107	16	1.979039	3.108498	-0.177725
108	16	11.968482	2.816493	-1.320344
109	16	-11.968482	-2.816493	-1.320344
110	16	-1.979039	-3.108498	-0.177725
111	16	8.022169	-2.854071	1.244526
112	16	18.075609	-2.958998	0.793985
113	1	-13.782340	4.857379	1.925299
114	1	-3.777533	5.131381	0.925825
115	1	6.221802	4.992964	-1.503563
116	1	16.280638	4.954465	-1.639851
117	1	-16.280638	4.954465	1.639851
118	1	-6.221802	4.992964	1.503563
119	1	3.777533	5.131381	-0.925825
120	1	13.782340	4.857379	-1.925299
121	1	-13.782340	-4.857379	-1.925299
122	1	-3.777533	-5.131381	-0.925825
123	1	6.221802	-4.992964	1.503563
124	1	16.280638	-4.954465	1.639851
125	1	-16.280638	-4.954465	-1.639851
126	1	-6.221802	-4.992964	-1.503563
127	1	3.777533	-5.131381	0.925825
128	1	13.782340	-4.857379	1.925299
129	1	20.237241	1.224707	-0.288093
130	1	20.237241	-1.224707	0.288093
131	1	-20.237241	1.224707	0.288093
132	1	-20.237241	-1.224707	-0.288093

Table S16. The optimized Cartesian coordinates of the **TTC** ribbon linked through four-membered ring with n=5 (type **III**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-19.357191	4.264744	0.561132
2	6	-9.340537	4.286013	-0.151843
3	6	0.665545	4.286075	0.156978
4	6	10.671061	4.285427	-0.164733
5	6	20.714215	4.279768	-0.400159
6	6	-20.714215	-4.279768	-0.400159
7	6	-10.671061	-4.285427	-0.164733
8	6	-0.665545	-4.286075	0.156978
9	6	9.340537	-4.286013	-0.151843
10	6	19.357191	-4.264744	0.561132
11	6	-24.323432	0.683168	-0.002699
12	6	-14.254611	0.678663	0.155410
13	6	-4.249215	0.679352	-0.152026
14	6	5.756816	0.679383	0.152050
15	6	15.762326	0.677828	-0.155720
16	6	-15.762326	-0.677828	-0.155720
17	6	-5.756816	-0.679383	0.152050
18	6	4.249215	-0.679352	-0.152026
19	6	14.254611	-0.678663	0.155410
20	6	24.323432	-0.683168	-0.002699
21	6	-19.357191	-4.264744	-0.561132
22	6	-9.340537	-4.286013	0.151843
23	6	0.665545	-4.286075	-0.156978
24	6	10.671061	-4.285427	0.164733
25	6	20.714215	-4.279768	0.400159
26	6	-20.714215	4.279768	0.400159
27	6	-10.671061	4.285427	0.164733
28	6	-0.665545	4.286075	-0.156978

29	6	9.340537	4.286013	0.151843
30	6	19.357191	4.264744	-0.561132
31	6	-24.323432	-0.683168	0.002699
32	6	-14.254611	-0.678663	-0.155410
33	6	-4.249215	-0.679352	0.152026
34	6	5.756816	-0.679383	-0.152050
35	6	15.762326	-0.677828	0.155720
36	6	-15.762326	0.677828	0.155720
37	6	-5.756816	0.679383	-0.152050
38	6	4.249215	0.679352	0.152026
39	6	14.254611	0.678663	-0.155410
40	6	24.323432	0.683168	0.002699
41	6	-21.793962	0.722179	0.030170
42	6	-11.777500	0.712629	0.103009
43	6	-1.772035	0.712972	-0.100691
44	6	8.233822	0.713004	0.100343
45	6	18.243945	0.709589	-0.132257
46	6	-18.243945	-0.709589	-0.132257
47	6	-8.233822	-0.713004	0.100343
48	6	1.772035	-0.712972	-0.100691
49	6	11.777500	-0.712629	0.103009
50	6	21.793962	-0.722179	0.030170
51	6	-20.744638	-1.762840	-0.147136
52	6	-10.722881	-1.758115	-0.105174
53	6	-0.717330	-1.758534	0.101399
54	6	9.288544	-1.758522	-0.099460
55	6	19.299315	-1.751961	0.249906
56	6	-19.299315	1.751961	0.249906
57	6	-9.288544	1.758522	-0.099460
58	6	0.717330	1.758534	0.101399
59	6	10.722881	1.758115	-0.105174
60	6	20.744638	1.762840	-0.147136
61	6	-21.793962	-0.722179	-0.030170
62	6	-11.777500	-0.712629	-0.103009
63	6	-1.772035	-0.712972	0.100691
64	6	8.233822	-0.713004	-0.100343
65	6	18.243945	-0.709589	0.132257
66	6	-18.243945	0.709589	0.132257
67	6	-8.233822	0.713004	-0.100343
68	6	1.772035	0.712972	0.100691
69	6	11.777500	0.712629	-0.103009
70	6	21.793962	0.722179	-0.030170
71	6	-20.744638	1.762840	0.147136
72	6	-10.722881	1.758115	0.105174
73	6	-0.717330	1.758534	-0.101399
74	6	9.288544	1.758522	0.099460
75	6	19.299315	1.751961	-0.249906
76	6	-19.299315	-1.751961	-0.249906
77	6	-9.288544	-1.758522	0.099460
78	6	0.717330	-1.758534	-0.101399
79	6	10.722881	-1.758115	0.105174
80	6	20.744638	-1.762840	0.147136
81	6	-23.084899	1.332051	0.016869
82	6	-13.070671	1.355897	0.271988
83	6	-3.065419	1.356987	-0.266492
84	6	6.940537	1.357133	0.266386
85	6	16.945994	1.350088	-0.291304
86	6	-16.945994	-1.350088	-0.291304
87	6	-6.940537	-1.357133	0.266386
88	6	3.065419	-1.356987	-0.266492
89	6	13.070671	-1.355897	0.271988
90	6	23.084899	-1.332051	0.016869
91	6	-21.354814	-3.053350	-0.209033
92	6	-11.311807	-3.048808	-0.270760
93	6	-1.306429	-3.049592	0.263651
94	6	8.699701	-3.049730	-0.261070
95	6	18.705477	-3.031588	0.478384
96	6	-18.705477	3.031588	0.478384
97	6	-8.699701	3.049730	-0.261070
98	6	1.306429	3.049592	0.263651
99	6	11.311807	3.048808	-0.270760
100	6	21.354814	3.053350	-0.209033
101	6	-23.084899	-1.332051	-0.016869
102	6	-13.070671	-1.355897	-0.271988
103	6	-3.065419	-1.356987	0.266492
104	6	6.940537	-1.357133	-0.266386
105	6	16.945994	-1.350088	0.291304
106	6	-16.945994	1.350088	0.291304
107	6	-6.940537	1.357133	-0.266386

108	6	3.065419	1.356987	0.266492
109	6	13.070671	1.355897	-0.271988
110	6	23.084899	1.332051	-0.016869
111	6	-21.354814	3.053350	0.209033
112	6	-11.311807	3.048808	0.270760
113	6	-1.306429	3.049592	-0.263651
114	6	8.699701	3.049730	0.261070
115	6	18.705477	3.031588	-0.478384
116	6	-18.705477	-3.031588	-0.478384
117	6	-8.699701	-3.049730	0.261070
118	6	1.306429	-3.049592	-0.263651
119	6	11.311807	-3.048808	0.270760
120	6	21.354814	-3.053350	0.209033
121	16	-16.974768	3.048589	0.617704
122	16	-6.981428	3.068625	-0.524299
123	16	3.024876	3.068354	0.524910
124	16	13.029711	3.066630	-0.535657
125	16	23.082738	3.062424	-0.084192
126	16	-23.082738	-3.062424	-0.084192
127	16	-13.029711	-3.066630	-0.535657
128	16	-3.024876	-3.068354	0.524910
129	16	6.981428	-3.068625	-0.524299
130	16	16.974768	-3.048589	0.617704
131	16	-23.082738	3.062424	0.084192
132	16	-13.029711	3.066630	0.535657
133	16	-3.024876	3.068354	-0.524910
134	16	6.981428	3.068625	0.524299
135	16	16.974768	3.048589	-0.617704
136	16	-16.974768	-3.048589	-0.617704
137	16	-6.981428	-3.068625	0.524299
138	16	3.024876	-3.068354	-0.524910
139	16	13.029711	-3.066630	0.535657
140	16	23.082738	-3.062424	0.084192
141	1	-18.788670	5.173919	0.729976
142	1	-8.781647	5.207484	-0.280965
143	1	1.224775	5.207308	0.286336
144	1	11.230076	5.206461	-0.296454
145	1	21.287753	5.200664	-0.436220
146	1	-21.287753	5.200664	0.436220
147	1	-11.230076	5.206461	0.296454
148	1	-1.224775	5.207308	-0.286336
149	1	8.781647	5.207484	0.280965
150	1	18.788670	5.173919	-0.729976
151	1	-18.788670	-5.173919	-0.729976
152	1	-8.781647	-5.207484	0.280965
153	1	1.224775	-5.207308	-0.286336
154	1	11.230076	-5.206461	0.296454
155	1	21.287753	-5.200664	0.436220
156	1	-21.287753	-5.200664	-0.436220
157	1	-11.230076	-5.206461	-0.296454
158	1	-1.224775	-5.207308	0.286336
159	1	8.781647	-5.207484	-0.280965
160	1	18.788670	-5.173919	0.729976
161	1	-25.244183	1.258116	-0.003651
162	1	-25.244183	-1.258116	0.003651
163	1	25.244183	1.258116	0.003651
164	1	25.244183	-1.258116	-0.003651

Table S17. The optimized Cartesian coordinates of the tetraselena[8]circulene (**TSC**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.108462	4.308998	-0.279297
2	6	-4.159280	1.127542	-0.291498
3	6	-0.484596	1.820847	-0.186093
4	6	-1.653225	0.903211	-0.188608
5	6	-0.874802	3.160106	-0.480392
6	6	-2.860701	1.600087	-0.486597
7	34	-2.647581	3.374998	-1.019904
8	1	-0.512822	5.288481	-0.514367
9	1	-5.014111	1.752443	-0.530076

10	6	4.308998	0.108462	0.279297
11	6	1.127542	4.159280	0.291498
12	6	1.820847	0.484596	0.186093
13	6	0.903211	1.653225	0.188608
14	6	3.160106	0.874802	0.480392
15	6	1.600087	2.860701	0.486597
16	34	3.374998	2.647581	1.019904
17	1	5.288481	0.512822	0.514367
18	1	1.752443	5.014111	0.530076
19	6	-4.308998	-0.108462	0.279297
20	6	-1.127542	-4.159280	0.291498
21	6	-1.820847	-0.484596	0.186093
22	6	-0.903211	-1.653225	0.188608
23	6	-3.160106	-0.874802	0.480392
24	6	-1.600087	-2.860701	0.486597
25	34	-3.374998	-2.647581	1.019904
26	1	-5.288481	-0.512822	0.514367
27	1	-1.752443	-5.014111	0.530076
28	6	0.108462	-4.308998	-0.279297
29	6	4.159280	-1.127542	-0.291498
30	6	0.484596	-1.820847	-0.186093
31	6	1.653225	-0.903211	-0.188608
32	6	0.874802	-3.160106	-0.480392
33	6	2.860701	-1.600087	-0.486597
34	34	2.647581	-3.374998	-1.019904
35	1	5.014111	-1.752443	-0.530076
36	1	0.512822	-5.288481	-0.514367

Table S18. The optimized Cartesian coordinates of the directly fused **TSC**-based ribbon with n=2 (type **I**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.931747	-1.216252	-1.261462
2	6	-5.982423	-0.410233	0.595217
3	6	-4.931542	-1.216097	1.261893
4	6	5.982541	-0.410429	-0.594600
5	6	-4.931721	1.215970	-1.261833
6	6	5.982398	0.410278	0.595334
7	6	4.931515	1.216378	1.261720
8	6	-5.982517	0.410209	-0.594899
9	6	3.546508	1.477396	0.940349
10	6	-2.508202	0.685719	-0.251854
11	6	-3.546635	1.477034	-0.940838
12	6	2.508160	0.685842	0.251513
13	6	-3.546505	-1.477140	0.940669
14	6	2.508200	-0.685731	-0.251685
15	6	3.546633	-1.477199	-0.940496
16	6	-2.508159	-0.685742	0.251651
17	6	5.466159	2.006840	2.318804
18	6	-1.251838	-1.326509	0.242727
19	6	-5.466522	2.006025	-2.319140
20	6	1.251888	-1.326510	-0.242819
21	6	-5.466214	-2.006304	2.319151
22	6	1.251845	1.326624	0.242414
23	6	5.466577	-2.006525	-2.318592
24	6	-1.251896	1.326515	-0.243097
25	6	3.001998	-2.667511	-1.499319
26	6	-7.262255	0.635038	-1.180071
27	6	-3.001832	-2.667469	1.499427
28	6	7.262009	0.635170	1.180757
29	6	-3.002020	2.667269	-1.499845
30	6	7.262314	-0.635469	-1.179613
31	6	3.001856	2.667898	1.498757
32	6	-7.262070	-0.635078	1.180580
33	6	-4.836752	3.087878	-2.937939
34	6	4.836367	3.089038	2.936974
35	6	0.000011	-0.696377	-0.000113
36	6	4.836784	-3.088444	-2.937251
37	6	-4.836398	-3.088292	2.937668

38	6	-0.000010	0.696442	-0.000268
39	6	3.612042	-3.477428	-2.458072
40	6	-3.611772	-3.477364	2.458264
41	6	-8.493165	0.288104	-0.621971
42	6	8.493029	0.287935	0.623086
43	6	-3.612056	3.477003	-2.458757
44	6	3.611788	3.478039	2.457392
45	6	-8.493065	-0.288074	0.622711
46	6	8.493200	-0.288519	-0.621469
47	34	7.248931	-1.649993	-2.748208
48	34	-7.248404	-1.649517	2.749226
49	34	-7.248812	1.649284	-2.748846
50	34	7.248282	1.650026	2.749133
51	34	1.249073	3.044445	0.989749
52	34	-1.249181	3.044013	-0.991184
53	34	-1.249029	-3.044115	0.990561
54	34	1.249140	-3.044130	-0.990630
55	1	3.102759	-4.353397	-2.847619
56	1	3.102521	4.354183	2.846569
57	1	-3.102792	4.352929	-2.848428
58	1	-5.340674	3.641906	-3.723549
59	1	-5.340235	-3.642449	3.723241
60	1	-3.102483	-4.353375	2.847711
61	1	5.340723	-3.642633	-3.722737
62	1	5.340185	3.643386	3.722425
63	1	9.418372	-0.527897	-1.136159
64	1	9.418062	0.527165	1.138095
65	1	-9.418128	-0.527259	1.137689
66	1	-9.418308	0.527301	-1.136798

Table S19. The optimized Cartesian coordinates of the directly fused **TSC**-based ribbon with n=3 (type **I**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-7.396946	1.713764	-0.997754
2	6	8.840250	1.722917	-0.994605
3	6	-1.715986	0.725691	1.327414
4	6	-0.720205	1.687129	1.851987
5	6	-6.396488	0.727432	-0.516523
6	6	9.858106	0.721085	-0.589752
7	6	-0.720205	-1.687129	1.851987
8	6	-6.396488	-0.727432	-0.516523
9	6	9.858106	-0.721085	-0.589752
10	6	-7.396946	-1.713764	-0.997754
11	6	8.840250	-1.722917	-0.994605
12	6	-1.715986	-0.725691	1.327414
13	6	-8.840250	-1.722917	-0.994605
14	6	7.396946	-1.713764	-0.997754
15	6	1.715986	-0.725691	1.327414
16	6	0.720205	-1.687129	1.851987
17	6	-9.858106	-0.721085	-0.589752
18	6	6.396488	-0.727432	-0.516523
19	6	0.720205	1.687129	1.851987
20	6	-9.858106	0.721085	-0.589752
21	6	6.396488	0.727432	-0.516523
22	6	-8.840250	1.722917	-0.994605
23	6	7.396946	1.713764	-0.997754
24	6	1.715986	0.725691	1.327414
25	6	-6.771700	-2.940378	-1.355354
26	6	9.442642	-2.977729	-1.299632
27	6	2.942969	1.346992	1.012077
28	6	-1.340103	-2.900927	2.252303
29	6	-11.113484	1.336573	-0.315145
30	6	5.162155	1.340901	-0.204900
31	6	-1.340103	2.900927	2.252303
32	6	-11.113484	-1.336573	-0.315145
33	6	5.162155	-1.340901	-0.204900
34	6	-6.771700	2.940378	-1.355354
35	6	9.442642	2.977729	-1.299632

36	6	2.942969	-1.346992	1.012077
37	6	-9.442642	2.977729	-1.299632
38	6	6.771700	2.940378	-1.355354
39	6	-2.942969	-1.346992	1.012077
40	6	1.340103	2.900927	2.252303
41	6	-5.162155	-1.340901	-0.204900
42	6	11.113484	-1.336573	-0.315145
43	6	1.340103	-2.900927	2.252303
44	6	-5.162155	1.340901	-0.204900
45	6	11.113484	1.336573	-0.315145
46	6	-9.442642	-2.977729	-1.299632
47	6	6.771700	-2.940378	-1.355354
48	6	-2.942969	1.346992	1.012077
49	6	-0.686387	-3.993395	2.826787
50	6	-7.416197	-4.074459	-1.852198
51	6	8.786423	-4.097652	-1.812749
52	6	-12.260547	0.685798	0.140278
53	6	4.050245	0.699456	0.401746
54	6	-7.416197	4.074459	-1.852198
55	6	8.786423	4.097652	-1.812749
56	6	-0.686387	3.993395	2.826787
57	6	-12.260547	-0.685798	0.140278
58	6	4.050245	-0.699456	0.401746
59	6	-8.786423	4.097652	-1.812749
60	6	7.416197	4.074459	-1.852198
61	6	0.686387	3.993395	2.826787
62	6	-4.050245	-0.699456	0.401746
63	6	12.260547	-0.685798	0.140278
64	6	0.686387	-3.993395	2.826787
65	6	-8.786423	-4.097652	-1.812749
66	6	7.416197	-4.074459	-1.852198
67	6	-4.050245	0.699456	0.401746
68	6	12.260547	0.685798	0.140278
69	34	-4.972172	3.075601	-0.884604
70	34	11.235072	3.134254	-0.803599
71	34	-3.125838	3.072039	1.730659
72	34	-3.125838	-3.072039	1.730659
73	34	-4.972172	-3.075601	-0.884604
74	34	11.235072	-3.134254	-0.803599
75	34	-11.235072	-3.134254	-0.803599
76	34	4.972172	-3.075601	-0.884604
77	34	3.125838	-3.072039	1.730659
78	34	3.125838	3.072039	1.730659
79	34	-11.235072	3.134254	-0.803599
80	34	4.972172	3.075601	-0.884604
81	1	-9.346596	4.984991	-2.091390
82	1	6.844225	4.943811	-2.162384
83	1	-9.346596	-4.984991	-2.091390
84	1	6.844225	-4.943811	-2.162384
85	1	1.249397	-4.855900	3.170780
86	1	-1.249397	-4.855900	3.170780
87	1	-1.249397	4.855900	3.170780
88	1	1.249397	4.855900	3.170780
89	1	-6.844225	4.943811	-2.162384
90	1	9.346596	4.984991	-2.091390
91	1	-6.844225	-4.943811	-2.162384
92	1	9.346596	-4.984991	-2.091390
93	1	13.151176	1.251879	0.395606
94	1	13.151176	-1.251879	0.395606
95	1	-13.151176	1.251879	0.395606
96	1	-13.151176	-1.251879	0.395606

Table S20. The optimized Cartesian coordinates of the directly fused **TSC**-based ribbon with n=4 (type **I**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.620418	-3.249466	1.690180
2	6	-0.672641	12.957376	1.722721
3	6	0.208725	-13.949787	0.721068

4	6	1.048176	2.283219	0.725790
5	6	0.672650	-12.957373	1.722721
6	6	1.620408	3.249464	1.690180
7	6	-1.048187	-2.283221	0.725790
8	6	-0.208714	13.949789	0.721068
9	6	0.672650	-12.957373	-1.722721
10	6	1.620408	3.249464	-1.690180
11	6	-1.048187	-2.283221	-0.725790
12	6	-0.208714	13.949789	-0.721068
13	6	-1.620418	-3.249466	-1.690180
14	6	-0.672641	12.957376	-1.722721
15	6	0.208725	-13.949787	-0.721068
16	6	1.048176	2.283219	-0.725790
17	6	-1.701806	-4.687791	-1.689238
18	6	-0.760036	11.516745	-1.713447
19	6	0.336963	-10.490091	-0.727421
20	6	1.237144	5.711609	-0.725844
21	6	0.760042	-11.516742	-1.713447
22	6	1.701798	4.687789	-1.689238
23	6	-1.237151	-5.711610	-0.725844
24	6	-0.336959	10.490093	-0.727421
25	6	0.760042	-11.516742	1.713447
26	6	1.701798	4.687789	1.689238
27	6	-1.237151	-5.711610	0.725844
28	6	-0.336959	10.490093	0.727421
29	6	-1.701806	-4.687791	1.689238
30	6	-0.760036	11.516745	1.713447
31	6	0.336963	-10.490091	0.727421
32	6	1.237144	5.711609	0.725844
33	6	-1.978771	-2.609503	-2.907140
34	6	-0.942298	13.576477	-2.977474
35	6	0.097294	-9.239881	1.340991
36	6	0.991407	6.954904	1.346645
37	6	0.942307	-13.576474	-2.977474
38	6	1.978762	2.609500	-2.907140
39	6	-0.991410	-6.954905	1.346645
40	6	-0.097293	9.239882	1.340991
41	6	0.942307	-13.576474	2.977474
42	6	1.978762	2.609500	2.907140
43	6	-0.991410	-6.954905	-1.346645
44	6	-0.097293	9.239882	-1.340991
45	6	-1.978771	-2.609503	2.907140
46	6	-0.942298	13.576477	2.977474
47	6	0.097294	-9.239881	-1.340991
48	6	0.991407	6.954904	-1.346645
49	6	-2.133019	-5.284618	2.904156
50	6	-1.154254	10.913308	2.939694
51	6	-0.138860	-15.186891	-1.336613
52	6	0.667225	1.074338	-1.345834
53	6	1.154258	-10.913304	2.939694
54	6	2.133012	5.284615	2.904156
55	6	-0.667235	-1.074340	-1.345834
56	6	0.138872	15.186893	-1.336613
57	6	1.154258	-10.913304	-2.939694
58	6	2.133012	5.284615	-2.904156
59	6	-0.667235	-1.074340	1.345834
60	6	0.138872	15.186893	1.336613
61	6	-2.133019	-5.284618	-2.904156
62	6	-1.154254	10.913308	-2.939694
63	6	-0.138860	-15.186891	1.336613
64	6	0.667225	1.074338	1.345834
65	6	1.493430	-12.951232	-4.097077
66	6	2.584260	3.230235	-4.001903
67	6	-2.584268	-3.230238	-4.001903
68	6	-1.493422	12.951236	-4.097076
69	6	-0.444909	-8.095131	0.699396
70	6	0.444908	8.095131	0.699396
71	6	-2.584268	-3.230238	4.001903
72	6	-1.493422	12.951236	4.097076
73	6	1.493430	-12.951232	4.097077
74	6	2.584260	3.230235	4.001903
75	6	-0.444909	-8.095131	-0.699396
76	6	0.444908	8.095131	-0.699396
77	6	-2.664051	-4.600581	3.999975
78	6	-1.613104	11.585661	4.073636
79	6	1.613109	-11.585657	4.073636
80	6	2.664044	4.600577	3.999975
81	6	-0.660771	-16.305268	-0.685809
82	6	-0.000005	-0.000001	-0.700388

83	6	0.660784	16.305269	-0.685809
84	6	1.613109	-11.585657	-4.073636
85	6	2.664044	4.600577	-3.999975
86	6	-2.664051	-4.600581	-3.999975
87	6	-1.613104	11.585661	-4.073636
88	6	-0.660771	-16.305268	0.685809
89	6	-0.000005	-0.000001	0.700388
90	6	0.660784	16.305269	0.685809
91	34	-1.363205	-0.853690	3.074391
92	34	-0.342039	15.336780	3.134225
93	34	0.342051	-15.336778	3.134225
94	34	1.363196	0.853687	3.074391
95	34	0.342051	-15.336778	-3.134225
96	34	1.363196	0.853687	-3.074391
97	34	-1.363205	-0.853690	-3.074391
98	34	-0.342039	15.336780	-3.134225
99	34	-1.716027	-7.097617	-3.072659
100	34	-0.788694	9.089424	-3.075059
101	34	0.788695	-9.089422	-3.075059
102	34	1.716024	7.097615	-3.072659
103	34	0.788695	-9.089422	3.075059
104	34	1.716024	7.097615	3.072659
105	34	-1.716027	-7.097617	3.072659
106	34	-0.788694	9.089424	3.075059
107	1	-3.036344	-5.144209	4.863151
108	1	-1.956610	11.032748	4.942789
109	1	-3.036344	-5.144209	-4.863151
110	1	-1.956610	11.032748	-4.942789
111	1	1.956614	-11.032743	-4.942790
112	1	3.036338	5.144205	-4.863150
113	1	1.739128	-13.526612	-4.984418
114	1	2.891360	2.649351	-4.866449
115	1	1.739128	-13.526612	4.984418
116	1	2.891360	2.649351	4.866449
117	1	1.956614	-11.032743	4.942790
118	1	3.036338	5.144205	4.863150
119	1	-2.891368	-2.649355	4.866450
120	1	-1.739120	13.526617	4.984418
121	1	-2.891368	-2.649355	-4.866450
122	1	-1.739120	13.526617	-4.984418
123	1	0.967864	17.179420	1.251868
124	1	0.967864	17.179420	-1.251868
125	1	-0.967850	-17.179419	1.251868
126	1	-0.967850	-17.179419	-1.251868

Table S21. The optimized Cartesian coordinates of the directly fused **TSC**-based ribbon with n=5 (type **I**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-15.508882	1.713637	-1.163101
2	6	0.720396	1.692146	-1.181136
3	6	16.952197	1.722873	-1.159909
4	6	-9.828145	0.725832	1.164099
5	6	6.394911	0.725776	1.169561
6	6	-8.832462	1.688906	1.686731
7	6	7.391881	1.689780	1.687060
8	6	-14.508416	0.727433	-0.681636
9	6	1.717460	0.725941	-0.666862
10	6	17.970135	0.721086	-0.755236
11	6	-8.832462	-1.688906	1.686731
12	6	7.391881	-1.689780	1.687060
13	6	-14.508416	-0.727433	-0.681636
14	6	1.717460	-0.725941	-0.666862
15	6	17.970135	-0.721086	-0.755236
16	6	-15.508882	-1.713637	-1.163101
17	6	0.720396	-1.692146	-1.181136
18	6	16.952197	-1.722873	-1.159909
19	6	-9.828145	-0.725832	1.164099
20	6	6.394911	-0.725776	1.169561

21	6	-16.952197	-1.722873	-1.159909
22	6	-0.720396	-1.692146	-1.181136
23	6	15.508882	-1.713637	-1.163101
24	6	-6.394911	-0.725776	1.169561
25	6	9.828145	-0.725832	1.164099
26	6	-7.391881	-1.689780	1.687060
27	6	8.832462	-1.688906	1.686731
28	6	-17.970135	-0.721086	-0.755236
29	6	-1.717460	-0.725941	-0.666862
30	6	14.508416	-0.727433	-0.681636
31	6	-7.391881	1.689780	1.687060
32	6	8.832462	1.688906	1.686731
33	6	-17.970135	0.721086	-0.755236
34	6	-1.717460	0.725941	-0.666862
35	6	14.508416	0.727433	-0.681636
36	6	-16.952197	1.722873	-1.159909
37	6	-0.720396	1.692146	-1.181136
38	6	15.508882	1.713637	-1.163101
39	6	-6.394911	0.725776	1.169561
40	6	9.828145	0.725832	1.164099
41	6	-14.883600	-2.940118	-1.520990
42	6	1.339502	-2.910123	-1.571704
43	6	17.554484	-2.977741	-1.464895
44	6	-5.166563	1.345958	0.857415
45	6	11.055355	1.346718	0.848046
46	6	-9.452806	-2.903609	2.083942
47	6	6.773134	-2.906355	2.081946
48	6	-19.225552	1.336567	-0.480854
49	6	-2.946255	1.345503	-0.354315
50	6	13.274112	1.340935	-0.369927
51	6	-9.452806	2.903609	2.083942
52	6	6.773134	2.906355	2.081946
53	6	-19.225552	-1.336567	-0.480854
54	6	-2.946255	-1.345503	-0.354315
55	6	13.274112	-1.340935	-0.369927
56	6	-14.883600	2.940118	-1.520990
57	6	1.339502	2.910123	-1.571704
58	6	17.554484	2.977741	-1.464895
59	6	-5.166563	-1.345958	0.857415
60	6	11.055355	-1.346718	0.848046
61	6	-17.554484	2.977741	-1.464895
62	6	-1.339502	2.910123	-1.571704
63	6	14.883600	2.940118	-1.520990
64	6	-11.055355	-1.346718	0.848046
65	6	5.166563	-1.345958	0.857415
66	6	-6.773134	2.906355	2.081946
67	6	9.452806	2.903609	2.083942
68	6	-13.274112	-1.340935	-0.369927
69	6	2.946255	-1.345503	-0.354315
70	6	19.225552	-1.336567	-0.480854
71	6	-6.773134	-2.906355	2.081946
72	6	9.452806	-2.903609	2.083942
73	6	-13.274112	1.340935	-0.369927
74	6	2.946255	1.345503	-0.354315
75	6	19.225552	1.336567	-0.480854
76	6	-17.554484	-2.977741	-1.464895
77	6	-1.339502	-2.910123	-1.571704
78	6	14.883600	-2.940118	-1.520990
79	6	-11.055355	1.346718	0.848046
80	6	5.166563	1.345958	0.857415
81	6	-8.799897	-3.998941	2.653773
82	6	7.427215	-4.000715	2.652067
83	6	-15.528018	-4.074287	-2.017769
84	6	0.686289	-4.008010	-2.135851
85	6	16.898226	-4.097639	-1.978044
86	6	-20.372782	0.685795	-0.025826
87	6	-4.056523	0.700344	0.251464
88	6	12.162458	0.699404	0.237215
89	6	-15.528018	4.074287	-2.017769
90	6	0.686289	4.008010	-2.135851
91	6	16.898226	4.097639	-1.978044
92	6	-8.799897	3.998941	2.653773
93	6	7.427215	4.000715	2.652067
94	6	-20.372782	-0.685795	-0.025826
95	6	-4.056523	-0.700344	0.251464
96	6	12.162458	-0.699404	0.237215
97	6	-16.898226	4.097639	-1.978044
98	6	-0.686289	4.008010	-2.135851
99	6	15.528018	4.074287	-2.017769

100	6	-7.427215	4.000715	2.652067
101	6	8.799897	3.998941	2.653773
102	6	-12.162458	-0.699404	0.237215
103	6	4.056523	-0.700344	0.251464
104	6	20.372782	-0.685795	-0.025826
105	6	-7.427215	-4.000715	2.652067
106	6	8.799897	-3.998941	2.653773
107	6	-16.898226	-4.097639	-1.978044
108	6	-0.686289	-4.008010	-2.135851
109	6	15.528018	-4.074287	-2.017769
110	6	-12.162458	0.699404	0.237215
111	6	4.056523	0.700344	0.251464
112	6	20.372782	0.685795	-0.025826
113	34	-13.084025	3.075344	-1.050447
114	34	3.127937	3.074869	-1.058876
115	34	19.346946	3.134336	-0.969031
116	34	-11.239024	3.072503	1.564161
117	34	4.985487	3.074033	1.566219
118	34	-11.239024	-3.072503	1.564161
119	34	4.985487	-3.074033	1.566219
120	34	-13.084025	-3.075344	-1.050447
121	34	3.127937	-3.074869	-1.058876
122	34	19.346946	-3.134336	-0.969031
123	34	-19.346946	-3.134336	-0.969031
124	34	-3.127937	-3.074869	-1.058876
125	34	13.084025	-3.075344	-1.050447
126	34	-4.985487	-3.074033	1.566219
127	34	11.239024	-3.072503	1.564161
128	34	-4.985487	3.074033	1.566219
129	34	11.239024	3.072503	1.564161
130	34	-19.346946	3.134336	-0.969031
131	34	-3.127937	3.074869	-1.058876
132	34	13.084025	3.075344	-1.050447
133	1	-17.458381	4.985020	-2.256576
134	1	-1.249634	4.873139	-2.472524
135	1	14.955968	4.943557	-2.328032
136	1	-17.458381	-4.985020	-2.256576
137	1	-1.249634	-4.873139	-2.472524
138	1	14.955968	-4.943557	-2.328032
139	1	-6.864691	-4.864991	2.992319
140	1	9.363674	-4.861966	2.995167
141	1	-9.363674	-4.861966	2.995167
142	1	6.864691	-4.864991	2.992319
143	1	-9.363674	4.861966	2.995167
144	1	6.864691	4.864991	2.992319
145	1	-6.864691	4.864991	2.992319
146	1	9.363674	4.861966	2.995167
147	1	-14.955968	4.943557	-2.328032
148	1	1.249634	4.873139	-2.472524
149	1	17.458381	4.985020	-2.256576
150	1	-14.955968	-4.943557	-2.328032
151	1	1.249634	-4.873139	-2.472524
152	1	17.458381	-4.985020	-2.256576
153	1	-21.263492	1.251893	0.229177
154	1	-21.263492	-1.251893	0.229177
155	1	21.263492	1.251893	0.229177
156	1	21.263492	-1.251893	0.229177

Table S22. The optimized Cartesian coordinates of the **TSC**-based ribbon fused *via* benzene-core linker with n=2 (type **II**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.934469	4.274167	0.298617
2	6	-6.077018	4.268041	-0.134283
3	6	6.076828	-4.268065	0.135918
4	6	-4.934031	-4.274130	-0.298337
5	6	9.738537	0.572666	-0.387241
6	6	-1.205628	0.610750	-0.418503
7	6	1.205657	-0.610456	0.419235

8	6	-9.738811	-0.573076	0.384427
9	6	4.903446	-4.195480	0.842283
10	6	-6.234210	-4.196508	-0.723889
11	6	6.234898	4.196429	0.723378
12	6	-4.903447	4.195833	-0.840371
13	6	9.611946	-0.674912	-0.942352
14	6	-1.228326	-0.658548	0.220022
15	6	1.228354	0.658827	-0.219321
16	6	-9.612630	0.674296	0.940095
17	6	7.264506	0.661515	0.050194
18	6	-3.735269	0.673016	-0.399544
19	6	3.735284	-0.672816	0.400095
20	6	-7.264479	-0.661687	-0.051353
21	6	6.140099	-1.762894	-0.070301
22	6	-4.821020	-1.768174	-0.090416
23	6	4.821183	1.768241	0.090520
24	6	-6.140299	1.762760	0.070642
25	6	7.175006	-0.731858	-0.321621
26	6	-3.751647	-0.744101	-0.005616
27	6	3.751704	0.744252	0.005995
28	6	-7.175293	0.731570	0.320963
29	6	6.250473	1.711390	0.315611
30	6	-4.790298	1.711951	-0.446549
31	6	4.790268	-1.711787	0.447295
32	6	-6.250200	-1.711453	-0.316245
33	6	8.587694	1.189680	0.102637
34	6	-2.470441	1.194799	-0.729504
35	6	2.470468	-1.194462	0.730315
36	6	-8.587603	-1.189913	-0.104814
37	6	6.646386	-3.074274	-0.307423
38	6	-4.280927	-3.082991	0.018185
39	6	4.281133	3.083107	-0.017720
40	6	-6.646720	3.074007	0.308217
41	6	8.371193	-1.304855	-0.844245
42	6	-2.498841	-1.307438	0.293157
43	6	2.498880	1.307686	-0.292507
44	6	-8.371818	1.304298	0.843106
45	6	6.862375	2.951090	0.663623
46	6	-4.276687	2.952660	-0.923886
47	6	4.276709	-2.952263	0.925295
48	6	-6.861791	-2.951196	-0.664648
49	6	-0.026004	-1.239676	0.632819
50	6	0.026037	1.239957	-0.632112
51	34	2.497557	3.155378	-0.539554
52	34	-8.289512	3.137662	1.192834
53	34	8.288690	-3.138417	-1.192902
54	34	-2.497509	-3.155082	0.540588
55	34	8.723686	2.910207	0.811191
56	34	-2.499265	2.901497	-1.482937
57	34	2.499328	-2.900838	1.484474
58	34	-8.722993	-2.910385	-0.813628
59	1	-0.046680	-2.220235	1.101034
60	1	0.046740	2.220474	-1.100416
61	1	4.413534	5.224100	0.230632
62	1	-6.571504	5.216183	0.051504
63	1	6.794271	5.082244	1.007279
64	1	-4.424159	5.084523	-1.238822
65	1	6.571236	-5.216310	-0.049540
66	1	-4.413074	-5.224024	-0.229974
67	1	4.424241	-5.083966	1.241290
68	1	-6.793355	-5.082377	-1.008070
69	1	-10.465891	1.198433	1.358998
70	1	-10.696034	-1.083276	0.344159
71	1	10.695805	1.082844	-0.347790
72	1	10.464917	-1.199241	-1.361610

Table S23. The optimized Cartesian coordinates of the **TSC**-based ribbon fused *via* benzene-core linker with n=3 (type **II**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	4.201167	-8.285785	3.807053
2	6	3.942459	1.274579	-3.320174
3	6	1.253153	12.324304	-1.510853
4	6	-1.253153	-12.324304	-1.510853
5	6	-3.942459	-1.274579	-3.320174
6	6	-4.201167	8.285785	3.807053
7	6	2.660715	-14.101772	2.805741
8	6	1.285494	-3.941883	-1.086559
9	6	-0.212318	6.484374	-0.493167
10	6	0.212318	-6.484374	-0.493167
11	6	-1.285494	3.941883	-1.086559
12	6	-2.660715	14.101772	2.805741
13	6	-1.890253	-11.113514	-1.416315
14	6	-4.218706	0.038320	-3.037695
15	6	-3.986000	9.429104	4.531431
16	6	3.986000	-9.429104	4.531431
17	6	4.218706	-0.038320	-3.037695
18	6	1.890253	11.113514	-1.416315
19	6	2.243251	-14.517898	1.567421
20	6	-0.066266	-4.238795	-1.411035
21	6	-1.546042	6.164426	-0.119579
22	6	1.546042	-6.164426	-0.119579
23	6	0.066266	4.238795	-1.411035
24	6	-2.243251	14.517898	1.567421
25	6	2.152309	-11.713799	2.205932
26	6	0.994375	-1.576374	-1.928327
27	6	-0.563355	8.868231	0.284928
28	6	0.563355	-8.868231	0.284928
29	6	-0.994375	1.576374	-1.928327
30	6	-2.152309	11.713799	2.205932
31	6	0.524741	-11.544351	0.087666
32	6	-1.572877	-0.982692	-2.524525
33	6	-2.597988	9.073754	2.033839
34	6	2.597988	-9.073754	2.033839
35	6	1.572877	0.982692	-2.524525
36	6	-0.524741	11.544351	0.087666
37	6	1.498067	-12.182210	1.005705
38	6	-0.435751	-1.844989	-2.127229
39	6	-1.809769	8.449440	0.944893
40	6	1.809769	-8.449440	0.944893
41	6	0.435751	1.844989	-2.127229
42	6	-1.498067	12.182210	1.005705
43	6	2.564356	-10.369759	2.678545
44	6	1.834740	-0.427158	-2.339244
45	6	0.003572	10.201876	-0.021374
46	6	-0.003572	-10.201876	-0.021374
47	6	-1.834740	0.427158	-2.339244
48	6	-2.564356	10.369759	2.678545
49	6	2.598647	-12.738055	3.091444
50	6	1.771461	-2.673225	-1.518757
51	6	0.212318	7.827917	-0.258836
52	6	-0.212318	-7.827917	-0.258836
53	6	-1.771461	2.673225	-1.518757
54	6	-2.598647	12.738055	3.091444
55	6	-0.082089	-12.504092	-0.774199
56	6	-2.682641	-1.759973	-2.967058
57	6	-3.520506	8.144660	2.597737
58	6	3.520506	-8.144660	2.597737
59	6	2.682641	1.759973	-2.967058
60	6	0.082089	12.504092	-0.774199
61	6	1.640264	-13.574654	0.735230
62	6	-0.817402	-3.196001	-2.028951
63	6	-2.234752	7.139261	0.664710
64	6	2.234752	-7.139261	0.664710
65	6	0.817402	3.196001	-2.028951
66	6	-1.640264	13.574654	0.735230
67	6	3.230272	-10.440810	3.936946
68	6	3.197940	-0.816812	-2.491515
69	6	1.236103	10.091815	-0.728101
70	6	-1.236103	-10.091815	-0.728101
71	6	-3.197940	0.816812	-2.491515
72	6	-3.230272	10.440810	3.936946
73	6	-0.573623	-5.508419	-1.116854
74	6	-2.064481	4.905395	-0.440447
75	6	2.064481	-4.905395	-0.440447
76	6	0.573623	5.508419	-1.116854
77	34	3.702996	-6.552554	1.653018
78	34	2.459002	3.604436	-2.810198

79	34	-0.721275	14.189652	-0.770478
80	34	0.721275	-14.189652	-0.770478
81	34	-2.459002	-3.604436	-2.810198
82	34	-3.702996	6.552554	1.653018
83	34	3.268553	-12.133692	4.725035
84	34	3.602633	-2.505376	-1.818920
85	34	1.877315	8.352529	-0.917612
86	34	-1.877315	-8.352529	-0.917612
87	34	-3.602633	2.505376	-1.818920
88	34	-3.268553	12.133692	4.725035
89	1	-1.605924	-5.734681	-1.370737
90	1	-3.086647	4.657350	-0.163199
91	1	3.086647	-4.657350	-0.163199
92	1	1.605924	5.734681	-1.370737
93	1	4.849470	-7.494886	4.171037
94	1	4.706767	1.945412	-3.700294
95	1	1.661923	13.137314	-2.102378
96	1	4.456647	-9.587685	5.496546
97	1	5.211029	-0.453509	-3.184470
98	1	2.826781	10.922151	-1.930632
99	1	-1.661923	-13.137314	-2.102378
100	1	-4.706767	-1.945412	-3.700294
101	1	-4.849470	7.494886	4.171037
102	1	-2.826781	-10.922151	-1.930632
103	1	-5.211029	0.453509	-3.184470
104	1	-4.456647	9.587685	5.496546
105	1	-2.297154	15.560560	1.270517
106	1	-3.062061	14.799101	3.534308
107	1	3.062061	-14.799101	3.534308
108	1	2.297154	-15.560560	1.270517

Table S24. The optimized Cartesian coordinates of the **TSC**-based ribbon fused *via* benzene-core linker with n=4 (type **II**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-15.705896	3.705219	-1.331528
2	6	-4.232657	4.234869	-3.057299
3	6	5.593315	4.222471	3.195405
4	6	17.036136	3.399995	1.316941
5	6	-15.223711	-3.768621	2.932531
6	6	-5.497471	-3.967975	-3.446665
7	6	4.139990	-3.978742	3.230417
8	6	14.323619	-4.045929	-1.929797
9	6	-19.598606	0.368010	1.972408
10	6	-9.204565	0.745097	-1.584486
11	6	1.037860	0.815411	0.635760
12	6	11.524333	0.683542	0.835852
13	6	-11.498751	-0.736368	-0.860095
14	6	-1.038331	-0.603925	-0.643637
15	6	9.191543	-0.677567	1.651567
16	6	19.137261	-0.421191	-2.986091
17	6	-14.312258	-4.042424	1.945640
18	6	-4.140067	-3.966287	-3.255046
19	6	5.496361	-3.978480	3.429205
20	6	15.234540	-3.772845	-2.917375
21	6	-17.040178	3.392929	-1.315183
22	6	-5.597216	4.232308	-3.188090
23	6	4.228252	4.223162	3.069988
24	6	15.701280	3.709728	1.334152
25	6	-19.136922	-0.429059	2.988223
26	6	-9.191412	-0.674345	-1.652003
27	6	1.038940	-0.606685	0.630444
28	6	11.500093	-0.737381	0.862963
29	6	-11.525000	0.684565	-0.834999
30	6	-1.040817	0.818166	-0.636809
31	6	9.202854	0.741799	1.582198
32	6	19.597777	0.379236	-1.972395
33	6	-17.307864	0.421278	0.936375
34	6	-6.743485	0.818239	-2.152727

35	6	3.299280	0.835765	1.761884
36	6	13.955398	0.640740	0.119376
37	6	-13.817788	-0.799827	0.159374
38	6	-3.292904	-0.625631	-1.784031
39	6	6.727963	-0.654650	2.210591
40	6	16.895266	-0.601799	-1.859950
41	6	-15.751778	-1.551480	1.867179
42	6	-5.662511	-1.617775	-2.564314
43	6	4.229355	-1.620832	2.358689
44	6	14.619240	-1.732129	-0.982209
45	6	-15.150153	1.508688	-0.234166
46	6	-4.263579	1.837078	-2.296403
47	6	5.698578	1.823319	2.446384
48	6	16.562467	1.308882	-0.002566
49	6	-16.893275	-0.605652	1.864819
50	6	-6.728836	-0.648826	-2.215372
51	6	3.292704	-0.632503	1.772484
52	6	13.820332	-0.798943	-0.153844
53	6	-13.955274	0.639191	-0.116114
54	6	-3.301874	0.842521	-1.763625
55	6	6.741297	0.812472	2.148938
56	6	17.308054	0.427986	-0.933866
57	6	-16.563383	1.303029	0.005045
58	6	-5.701373	1.830561	-2.447218
59	6	4.260441	1.828668	2.298714
60	6	15.148975	1.512083	0.237251
61	6	-14.614166	-1.732445	0.990798
62	6	-4.229557	-1.612044	-2.373431
63	6	5.661635	-1.625341	2.554649
64	6	15.756438	-1.550867	-1.859065
65	6	-18.689304	0.769317	0.994098
66	6	-8.009584	1.408521	-1.988633
67	6	2.103419	1.446052	1.341809
68	6	12.779822	1.292531	0.531351
69	6	-12.650826	-1.404293	-0.343264
70	6	-2.097223	-1.233435	-1.360561
71	6	7.984750	-1.278447	2.114114
72	6	17.835214	-0.911168	-2.886529
73	6	-15.912517	-2.557329	2.864804
74	6	-6.215580	-2.854262	-3.009821
75	6	3.572600	-2.858942	2.621383
76	6	14.020046	-3.024514	-1.029979
77	6	-14.814092	2.770733	-0.805500
78	6	-3.629508	3.092761	-2.529297
79	6	6.281839	3.077263	2.793889
80	6	17.427060	2.251156	0.628000
81	6	-17.833250	-0.915234	2.891288
82	6	-7.984692	-1.274035	-2.116298
83	6	2.098744	-1.239514	1.343110
84	6	12.654009	-1.404395	0.349116
85	6	-12.780878	1.292240	-0.529465
86	6	-2.107504	1.452022	-1.338282
87	6	8.006790	1.404070	1.985043
88	6	18.688544	0.779483	-0.993604
89	6	-17.429371	2.243288	-0.626610
90	6	-6.285337	3.084752	-2.792619
91	6	3.625132	3.082262	2.539336
92	6	14.810941	2.773700	0.808383
93	6	-14.011798	-3.023208	1.042291
94	6	-3.571834	-2.847889	-2.644207
95	6	6.214626	-2.862168	2.999295
96	6	15.919779	-2.559313	-2.853649
97	6	-10.334655	-1.389272	-1.282863
98	6	0.001205	-1.292173	-0.009539
99	6	10.336308	-1.391366	1.284903
100	6	-10.371809	1.398163	-1.179100
101	6	-0.002367	1.503534	0.002387
102	6	10.369657	1.395975	1.177355
103	34	-12.989151	3.089871	-0.980244
104	34	-1.886906	3.219604	-1.882037
105	34	8.120405	3.186144	2.514720
106	34	19.248388	2.010716	0.292586
107	34	-17.302739	-2.258676	4.075130
108	34	-8.060626	-3.005926	-2.795863
109	34	1.851413	-2.992624	1.921451
110	34	12.553630	-3.249927	0.095510
111	34	-19.250552	1.998421	-0.293581
112	34	-8.124651	3.190859	-2.517040
113	34	1.880615	3.209710	1.897305

114	34	12.985522	3.090406	0.982267
115	34	-12.545996	-3.248798	-0.083935
116	34	-1.847945	-2.982236	-1.950943
117	34	8.060735	-3.010845	2.792383
118	34	17.308100	-2.259842	-4.065921
119	1	-10.291315	-2.475590	-1.273169
120	1	0.002490	-2.379981	-0.013991
121	1	10.294402	-2.477744	1.276131
122	1	-10.372017	2.483363	-1.109052
123	1	-0.003684	2.591234	0.006845
124	1	10.368396	2.481078	1.105736
125	1	-15.341823	4.623975	-1.780496
126	1	-3.644809	5.123308	-3.266799
127	1	6.133770	5.108474	3.514260
128	1	17.779065	4.061652	1.750896
129	1	-17.784066	4.053098	-1.749759
130	1	-6.137939	5.118596	-3.505697
131	1	3.639710	5.109782	3.285167
132	1	15.335741	4.627849	1.783226
133	1	-15.448795	-4.487372	3.713994
134	1	-6.013574	-4.839396	-3.837863
135	1	3.534054	-4.850683	3.456976
136	1	13.794064	-4.992613	-1.890435
137	1	-13.780216	-4.987828	1.909179
138	1	-3.533671	-4.836275	-3.487800
139	1	6.012079	-4.850252	3.820128
140	1	15.461700	-4.493472	-3.696506
141	1	20.623267	0.734141	-1.949557
142	1	19.781699	-0.731182	-3.802642
143	1	-20.625062	0.719994	1.947791
144	1	-19.781343	-0.739165	3.804744

Table S25. The optimized Cartesian coordinates of the **TSC**-based ribbon fused *via* benzene-core linker with n=5 (type **II**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.575578	21.197887	-1.777689
2	6	2.408043	9.890044	-3.698986
3	6	4.145092	-0.088462	2.386108
4	6	5.745577	-10.674168	-1.867723
5	6	3.440326	-20.228632	5.048663
6	6	-3.440326	20.228632	5.048663
7	6	-5.745577	10.674168	-1.867723
8	6	-4.145092	0.088462	2.386108
9	6	-2.408043	-9.890044	-3.698986
10	6	-1.575578	-21.197887	-1.777689
11	6	-1.713384	25.057812	1.667965
12	6	-0.891740	14.547195	-1.271541
13	6	0.110161	4.152920	0.179331
14	6	1.637042	-6.168215	-0.744097
15	6	2.085606	-16.646415	0.191344
16	6	-2.085606	16.646415	0.191344
17	6	-1.637042	6.168215	-0.744097
18	6	-0.110161	-4.152920	0.179331
19	6	0.891740	-14.547195	-1.271541
20	6	1.713384	-25.057812	1.667965
21	6	-3.872390	19.096813	4.407965
22	6	-5.631474	9.319192	-2.042942
23	6	-3.971330	-1.269150	2.307882
24	6	-2.205590	-11.228971	-3.912895
25	6	-1.051042	-22.464445	-1.817458
26	6	1.051042	22.464445	-1.817458
27	6	2.205590	11.228971	-3.912895
28	6	3.971330	1.269150	2.307882
29	6	5.631474	-9.319192	-2.042942
30	6	3.872390	-19.096813	4.407965
31	6	-1.973101	24.711579	2.969328
32	6	-2.196122	14.391524	-0.728546
33	6	-1.298179	3.976109	0.268397

34	6	0.228417	-6.338312	-0.842856
35	6	0.802580	-16.823978	-0.394628
36	6	-0.802580	16.823978	-0.394628
37	6	-0.228417	6.338312	-0.842856
38	6	1.298179	-3.976109	0.268397
39	6	2.196122	-14.391524	-0.728546
40	6	1.973101	-24.711579	2.969328
41	6	-1.285491	22.648646	1.085715
42	6	-0.873341	12.119635	-1.969157
43	6	0.483914	1.811784	1.052289
44	6	1.998655	-8.530311	-1.561481
45	6	1.957323	-18.965552	1.205957
46	6	-1.957323	18.965552	1.205957
47	6	-1.998655	8.530311	-1.561481
48	6	-0.483914	-1.811784	1.052289
49	6	0.873341	-12.119635	-1.969157
50	6	1.285491	-22.648646	1.085715
51	6	-2.245405	20.986114	2.965978
52	6	-3.248425	10.896521	-1.673301
53	6	-1.803966	0.473526	1.549883
54	6	-0.246931	-9.729251	-2.423317
55	6	0.154885	-20.507820	-0.084871
56	6	-0.154885	20.507820	-0.084871
57	6	0.246931	9.729251	-2.423317
58	6	1.803966	-0.473526	1.549883
59	6	3.248425	-10.896521	-1.673301
60	6	2.245405	-20.986114	2.965978
61	6	-1.788269	22.272847	2.387212
62	6	-2.259243	11.986768	-1.502155
63	6	-0.970151	1.616241	1.107362
64	6	0.550156	-8.673600	-1.754589
65	6	0.794640	-19.244280	0.348743
66	6	-0.794640	19.244280	0.348743
67	6	-0.550156	8.673600	-1.754589
68	6	0.970151	-1.616241	1.107362
69	6	2.259243	-11.986768	-1.502155
70	6	1.788269	-22.272847	2.387212
71	6	-0.528789	21.898371	0.055445
72	6	0.074043	11.156335	-2.577567
73	6	1.610518	0.958084	1.498556
74	6	3.133600	-9.458979	-1.774210
75	6	2.501381	-19.686537	2.381196
76	6	-2.501381	19.686537	2.381196
77	6	-3.133600	9.458979	-1.774210
78	6	-1.610518	-0.958084	1.498556
79	6	-0.074043	-11.156335	-2.577567
80	6	0.528789	-21.898371	0.055445
81	6	-1.335619	24.042202	0.789511
82	6	-0.360288	13.429929	-1.980168
83	6	0.912511	3.111887	0.730396
84	6	2.442388	-7.233652	-1.242443
85	6	2.544735	-17.699415	1.040078
86	6	-2.544735	17.699415	1.040078
87	6	-2.442388	7.233652	-1.242443
88	6	-0.912511	-3.111887	0.730396
89	6	0.360288	-13.429929	-1.980168
90	6	1.335619	-24.042202	0.789511
91	6	-2.696698	21.148965	4.308321
92	6	-4.581746	11.397559	-1.605616
93	6	-3.113300	0.902144	1.916499
94	6	-1.485877	-9.210805	-2.902237
95	6	-0.938433	-20.260544	-0.964759
96	6	0.938433	20.260544	-0.964759
97	6	1.485877	9.210805	-2.902237
98	6	3.113300	-0.902144	1.916499
99	6	4.581746	-11.397559	-1.605616
100	6	2.696698	-21.148965	4.308321
101	6	-1.994990	23.354919	3.292100
102	6	-2.859095	13.165296	-1.025889
103	6	-1.747311	2.764931	0.871301
104	6	-0.217488	-7.524581	-1.495845
105	6	0.217488	-18.121148	-0.271827
106	6	-0.217488	18.121148	-0.271827
107	6	0.217488	7.524581	-1.495845
108	6	1.747311	-2.764931	0.871301
109	6	2.859095	-13.165296	-1.025889
110	6	1.994990	-23.354919	3.292100
111	6	0.028360	22.775091	-0.920805
112	6	1.121228	11.829574	-3.271978

113	6	2.767031	1.741407	1.784940
114	6	4.365765	-8.751642	-1.890360
115	6	3.407105	-18.864715	3.113633
116	6	-3.407105	18.864715	3.113633
117	6	-4.365765	8.751642	-1.890360
118	6	-2.767031	-1.741407	1.784940
119	6	-1.121228	-11.829574	-3.271978
120	6	-0.028360	-22.775091	-0.920805
121	6	-2.767032	15.440092	-0.002158
122	6	-2.147178	4.987909	-0.192166
123	6	-0.621078	-5.330139	-0.376709
124	6	0.223630	-15.763774	-1.101886
125	6	-0.223630	15.763774	-1.101886
126	6	0.621078	5.330139	-0.376709
127	6	2.147178	-4.987909	-0.192166
128	6	2.767032	-15.440092	-0.002158
129	34	1.370379	18.461984	-1.190562
130	34	1.902603	7.502201	-2.290070
131	34	3.488582	-2.685750	1.527808
132	34	4.721816	-13.156134	-1.008514
133	34	2.455471	-22.854673	5.029941
134	34	-2.455471	22.854673	5.029941
135	34	-4.721816	13.156134	-1.008514
136	34	-3.488582	2.685750	1.527808
137	34	-1.902603	-7.502201	-2.290070
138	34	-1.370379	-18.461984	-1.190562
139	34	-0.602052	24.531520	-0.857443
140	34	1.117876	13.684286	-3.085024
141	34	2.651932	3.523410	1.254391
142	34	4.247962	-6.917937	-1.575118
143	34	3.887141	-17.280683	2.264523
144	34	-3.887141	17.280683	2.264523
145	34	-4.247962	6.917937	-1.575118
146	34	-2.651932	-3.523410	1.254391
147	34	-1.117876	-13.684286	-3.085024
148	34	0.602052	-24.531520	-0.857443
149	1	-3.750298	15.299673	0.441284
150	1	-3.223995	4.855555	-0.116586
151	1	-1.698390	-5.461772	-0.451907
152	1	-0.771190	-15.880986	-1.523824
153	1	0.771190	15.880986	-1.523824
154	1	1.698390	5.461772	-0.451907
155	1	3.223995	-4.855555	-0.116586
156	1	3.750298	-15.299673	0.441284
157	1	2.399754	20.903444	-2.419766
158	1	3.288210	9.381519	-4.080306
159	1	5.086985	-0.521543	2.708704
160	1	6.713233	-11.166450	-1.867820
161	1	3.736722	-20.452894	6.068446
162	1	1.441022	23.220526	-2.491427
163	1	2.918679	11.827886	-4.471054
164	1	4.769393	1.958583	2.565845
165	1	6.505060	-8.690997	-2.187713
166	1	4.526553	-18.381081	4.895922
167	1	-3.736722	20.452894	6.068446
168	1	-6.713233	11.166450	-1.867820
169	1	-5.086985	0.521543	2.708704
170	1	-3.288210	-9.381519	-4.080306
171	1	-2.399754	-20.903444	-2.419766
172	1	-4.526553	18.381081	4.895922
173	1	-6.505060	8.690997	-2.187713
174	1	-4.769393	-1.958583	2.565845
175	1	-2.918679	-11.827886	-4.471054
176	1	-1.441022	-23.220526	-2.491427
177	1	-1.714244	26.094070	1.344896
178	1	-2.190745	25.460555	3.724195
179	1	2.190745	-25.460555	3.724195
180	1	1.714244	-26.094070	1.344896

Table S26. The optimized Cartesian coordinates of the **TSC**-based ribbon fused through four-membered ring with n=2 (type **III**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.345848	4.004056	-1.484634
2	6	5.577755	3.754418	2.031595
3	6	-5.577755	-3.754419	2.031595
4	6	4.345848	-4.004057	-1.484635
5	6	-9.216397	0.440119	-0.524704
6	6	0.749794	0.697837	-0.001354
7	6	-0.749794	-0.697837	-0.001354
8	6	9.216397	-0.440121	-0.524702
9	6	-4.345852	-4.004064	1.484618
10	6	5.577752	-3.754411	-2.031609
11	6	-5.577752	3.754410	-2.031608
12	6	4.345852	4.004064	1.484618
13	6	-9.216397	-0.440109	0.524722
14	6	0.749795	-0.697836	0.001365
15	6	-0.749795	0.697836	0.001365
16	6	9.216396	0.440108	0.524724
17	6	-6.703099	0.553771	-0.464655
18	6	3.211531	0.714178	0.101197
19	6	-3.211531	-0.714178	0.101196
20	6	6.703099	-0.553771	-0.464654
21	6	-5.653182	-1.511023	0.896100
22	6	4.262023	-1.674886	-0.533243
23	6	-4.262023	1.674885	-0.533242
24	6	5.653182	1.511023	0.896101
25	6	-6.703099	-0.553769	0.464659
26	6	3.211532	-0.714176	-0.101196
27	6	-3.211532	0.714176	-0.101196
28	6	6.703099	0.553769	0.464660
29	6	-5.653181	1.511020	-0.896102
30	6	4.262024	1.674888	0.533238
31	6	-4.262024	-1.674889	0.533238
32	6	5.653181	-1.511020	-0.896102
33	6	-7.983440	0.921810	-0.969513
34	6	1.924321	1.385031	0.054351
35	6	-1.924321	-1.385031	0.054350
36	6	7.983440	-0.921811	-0.969512
37	6	-6.197879	-2.547578	1.708560
38	6	3.724242	-2.974428	-0.778610
39	6	-3.724242	2.974428	-0.778609
40	6	6.197879	2.547578	1.708561
41	6	-7.983438	-0.921806	0.969523
42	6	1.924321	-1.385029	-0.054346
43	6	-1.924321	1.385029	-0.054346
44	6	7.983437	0.921805	0.969525
45	6	-6.197878	2.547573	-1.708565
46	6	3.724245	2.974433	0.778599
47	6	-3.724245	-2.974433	0.778600
48	6	6.197878	-2.547573	-1.708565
49	34	-1.947531	3.237232	-0.236417
50	34	7.979051	2.312122	2.213923
51	34	-7.979051	-2.312123	2.213922
52	34	1.947531	-3.237231	-0.236418
53	34	-7.979054	2.312122	-2.213917
54	34	1.947530	3.237234	0.236412
55	34	-1.947530	-3.237234	0.236412
56	34	7.979055	-2.312123	-2.213916
57	1	-3.835436	4.948806	-1.642558
58	1	6.089251	4.491399	2.642549
59	1	-6.089249	4.491389	-2.642565
60	1	3.835442	4.948815	1.642537
61	1	-3.835442	-4.948814	1.642538
62	1	6.089249	-4.491389	-2.642566
63	1	-6.089251	-4.491399	2.642550
64	1	3.835436	-4.948805	-1.642560
65	1	10.140343	0.806415	0.960875
66	1	10.140346	-0.806432	-0.960848
67	1	-10.140346	0.806431	-0.960850
68	1	-10.140343	-0.806416	0.960873

Table S27. The optimized Cartesian coordinates of the **TSC**-based ribbon fused through four-membered ring with n=3 (type **III**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.373353	-9.307816	4.254056
2	6	-0.314884	0.608926	4.253099
3	6	0.227799	10.539348	4.262332
4	6	0.227799	-10.539349	-4.262331
5	6	-0.314884	-0.608926	-4.253099
6	6	0.373355	9.307817	-4.254056
7	6	-0.286379	-14.176179	0.622085
8	6	0.305420	-4.205308	0.627265
9	6	-0.305574	5.706558	0.627062
10	6	-0.305573	-5.706558	-0.627063
11	6	0.305419	4.205308	-0.627266
12	6	-0.286385	14.176179	-0.622085
13	6	-0.373355	-9.307817	-4.254056
14	6	0.314884	0.608926	-4.253099
15	6	-0.227799	10.539349	-4.262331
16	6	-0.227799	-10.539348	4.262332
17	6	0.314884	-0.608926	4.253099
18	6	-0.373353	9.307816	4.254056
19	6	0.286385	-14.176179	-0.622085
20	6	-0.305419	-4.205308	-0.627266
21	6	0.305573	5.706558	-0.627063
22	6	0.305574	-5.706558	0.627062
23	6	-0.305420	4.205308	0.627265
24	6	0.286379	14.176179	0.622085
25	6	-0.183395	-11.662765	0.699145
26	6	0.208635	-1.744673	0.689863
27	6	-0.212869	8.168842	0.689436
28	6	-0.212868	-8.168842	-0.689436
29	6	0.208634	1.744673	-0.689863
30	6	-0.183399	11.662765	-0.699144
31	6	0.164306	-10.612601	-1.748433
32	6	-0.209754	-0.692886	-1.740979
33	6	0.233175	9.220706	-1.741414
34	6	0.233174	-9.220706	1.741414
35	6	-0.209755	0.692886	1.740978
36	6	0.164304	10.612601	1.748433
37	6	0.183399	-11.662765	-0.699144
38	6	-0.208634	-1.744673	-0.689863
39	6	0.212868	8.168842	-0.689436
40	6	0.212869	-8.168842	0.689436
41	6	-0.208635	1.744673	0.689863
42	6	0.183395	11.662765	0.699145
43	6	-0.164304	-10.612601	1.748433
44	6	0.209755	-0.692886	1.740978
45	6	-0.233174	9.220706	1.741414
46	6	-0.233175	-9.220706	-1.741414
47	6	0.209754	0.692886	-1.740979
48	6	-0.164306	10.612601	-1.748433
49	6	-0.482546	-12.943195	1.247582
50	6	0.540218	-3.029825	1.277170
51	6	-0.542845	6.881404	1.275556
52	6	-0.542845	-6.881404	-1.275556
53	6	0.540218	3.029825	-1.277171
54	6	-0.482551	12.943195	-1.247581
55	6	0.454386	-11.157918	-3.032831
56	6	-0.537821	-1.226410	-3.022850
57	6	0.568321	8.684924	-3.021194
58	6	0.568320	-8.684923	3.021194
59	6	-0.537821	1.226410	3.022849
60	6	0.454385	11.157918	3.032831
61	6	0.482551	-12.943195	-1.247581
62	6	-0.540218	-3.029825	-1.277171
63	6	0.542845	6.881404	-1.275556
64	6	0.542845	-6.881404	1.275556

65	6	-0.540218	3.029825	1.277170
66	6	0.482546	12.943195	1.247582
67	6	-0.454385	-11.157918	3.032831
68	6	0.537821	-1.226410	3.022849
69	6	-0.568320	8.684923	3.021194
70	6	-0.568321	-8.684924	-3.021194
71	6	0.537821	1.226410	-3.022850
72	6	-0.454386	11.157918	-3.032831
73	34	1.153053	-6.903799	3.033807
74	34	-1.142670	3.001547	3.038495
75	34	1.012329	12.938843	3.036453
76	34	1.012333	-12.938842	-3.036453
77	34	-1.142669	-3.001548	-3.038495
78	34	1.153054	6.903800	-3.033806
79	34	-1.012329	-12.938843	3.036453
80	34	1.142670	-3.001547	3.038495
81	34	-1.153053	6.903799	3.033807
82	34	-1.153054	-6.903800	-3.033806
83	34	1.142669	3.001548	-3.038495
84	34	-1.012333	12.938842	-3.036453
85	1	0.635739	-8.797687	5.175448
86	1	-0.575070	1.113465	5.178123
87	1	0.463141	11.051921	5.189638
88	1	-0.463141	-11.051921	5.189638
89	1	0.575070	-1.113465	5.178123
90	1	-0.635739	8.797687	5.175448
91	1	-0.635742	-8.797689	-5.175447
92	1	0.575071	1.113465	-5.178123
93	1	-0.463141	11.051921	-5.189638
94	1	0.463141	-11.051921	-5.189638
95	1	-0.575071	-1.113465	-5.178123
96	1	0.635742	8.797689	-5.175447
97	1	0.524165	15.100094	1.139691
98	1	-0.524173	15.100094	-1.139690
99	1	-0.524165	-15.100094	1.139691
100	1	0.524173	-15.100094	-1.139690

Table S28. The optimized Cartesian coordinates of the **TSC**-based ribbon fused through four-membered ring with n=4 (type **III**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-14.259973	3.691241	2.147505
2	6	-4.340341	3.981084	1.530319
3	6	5.558985	3.713026	-2.099278
4	6	15.491670	3.954296	-1.607272
5	6	-15.491669	-3.954300	-1.607269
6	6	-5.558983	-3.713021	-2.099285
7	6	4.340339	-3.981079	1.530326
8	6	14.259972	-3.691245	2.147503
9	6	-19.128509	0.684809	0.005631
10	6	-9.157472	0.437983	0.543010
11	6	0.749806	0.697903	0.001335
12	6	10.658762	0.437683	-0.543145
13	6	-10.658762	-0.437683	-0.543146
14	6	-0.749806	-0.697900	0.001334
15	6	9.157472	-0.437983	0.543012
16	6	19.128509	-0.684814	0.005630
17	6	-14.259973	-3.691245	-2.147497
18	6	-4.340340	-3.981078	-1.530333
19	6	5.558982	-3.713024	2.099279
20	6	15.491668	-3.954300	1.607276
21	6	-15.491670	3.954296	1.607278
22	6	-5.558984	3.713028	2.099272
23	6	4.340342	3.981082	-1.530326
24	6	14.259975	3.691242	-2.147499
25	6	-19.128509	-0.684813	-0.005625
26	6	-9.157473	-0.437983	-0.543012
27	6	0.749806	-0.697900	-0.001339
28	6	10.658761	-0.437683	0.543146

29	6	-10.658761	0.437683	0.543146
30	6	-0.749806	0.697904	-0.001340
31	6	9.157472	0.437984	-0.543011
32	6	19.128509	0.684808	-0.005626
33	6	-16.615072	0.710724	0.131567
34	6	-6.696876	0.535793	0.482206
35	6	3.209731	0.712811	-0.104378
36	6	13.121040	0.533480	-0.485818
37	6	-13.121040	-0.533483	-0.485817
38	6	-3.209731	-0.712807	-0.104382
39	6	6.696876	-0.535790	0.482210
40	6	16.615072	-0.710728	0.131565
41	6	-15.564901	-1.652213	-0.595231
42	6	-5.645378	-1.486985	-0.930852
43	6	4.260138	-1.665653	0.551393
44	6	14.172932	-1.476897	0.951749
45	6	-14.172932	1.476894	0.951750
46	6	-4.260138	1.665656	0.551388
47	6	5.645379	1.486988	-0.930847
48	6	15.564902	1.652210	-0.595233
49	6	-16.615072	-0.710727	-0.131560
50	6	-6.696876	-0.535789	-0.482213
51	6	3.209730	-0.712808	0.104377
52	6	13.121040	-0.533483	0.485820
53	6	-13.121040	0.533481	0.485821
54	6	-3.209731	0.712811	0.104373
55	6	6.696876	0.535792	-0.482210
56	6	16.615072	0.710723	-0.131562
57	6	-15.564901	1.652210	0.595238
58	6	-5.645378	1.486989	0.930843
59	6	4.260138	1.665655	-0.551393
60	6	14.172933	1.476894	-0.951746
61	6	-14.172932	-1.476897	-0.951745
62	6	-4.260138	-1.665652	-0.551398
63	6	5.645378	-1.486986	0.930847
64	6	15.564901	-1.652214	0.595236
65	6	-17.895517	1.334316	0.094328
66	6	-7.981953	0.926521	1.031897
67	6	1.924528	1.385554	-0.056267
68	6	11.833563	0.923720	-1.033681
69	6	-11.833563	-0.923720	-1.033681
70	6	-1.924528	-1.385551	-0.056269
71	6	7.981953	-0.926520	1.031900
72	6	17.895516	-1.334320	0.094326
73	6	-16.110294	-2.937932	-0.879306
74	6	-6.178369	-2.506766	-1.774410
75	6	3.724269	-2.964277	0.802293
76	6	13.637084	-2.492610	1.799339
77	6	-13.637085	2.492606	1.799341
78	6	-3.724270	2.964281	0.802288
79	6	6.178370	2.506770	-1.774405
80	6	16.110295	2.937929	-0.879307
81	6	-17.895517	-1.334319	-0.094321
82	6	-7.981954	-0.926519	-1.031902
83	6	1.924527	-1.385551	0.056264
84	6	11.833562	-0.923720	1.033683
85	6	-11.833562	0.923719	1.033684
86	6	-1.924528	1.385554	0.056262
87	6	7.981954	0.926521	-1.031899
88	6	17.895517	1.334315	-0.094322
89	6	-16.110295	2.937929	0.879314
90	6	-6.178369	2.506771	1.774400
91	6	3.724271	2.964280	-0.802294
92	6	13.637086	2.492607	-1.799336
93	6	-13.637085	-2.492610	-1.799335
94	6	-3.724270	-2.964276	-0.802299
95	6	6.178368	-2.506767	1.774405
96	6	16.110294	-2.937933	0.879311
97	34	-11.855938	2.255350	2.333843
98	34	-1.953217	3.237370	0.243787
99	34	7.954043	2.264034	-2.326721
100	34	17.891244	3.178529	-0.376188
101	34	-17.891243	-3.178533	-0.376187
102	34	-7.954043	-2.264031	-2.326725
103	34	1.953217	-3.237366	0.243790
104	34	11.855937	-2.255351	2.333842
105	34	-17.891243	3.178529	0.376195
106	34	-7.954042	2.264035	2.326718
107	34	1.953217	3.237369	-0.243793

108	34	11.855939	2.255351	-2.333839
109	34	-11.855939	-2.255352	-2.333839
110	34	-1.953217	-3.237366	-0.243797
111	34	7.954042	-2.264033	2.326722
112	34	17.891242	-3.178534	0.376193
113	1	-13.749785	4.413520	2.776837
114	1	-3.835282	4.928252	1.690488
115	1	6.062462	4.438533	-2.730223
116	1	16.004298	4.893579	-1.788858
117	1	-16.004297	4.893579	1.788866
118	1	-6.062461	4.438535	2.730217
119	1	3.835282	4.928250	-1.690496
120	1	13.749787	4.413521	-2.776830
121	1	-13.749785	-4.413524	-2.776828
122	1	-3.835280	-4.928245	-1.690504
123	1	6.062459	-4.438530	2.730225
124	1	16.004295	-4.893583	1.788863
125	1	-16.004296	-4.893583	-1.788856
126	1	-6.062460	-4.438528	-2.730232
127	1	3.835280	-4.928247	1.690496
128	1	13.749784	-4.413524	2.776834
129	1	20.052421	1.254401	-0.010715
130	1	20.052420	-1.254407	0.010719
131	1	-20.052421	1.254402	0.010720
132	1	-20.052421	-1.254405	-0.010714

Table S29. The optimized Cartesian coordinates of the **TSC**-based ribbon fused through four-membered ring with n=5 (type **III**) in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-19.219271	4.253878	0.374831
2	6	-9.302408	4.253341	-0.312498
3	6	0.609045	4.253235	0.314638
4	6	10.520349	4.252948	-0.317091
5	6	20.450709	4.262338	0.226539
6	6	-20.450709	-4.262338	0.226539
7	6	-10.520349	-4.252948	-0.317091
8	6	-0.609045	-4.253235	0.314638
9	6	9.302408	-4.253341	-0.312498
10	6	19.219271	-4.253878	0.374831
11	6	-24.087579	0.622148	-0.286251
12	6	-14.116893	0.627125	0.305675
13	6	-4.205191	0.627345	-0.305167
14	6	5.706476	0.627404	0.305083
15	6	15.618137	0.626902	-0.305903
16	6	-15.618137	-0.626902	-0.305903
17	6	-5.706476	-0.627404	0.305083
18	6	4.205191	-0.627345	-0.305167
19	6	14.116893	-0.627125	0.305675
20	6	24.087579	-0.622148	-0.286251
21	6	-19.219271	-4.253878	-0.374831
22	6	-9.302408	-4.253341	0.312498
23	6	0.609045	-4.253235	-0.314638
24	6	10.520349	-4.252948	0.317091
25	6	20.450709	-4.262338	-0.226539
26	6	-20.450709	4.262338	-0.226539
27	6	-10.520349	4.252948	0.317091
28	6	-0.609045	4.253235	-0.314638
29	6	9.302408	4.253341	0.312498
30	6	19.219271	4.253878	-0.374831
31	6	-24.087579	-0.622148	0.286251
32	6	-14.116893	-0.627125	-0.305675
33	6	-4.205191	-0.627345	0.305167
34	6	5.706476	-0.627404	-0.305083
35	6	15.618137	-0.626902	0.305903
36	6	-15.618137	0.626902	0.305903
37	6	-5.706476	0.627404	-0.305083
38	6	4.205191	0.627345	0.305167
39	6	14.116893	0.627125	-0.305675

40	6	24.087579	0.622148	0.286251
41	6	-21.574173	0.699177	-0.183246
42	6	-11.656231	0.689785	0.208934
43	6	-1.744640	0.689897	-0.208470
44	6	8.166942	0.689965	0.208227
45	6	18.080361	0.689339	-0.213238
46	6	-18.080361	-0.689339	-0.213238
47	6	-8.166942	-0.689965	0.208227
48	6	1.744640	-0.689897	-0.208470
49	6	11.656231	-0.689785	0.208934
50	6	21.574173	-0.699177	-0.183246
51	6	-20.524036	-1.748433	0.163811
52	6	-10.604491	-1.740867	-0.210555
53	6	-0.692929	-1.741053	0.209603
54	6	9.218691	-1.741112	-0.208855
55	6	19.132214	-1.741282	0.233857
56	6	-19.132214	1.741282	0.233857
57	6	-9.218691	1.741112	-0.208855
58	6	0.692929	1.741053	0.209603
59	6	10.604491	1.740867	-0.210555
60	6	20.524036	1.748433	0.163811
61	6	-21.574173	-0.699177	0.183246
62	6	-11.656231	-0.689785	-0.208934
63	6	-1.744640	-0.689897	0.208470
64	6	8.166942	-0.689965	-0.208227
65	6	18.080361	-0.689339	0.213238
66	6	-18.080361	0.689339	0.213238
67	6	-8.166942	0.689965	-0.208227
68	6	1.744640	0.689897	0.208470
69	6	11.656231	0.689785	-0.208934
70	6	21.574173	0.699177	0.183246
71	6	-20.524036	1.748433	-0.163811
72	6	-10.604491	1.740867	0.210555
73	6	-0.692929	1.741053	-0.209603
74	6	9.218691	1.741112	0.208855
75	6	19.132214	1.741282	-0.233857
76	6	-19.132214	-1.741282	-0.233857
77	6	-9.218691	-1.741112	0.208855
78	6	0.692929	-1.741053	-0.209603
79	6	10.604491	-1.740867	0.210555
80	6	20.524036	-1.748433	-0.163811
81	6	-22.854583	1.247686	-0.482285
82	6	-12.941360	1.276944	0.540655
83	6	-3.029870	1.277382	-0.539821
84	6	6.881735	1.277539	0.539582
85	6	16.792970	1.275270	-0.543580
86	6	-16.792970	-1.275270	-0.543580
87	6	-6.881735	-1.277539	0.539582
88	6	3.029870	-1.277382	-0.539821
89	6	12.941360	-1.276944	0.540655
90	6	22.854583	-1.247686	-0.482285
91	6	-21.069283	-3.032919	0.453578
92	6	-11.137976	-3.022599	-0.539217
93	6	-1.226550	-3.022956	0.537382
94	6	8.685088	-3.023135	-0.536098
95	6	18.596471	-3.020929	0.569522
96	6	-18.596471	3.020929	0.569522
97	6	-8.685088	3.023135	-0.536098
98	6	1.226550	3.022956	0.537382
99	6	11.137976	3.022599	-0.539217
100	6	21.069283	3.032919	0.453578
101	6	-22.854583	-1.247686	0.482285
102	6	-12.941360	-1.276944	-0.540655
103	6	-3.029870	-1.277382	0.539821
104	6	6.881735	-1.277539	-0.539582
105	6	16.792970	-1.275270	0.543580
106	6	-16.792970	1.275270	0.543580
107	6	-6.881735	1.277539	-0.539582
108	6	3.029870	1.277382	0.539821
109	6	12.941360	1.276944	-0.540655
110	6	22.854583	1.247686	0.482285
111	6	-21.069283	3.032919	-0.453578
112	6	-11.137976	3.022599	0.539217
113	6	-1.226550	3.022956	-0.537382
114	6	8.685088	3.023135	0.536098
115	6	18.596471	3.020929	-0.569522
116	6	-18.596471	-3.020929	-0.569522
117	6	-8.685088	-3.023135	0.536098
118	6	1.226550	-3.022956	-0.537382

119	6	11.137976	-3.022599	0.539217
120	6	21.069283	-3.032919	-0.453578
121	34	-16.815456	3.033198	1.154761
122	34	-6.909935	3.039041	-1.141300
123	34	3.001871	3.038782	1.141806
124	34	12.913213	3.038097	-1.143619
125	34	22.850182	3.036701	1.011653
126	34	-22.850182	-3.036701	1.011653
127	34	-12.913213	-3.038097	-1.143619
128	34	-3.001871	-3.038782	1.141806
129	34	6.909935	-3.039041	-1.141300
130	34	16.815456	-3.033198	1.154761
131	34	-22.850182	3.036701	-1.011653
132	34	-12.913213	3.038097	1.143619
133	34	-3.001871	3.038782	-1.141806
134	34	6.909935	3.039041	1.141300
135	34	16.815456	3.033198	-1.154761
136	34	-16.815456	-3.033198	-1.154761
137	34	-6.909935	-3.039041	1.141300
138	34	3.001871	-3.038782	-1.141806
139	34	12.913213	-3.038097	1.143619
140	34	22.850182	-3.036701	-1.011653
141	1	-18.709181	5.175162	0.637650
142	1	-8.797788	5.178461	-0.572136
143	1	1.113669	5.178229	0.574722
144	1	11.024874	5.177815	-0.577845
145	1	20.963216	5.189708	0.461755
146	1	-20.963216	5.189708	-0.461755
147	1	-11.024874	5.177815	0.577845
148	1	-1.113669	5.178229	-0.574722
149	1	8.797788	5.178461	0.572136
150	1	18.709181	5.175162	-0.637650
151	1	-18.709181	-5.175162	-0.637650
152	1	-8.797788	-5.178461	0.572136
153	1	1.113669	-5.178229	-0.574722
154	1	11.024874	-5.177815	0.577845
155	1	20.963216	-5.189708	-0.461755
156	1	-20.963216	-5.189708	0.461755
157	1	-11.024874	-5.177815	-0.577845
158	1	-1.113669	-5.178229	0.574722
159	1	8.797788	-5.178461	-0.572136
160	1	18.709181	-5.175162	0.637650
161	1	-25.011476	1.139803	-0.523979
162	1	-25.011476	-1.139803	0.523979
163	1	25.011476	1.139803	0.523979
164	1	25.011476	-1.139803	-0.523979

Table S30. The optimized Cartesian coordinates of the periodic **TTC** ribbon of type **I** calculated at the PBE level of theory.

TThC#1
1.00000000000000
16.4046401977999992 0.0000000000000000 0.0000000000000000
0.0000000000000000 16.5120000000000005 0.0000000000000000
0.0000000000000000 0.0000000000000000 18.2538900374999997
C S H
44 8 8
Direct
0.8962129594579984 0.5434753111701448 0.9372215582691091
0.9560083259010929 0.8956892120825524 0.0405111556724230
0.8962135057473766 0.9565246512248570 0.0623611625666895
0.9560083225044499 0.6043109517736189 0.9590702516560808
0.1037864942527067 0.9565246512248570 0.0623611625666895
0.0439916774956153 0.6043109517736189 0.9590702516560808
0.1037870405420920 0.5434753111701448 0.9372215582691091
0.0439916740989652 0.8956892120825524 0.0405111556724230
0.1037870405420920 0.4565246888299775 0.9372215582691091
0.0439916740989652 0.1043107879174776 0.0405111556724230
0.1037864942527067 0.0434753487750364 0.0623611625666895
0.0439916774956153 0.3956890482263348 0.9590702516560808
0.8962135057473766 0.0434753487750364 0.0623611625666895
0.9560083225044499 0.3956890482263348 0.9590702516560808
0.8962129594579984 0.4565246888299775 0.9372215582691091
0.9560083259010929 0.1043107879174776 0.0405111556724230
0.1802522905361675 0.5811507511602234 0.9225202030285108
0.9174143663483222 0.1799399745537316 0.0276606265210566
0.1802510956272988 0.9188492047189238 0.0770644765560673
0.9174145045022727 0.3200597618807290 0.9719208732860677
0.8197489043726873 0.9188492047189238 0.0770644765560673
0.0825854954976912 0.3200597618807290 0.9719208732860677
0.8197477094638328 0.5811507511602234 0.9225202030285108
0.0825856336516275 0.1799399745537316 0.0276606265210566
0.8197477094638328 0.4188492488396899 0.9225202030285108
0.0825856336516275 0.8200600254462729 0.0276606265210566
0.8197489043726873 0.0811507952811393 0.0770644765560673
0.0825854954976912 0.6799402381193089 0.9719208732860677
0.1802510956272988 0.0811507952811393 0.0770644765560673
0.9174145045022727 0.6799402381193089 0.9719208732860677
0.1802522905361675 0.4188492488396899 0.9225202030285108
0.9174143663483222 0.8200600254462729 0.0276606265210566
0.2514982752038836 0.9583734755680726 0.0999610884393449
0.2515002003402077 0.5416262748007565 0.8996253589941575
0.9570877770809100 0.2499997378286025 0.9997905714326194
0.7484997996596953 0.5416262748007565 0.8996253589941575
0.7485017247960336 0.9583734755680726 0.0999610884393449
0.0429122229191405 0.2499997378286025 0.9997905714326194
0.7484997996596953 0.4583737251991015 0.8996253589941575
0.7485017247960336 0.0416265244320777 0.0999610884393449
0.0429122229191405 0.7500002621714046 0.9997905714326194
0.2514982752038836 0.0416265244320777 0.0999610884393449
0.2515002003402077 0.4583737251991015 0.8996253589941575
0.9570877770809100 0.7500002621714046 0.9997905714326194
0.8169355067574319 0.6824304561753459 0.9439962554427024
0.8169359957117738 0.8175694873797786 0.0555878077774865
0.1830640042881058 0.8175694873797786 0.0555878077774865
0.1830644932424619 0.6824304561753459 0.9439962554427024
0.1830644932424619 0.3175695438247259 0.9439962554427024
0.1830640042881058 0.1824305126201525 0.0555878077774865

0.8169359957117738 0.1824305126201525 0.0555878077774865
0.8169355067574319 0.3175695438247259 0.9439962554427024
0.6937856547024499 0.4237333351644807 0.8865126943080480
0.3062143452976166 0.4237333351644807 0.8865126943080480
0.3062121927600195 0.0762665881390234 0.1130745428037116
0.3062121927600195 0.9237334118610845 0.1130745428037116
0.6937878072400683 0.9237334118610845 0.1130745428037116
0.6937878072400683 0.0762665881390234 0.1130745428037116
0.6937856547024499 0.5762666648353532 0.8865126943080480
0.3062143452976166 0.5762666648353532 0.8865126943080480

Table S31. The optimized Cartesian coordinates of the periodic **TTC** ribbon of type **II** calculated at the PBE level of theory.

TThC#3
1.00000000000000
21.1000000000000050 0.0000000000000000 0.0000000000000000
0.0000000000000000 17.8500000000000014 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C S H
52 8 12
Direct
0.9687437038242949 0.2349811040018194 0.8795065770489002
0.4686998280167438 0.2348838256071330 0.0872744302963399
0.0338405147751864 0.7648500578213004 0.8811620328104479
0.5338335049353513 0.7649609995340891 0.0852620224815952
0.1966812727633198 0.0398859560628997 0.9637912108852433
0.6963572734987783 0.0399272484121485 0.0017485129909875
0.8031192394406467 0.9600196393004802 0.9557652543553866
0.3032246158706750 0.9599955505219607 0.0103079530949679
0.9687236580136380 0.7648970851755049 0.8795584180125905
0.4687227977846164 0.7650153458742568 0.0871814518693202
0.0338604016993204 0.2350001045881470 0.8810369216345197
0.5338099939485478 0.2349598829200878 0.0853201029596032
0.1966758312105864 0.9599919200646715 0.9638272701992111
0.6963596108932896 0.9600317929720984 0.0017524502648382
0.8031220505661888 0.0399166229520059 0.9557687955374149
0.3032188493365194 0.0399147247288352 0.0103054525462546
0.0823426073902261 0.0407557418809983 0.9261095309927453
0.5821276170016848 0.0408033798326799 0.0398036253040459
0.9185661052129215 0.9591309796015464 0.9223355017170142
0.4185136104017586 0.9591469467923158 0.0441388092460995
0.0348413352434509 0.9028968319420043 0.9085538415528814
0.5347446018636711 0.9029675586129847 0.0577680949923099
0.9667124606651305 0.0969680565679293 0.9068785162512188
0.4666170723651354 0.0969490348354630 0.0596866397416410
0.0823371772566553 0.9591022274719514 0.9261588162716251
0.5821313149358459 0.9591490498881562 0.0398090070921212
0.9185695366391207 0.0407737121033832 0.9223314529590264
0.4185068009065995 0.0407732960925554 0.0441448104669774
0.0348530914968422 0.0969595810547572 0.9084669070297368
0.5347344982649920 0.0969719269244217 0.0577724084324229
0.9667043097713715 0.9029157187676220 0.9069135843427257
0.4666287523410261 0.9029724574426309 0.0596677435003821
0.1413690626029738 0.0757163142546270 0.9383463398571553
0.6410759103159631 0.0757870865353222 0.0272440074583315
0.8591184628346700 0.9241922617612329 0.9320301254014969
0.3590856829832288 0.9241891318071470 0.0344401907142076
0.0643975699071586 0.8315455599727646 0.8992324904339319
0.5643307637171859 0.8316370052297872 0.0670338391450572
0.9375147930944950 0.1682662529232514 0.8961275622690094

0.4374135351530949 0.1681914369800191 0.0706946264454565
0.1413520524041748 0.9241330211797451 0.9384530704144561
0.6410830482886067 0.9241733475278526 0.0272541774434838
0.8591288580106211 0.0757297015275928 0.9320374779144052
0.3590729986059342 0.0757255380542982 0.0344522048587840
0.0644189519085519 0.1682949077263259 0.8990778397362855
0.5643146718392257 0.1683035684684683 0.0670472326609149
0.9374973810133702 0.8316217675732662 0.8961541053283180
0.4374342140627338 0.8317173688669226 0.0706409140210538
0.2499006126571088 0.9214321882937211 0.9872307544553385
0.7496442158016878 0.9214733660649176 0.9784884294633037
0.2498965138858334 0.0784662265341740 0.9872002448510964
0.7496474055219067 0.0784736253656691 0.9784840523912467
0.8575044835638465 0.1692169763970623 0.9119633616706458
0.3573541955130949 0.1690943496646066 0.0550122983148375
0.1436725230867826 0.8305489394882384 0.9186865528891929
0.6435176404463548 0.8306336242081563 0.0471667509128172
0.1437210796809890 0.1692481305939062 0.9184067620980775
0.6434979504197557 0.1693289539379464 0.0471573854574045
0.8574809908640993 0.8307053940726168 0.9119597378316151
0.3573821506391748 0.8308080098911588 0.0549418649454986
0.2499720590281608 0.8601862520754412 0.9871301145956898
0.7496951785545630 0.8602273601451792 0.9785957532675881
0.2499578993788354 0.1397124171335359 0.9870872043529809
0.7497041530889694 0.1397192430500104 0.9785751925959252
0.9417938223631124 0.2858660956097340 0.8693180010110546
0.4417841167514935 0.2857494762795752 0.0976396358554099
0.0611740541428130 0.2859146478105667 0.8721299045851963
0.5611349286432701 0.2858963536491571 0.0940840015858776
0.0611494087394973 0.7139235403839292 0.8722879972949467
0.5611660261272005 0.7140240418272470 0.0940019523290042
0.9417712515398388 0.7140172487576099 0.8693502790966873
0.4418140859042790 0.7141299836580831 0.0974935171655441

Table S32. The optimized Cartesian coordinates of the periodic **TSC** ribbon of type **I** calculated at the PBE level of theory.

TSeC#1
1.00000000000000
15.7000000000000028 0.0000000000000000 0.0000000000000000
0.0000000000000000 16.5065038860986171 0.0000000000000000
0.0000000000000000 0.0000000000000000 18.1569750575711346
C Se H
44 8 8
Direct
0.5445767882975586 0.1014806762510986 0.9319069344214741
0.8924990737053785 0.0438491871723658 0.0834697775325296
0.9532415669073151 0.1015797629521417 0.1154350631356776
0.6054939578628810 0.0438469053581766 0.9636929410305900
0.9532415669073151 0.8984202370484812 0.1154350631356776
0.6054939578628810 0.9561530946423588 0.9636929410305900
0.5445767882975586 0.8985193237490926 0.9319069344214741
0.8924990737053785 0.9561508128286443 0.0834697775325296
0.4532104510292933 0.8985444700149073 0.9321439874957007
0.1055840384741031 0.9561436660235051 0.0841243825256873
0.0446280208418952 0.8983899716078743 0.1157028222479262
0.3925363026380842 0.9561632984295307 0.9643037266668549
0.0446280208418952 0.1016100283930835 0.1157028222479262
0.3925363026380842 0.0438367015703081 0.9643037266668549
0.4532104510292933 0.1014555299849204 0.9321439874957007

0.1055840384741031 0.0438563339766574 0.0841243825256873
0.5843277470884649 0.8247939518433001 0.9105818277839068
0.1822766156918951 0.0818468919185178 0.0628359798487067
0.9133037171766465 0.8246564374522396 0.1364054576553545
0.3160413419152567 0.0818661515734302 0.9860359061026399
0.9133037171766465 0.1753435625469248 0.1364054576553545
0.3160413419152567 0.9181338484270747 0.9860359061026399
0.5843277470884649 0.1752060481554165 0.9105818277839068
0.1822766156918951 0.9181531080805554 0.0628359798487067
0.4132575171587069 0.1751291076635811 0.9109843292479892
0.8159407528032288 0.9181590226843711 0.0617895386868745
0.0843783140962008 0.1754198186867585 0.1368425554404452
0.6821243374986810 0.9181195722231449 0.9850544799540573
0.0843783140962008 0.8245801813118431 0.1368425554404452
0.6821243374986810 0.0818804277758667 0.9850544799540573
0.4132575171587069 0.8248708923370832 0.9109843292479892
0.8159407528032288 0.0818409773151444 0.0617895386868745
0.9547682427549087 0.7583443121676496 0.1682712780864522
0.5425864661708011 0.7586834815977963 0.8786164346508220
0.2492401541597256 0.0427534401405984 0.0245279912169504
0.5425864661708011 0.2413165184032774 0.8786164346508220
0.9547682427549087 0.2416556878318639 0.1682712780864522
0.2492401541597256 0.9572465598587521 0.0245279912169504
0.4547210053820436 0.2412723528961775 0.8788107935458934
0.0426267590763676 0.2417047630539599 0.1684753546123357
0.7490755065872181 0.9572466526077525 0.0233634078934656
0.0426267590763676 0.7582952369461184 0.1684753546123357
0.4547210053820436 0.7587276471041666 0.8788107935458934
0.7490755065872181 0.0427533473920410 0.0233634078934656
0.6967252391462050 0.1865387545580236 0.9450722853392194
0.8010777064863868 0.1865298021875499 0.1015647697515221
0.8010777064863868 0.8134701978118343 0.1015647697515221
0.6967252391462050 0.8134612454427921 0.9450722853392194
0.3011353213459907 0.8135178132128230 0.9460842896232753
0.1969251524885523 0.8134346049446077 0.1026553982207741
0.1969251524885523 0.1865653950561027 0.1026553982207741
0.3011353213459907 0.1864821867867202 0.9460842896232753
0.4188200930796107 0.2940265982078451 0.8601381921558338
0.4188200930796107 0.7059734017925834 0.8601381921558338
0.0783481679878059 0.7054046407534734 0.1870873756426291
0.9188597671005275 0.7054988066031145 0.1867197963993801
0.9188597671005275 0.2945011933959928 0.1867197963993801
0.0783481679878059 0.2945953592456012 0.1870873756426291
0.5783128934893365 0.2941069226193299 0.8597783994555324
0.5783128934893365 0.7058930773809687 0.8597783994555324

Table S33. The optimized Cartesian coordinates of the periodic **TSC** ribbon of type **II** calculated at the PBE level of theory.

TSeC#2
1.00000000000000
19.4050000000000011 0.0000000000000000 0.0000000000000000
0.0000000000000000 16.4046401977999992 0.0000000000000000
0.0000000000000000 0.0000000000000000 18.2538900374999997
C Se H
52 8 12
Direct
0.9653945592800581 0.2318927305711070 0.8053244239734567
0.4649459540428920 0.2865403825233453 0.1665711772196752
0.0355950797460001 0.7429973894403215 0.8642794025457519
0.5359409095316535 0.7979067000156368 0.2271288598407216

0.2014678585702675 0.0513651030118338 0.9689403330326830
0.7013199294336586 0.0643339371041507 0.0519301136361098
0.3014482872621608 0.9772915359221381 0.0595881406967018
0.8015682837902779 0.9660982449630712 0.9828261611919903
0.9644746246627387 0.7435078824514150 0.8639157666073307
0.4648197365979100 0.7981763533529950 0.2272112063184157
0.0364946623796594 0.2309992381004934 0.8036209345368356
0.5360596684169256 0.2864786306404207 0.1678454930268614
0.2008923655246415 0.9650460940078965 0.9806908202666518
0.7009517613126772 0.9777186331748503 0.0617135383817171
0.3019226012770479 0.0636224748429371 0.0479724366611375
0.8020605050142144 0.0527388067164988 0.9732166169288691
0.0871899890544550 0.0426344415484926 0.9059282551428067
0.5869906672159442 0.0745382538633063 0.1147695451917184
0.9150652320207078 0.9555109138679169 0.9183292861042913
0.4149814338993166 0.9864114236848163 0.1241950961441745
0.0376182335187126 0.8918732574821721 0.8946977144694552
0.5376901207061926 0.9324458111011140 0.1621559497635122
0.9641381833372572 0.0973395741934137 0.8702987894515190
0.4638603579416509 0.1375679637793389 0.1363464018341622
0.0868136158544781 0.9547168862716165 0.9174654532829132
0.5868003242079880 0.9864043443613618 0.1251123464610860
0.9154380520768870 0.0436613063307980 0.9082285951439649
0.4152182362679593 0.0743926281668987 0.1128397875472957
0.0381188023928642 0.0966423509069311 0.8689122701617504
0.5378619661499918 0.1375642036720834 0.1374039086273783
0.9636235880894370 0.8923306474414467 0.8946993521559725
0.4636821629311321 0.9325936315363624 0.1619986649428002
0.1492101959929923 0.0830308026468887 0.9223449819784195
0.6488702573991618 0.1086761681229983 0.0889180837160547
0.8534381895958738 0.9215951741077414 0.9450710714998778
0.3533870044505710 0.9456667380044643 0.1066044588341300
0.0695039331437591 0.8143223653138019 0.8857191592187281
0.5697221239748448 0.8604827971676159 0.1894860836282155
0.9320080624617627 0.1695665811636287 0.8436994616084846
0.4315862363015484 0.2149789148734264 0.1447731944705518
0.1482871750186731 0.9204350996998663 0.9442057931677306
0.6483973920517254 0.9455979376321902 0.1076897331078630
0.8542926783703901 0.0847654792935550 0.9268144927172883
0.3540044596551244 0.1083726837944603 0.0851446432764780
0.0703411991319806 0.1680032500921623 0.8406229128410032
0.5699634065723141 0.2148961428543454 0.1470745318913228
0.9311030948053229 0.8152313313208014 0.8852540019635562
0.4313302682388747 0.8609172014239360 0.1894942390334889
0.2509353702025577 0.9297185407326480 0.0256613864510680
0.7510952516637999 0.9303312346804050 0.0269973431699318
0.2520366438133236 0.0989252187667240 0.0027691537275303
0.7519622264664678 0.1001348818882606 0.0080156203294683
0.8418239432253289 0.1848930831970619 0.8788429229084100
0.3412432606256899 0.2190382085885218 0.1075249671053009
0.1602987468464479 0.8096821212876301 0.9216741017261793
0.6606468130008134 0.8457436731011809 0.1562241904712240
0.1618870730496109 0.1817840256281325 0.8722288833961112
0.6612488506991600 0.2190724147797478 0.1125271510656154
0.8402354196495314 0.8114058516941567 0.9210660751318154
0.3404841250155529 0.8463991813134255 0.1559465672227373
0.2504845729106734 0.8637560004351975 0.0345304237276529
0.7507599938071076 0.8641445652795737 0.0344051981220627
0.2524423014440391 0.1648911821200493 0.9939179770580514
0.7522406598585240 0.1663160566707798 0.0005533174053151
0.9364165220571108 0.2830765736157589 0.7827820390688501
0.4358992318309726 0.3424850874697931 0.1761616008077969

0.0653966441246663 0.2814474147042052 0.7796663245353121
0.5648634211548604 0.3423674891860209 0.1784730251341679
0.0642848931078527 0.6868967384914184 0.8542414487860764
0.5647747100787416 0.7469843169293107 0.2503515470749453
0.9353083253515384 0.6878199442733983 0.8535759894526364
0.4357582537734553 0.7474775643271343 0.2505046916616282

Table S34. Total energies of the studied **TTC** and **TSC** systems calculated at the B3LYP/6-31(d) level of theory

	E_{tot}, *a.u.*		E_{tot}, *a.u.*		E_{tot}, *a.u.*
TTC-based systems					
TTC	–2512.1824				
Type I		**Type II**		**Type III**	
n=2	–4945.7418	**n=2**	–5099.3951	**n=2**	–5021.8823
n=3	–7379.2979	**n=3**	–7686.6084	**n=3**	–7531.5820
n=4	–9812.8576	**n=4**	–10273.8218	**n=4**	–10041.2819
n=5	–12246.4174	**n=5**	–12861.0350	**n=5**	–12550.9815
TSC-based systems					
TSC	–10516.9065				
Type I		**Type II**		**Type III**	
n=2	–20955.2114	**n=2**	–21108.8496	**n=2**	–21031.3473
n=3	–31393.5132	**n=3**	–31700.7944	**n=3**	–31545.7865
n=4	–41831.8182	**n=4**	–42292.7387	**n=4**	–42060.2271
n=5	–52270.1233	**n=5**	–52884.6833	**n=5**	–52574.6663

TTC – tetrathia[8]circulene;
TSC – tetraselena[8]circulene.