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

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Abstract

Conjugated polymers gain much attention due to the promising applications in organic electronic device technology. In this work, we theoretically study structures and electronic properties of a novel class of nanostructures, namely one-dimensional tetrathia[8]circulenes (**TTC**) and tetraselena[8]circulenes (**TSC**) predicted to be promising semiconducting soft materials. It is found that all nanoribbons are thermodynamically stable and that their electronic properties depend significantly on the type of fusing between the monomers. In particular, the band gap tends to decrease while moving from the directly fused **TTC/TSC** ribbons to the structures coupled *via* a benzene-core linker and then to the ribbons fused through a four-membered ring. Therefore, both coupling type and length of oligomers allow one to manipulate the electronic and optical properties of the

studied ribbons. The band structure calculations of infinite nanoribbons reveal direct band gaps that decrease from 2.28 to 2.14 eV for the **TTC** ribbons of the first and second fusion types. The **TSC** structures demonstrate the same trend exhibiting band gap narrowing from 2.41 (type **I**) up to 2.11 eV (type **II**). The type **III** ribbons possess the lack of periodicity due to the close-lying energy minima for the possible twisting configurations of **TTC** and **TSC** moieties relative to the linking four-membered ring.

Keywords: tetrathia[8]circulene, tetraselena[8]circulene, band gap engineering, π-conjugation, band structure, nanoribbons.
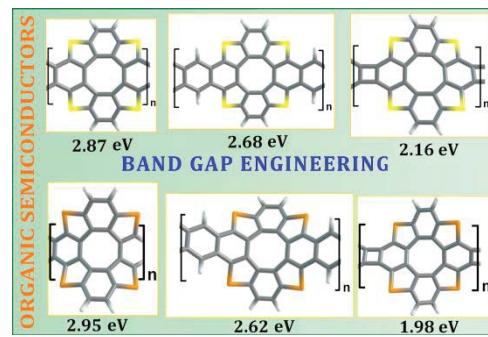
Graphical abstract

1. Introduction

One- (1D) and two-dimensional (2D) conjugated polymers currently represent a rapidly developing research branch due to their potential applications in organic electronics possessing advantages over inorganic and small-molecule organic semiconductors. [1-8] Modern molecular design methods make it possible to alter and engineer materials of different architectures with certain desired properties and functionality through controlled and directed assemblies of molecular building blocks in order to meet the requirements of certain organic devices. Recently, a wide range of molecules including benzene, furan, thiophene, pyridine, acetylene, *etc*., as well as bulky polycyclic aromatic hydrocarbons (PAHs) and polyheterocyclic structures have been successfully used as appropriate building blocks for synthetic preparation of the shape-persistent conjugated macrocycles with different dimensionality. [1] The self-assembly and self-organization of porphyrins, metalloporphyrins and phthalocyanines prove the possibility to build ideal 1D or 2D extended polymers, [2–6] for prospective catalytic, photovoltaic and electronic applications. Such materials can provide an efficient optical coupling leading to significantly higher optical absorption and photocatalytic activity compared to the original monomers. [7, 8]

Recently, Osuka *et al*. [9, 10] have reported the synthesis of a free base porphyrin sheet (Fig. 1, **a**) consisting of four *meso-meso* fused porphyrin molecules as initial building units. It was shown that anomalous electronic properties including the unusual aromaticity of the porphyrin sheet arise from the central strongly antiaromatic cyclooctatetraene (COT) core which prefers to be planar due to the direct fusion of the porphyrins. Much attention has also been paid to study optoelectronic properties and the self-assembly phenomenon of phthalocyanines, which are of paramount importance for their incorporation into photovoltaic devices.[11–13] In particular, phthalocyanines have a larger π-conjugated system compared to porphyrins, which leads to a radiation absorption of a longer wavelength. [14, 15] The high stability and insolubility of phthalocyanines in most solvents makes these compounds applicable as useful dyestuff. [16, 17]

An interesting alternative class of polyheteroaromatic systems contained antiaromatic COT-cores are heterocirculenes. [18–21] The electronic spectral and photophysical properties of these compounds are in the spotlight of current studies [22–27] due to their promising application in organic light-emitting diodes (OLEDs) [28–30] and organic field-effect transistors (OFETs)[31–33] technologies. Similar to porphyrins and phthalocyanines, the inherent functionalities stored within the heterocirculene systems make them attractive building blocks for novel tailor-made π-conjugated polymers. Recently, tetraoxa[8]circulene (**TOC**) was predicted as an initial building unit in formation of the stable 1D and 2D **TOC**-based materials (Fig. 1, **b-e**) [34–37] which represent biomimetic-type nanopores in the context of their ability to capture s- and d-block metal ions. [38, 39] In contrast to the parent tetraoxa[8]circulene molecule, **TOC**-polymers show strong absorption in the visible region due to the consistent growth of π-conjugation. [34, 35] Moreover, the electronic properties of these polymers depend significantly on the type of fusing between monomers. In particular, among **TOC**-polymers with three different fusion principles discussed in Ref. 37 only **TOC**-polymers with directly linked **TOC**-molecules and **TOC**-polymers with benzene-core linkers demonstrate semiconducting properties with 1.37 and 1.84 eV direct band gaps, while another one in which **TOC** moieties linked through the four-membered ring was found to be a semimetal with ~87 meV band gap induced by spin-orbit coupling. [37]
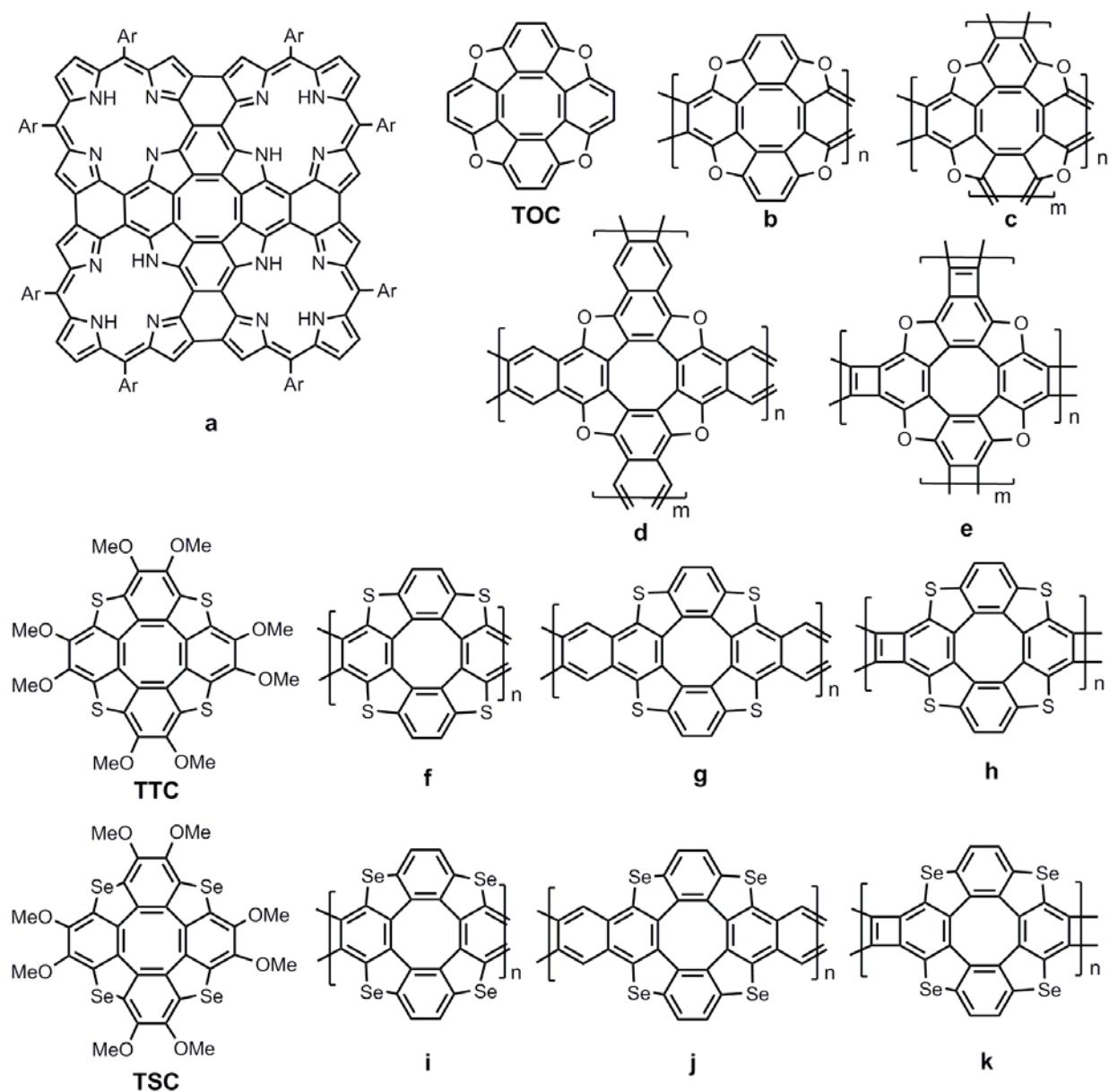
Fig. 1 Some examples of the 1D and 2D polymers containing porphyrin (**a**),[9, 10] tetraoxa[8]circulene (**b–e**),[34–37] tetrathia[8]circulene (**f–h**) and tetraselena[8]circulene (**i–k**) monomers studied in this paper.

The methoxy-substituted **TTC** and **TSC** hetero[8]circulenes (Fig. 1) have been prepared in 2015 [40] and their electronic and spectral properties have also been interpreted in detail. [41–43] In 2019 Miyake *et al.* reported a diversity-oriented approach for the synthetic preparation of tetrathia[8]circulenes which enables a convenient installation of various peripheral substituents. [44] This is an effective way to fine tune the photophysical properties and control the solid-state packing of

tetraheterocirculenes. Moreover, a great advantage of the tetrahetero[8]circulenes being effective for their functionalization is the presence of CH bonds which serve as the main functionalization centers in chemical transformations and possible formation of n-dimensional materials.

In this paper, we perform a comprehensive study of two new families of 1D covalent organic polymers based on tetrathia[8]circulene (**TTC**) and tetraselena[8]circulene (**TSC**) as initial building units with different types of intermonomer fusion (Fig. 1, **f-k**). Depending on the fusion type between tetrahetero[8]circulene (**TTC** and **TSC**) molecules, various materials can be obtained. Such inter-monomer coupling can proceed through intermolecular dehydrohalogenation or the Ullman-type polymerization reactions which have been shown to be thermodynamically allowed. [35] The ability to control intermonomer fusion significantly expands the design possibilities of novel polymers with targeted functional properties.

2. Computational details

The structure, UV-visible absorption spectra and band structure origin were investigated for the two series of designed 1D oligomers based on **TTC** and **TSC** building units. Both these species were constructed by n-repeating **TTC** and **TSC** monomers (n = 2 – 5, and infinite band) along the 1D direction. In accordance with this principle, we have designed various **TTC** and **TSC**-based materials with three different types of fusion between monomers including the **TTC** or **TSC**-materials with directly linked **TTC**/**TSC** units (type I), fused *via* a benzene-core linker (type **II**) or through a four-membered ring (type **III**).

The finite **TTC** and **TSC**-based 1D structures were optimized at the B3LYP/6-31G(d) level of density functional theory (DFT) [45-49] using the Gaussian 16 software package. [50] The absence of imaginary vibrational wavenumbers in the calculated IR spectra indicates that a true minimum on the hypersurface of the total energy was found. The electronic absorption spectra of all the studied molecules

were calculated by the time-dependent (TD) DFT method [51] in the vacuum approximation with the same B3LYP/6-31G(d) method. [45-49]

The infinite units were calculated in periodic boundary conditions (PBC) within the generalized gradient approximation (DFT GGA) as realized in the Vienna Ab initio Simulation Package (VASP). [52,53] The projector augmented wave (PAW) [54] method and the Perdew-Burke-Ernzerhof (PBE) [55] exchange functionals were employed. To correctly describe electronic properties, the long-corrected hybrid functional proposed by Heyd, Scuseria, and Ernzerhof (HSE06) was employed. [56] The cutoff energy utilized for the plane wave expansion of the wave functions was set to 400 eV. The vacuum region of 15 Å was set along the z-direction to avoid interactions between neighboring images. A set of $1\times40\times1$ k-points was applied according to the Monkhorst-Pack scheme [57] for electronic structure calculations in the PBE approximation, while $1\times6\times1$ k-points were used utilizing the HSE06 functional. The convergence tolerances of the force and electronic minimizations were set to 10^{-5} eV/Å and 10^{-6} eV, respectively.

3. Results and discussion

3.1. Structural features

According to X-ray data [40] the free methoxy-substituted **TTC** and **TSC** molecules represent non-planar species (the D_2 symmetry point group) which was also well reproduced by our DFT calculations. [41] In the case of **TTC**, the deviation from planarity is very slight, about 2°, while **TSC** has a more pronounced saddle-shaped structure with a bent angle of the COT core of 12°. Such structural perturbations have been explained by insertion of more massive sulfur or selenium heteroatoms into the outer framework of the heterocirculenes.[42] Therefore, it can be assumed that these circulenes being building blocks in the **TTC** and **TSC**-based structures will adopt to the shape of the free molecules along the corresponding ribbon. Indeed, our DFT calculations predict more distorted shapes for the **TSC**-based structures compared to those of **TTC** ones due to the inherent saddle shape of the initial **TSC**-building unit. The optimized structures of the predicted 1D

ribbons (n = 2 and 5) are shown in Fig. 2. Their general size parameters (length and width) are presented in Table 1.

As one can see from Fig. 2, direct fusion of the **TTC** monomers (the first fusion type) provides a steric hindrance in the **TTC**-structures; therefore, the shape of ribbon with n = 2 is twisted in such a way that the sulfur atoms of adjacent thiophene rings are located as far as possible with S--S distances equal to 3.07 Å. Further inclusion of the **TTC** building unit into the molecular skeleton (n = 3–5) leads to the formation of the regular wave-like ribbons with distances between adjacent ridges (wavelength) of 16.7 Å (Fig. 2), herewith, the S--S distances decrease to 3.02 – 3.06 Å. It should be noted that the terminal **TTC** fragments are more planar than the inner ones. The deviations from planarity of the COT core are ≈10° and ≈15° for the terminal and inner **TTC** macrocycles, respectively. A continuous attaching of the same building blocks in the second dimension should lead to a porous 3D structure with high thermoelectric performance. [58]

The inclusion of a benzene-core linker into the **TTC** ribbons (second fusion type) eliminates the problem of steric complications between **TTC** building blocks. The **TTC** ribbons remain a wave-like structure with wavelength 21.8 Å with formation strongly planar acene structural part (Fig. 2). In this case, the structure of the **TTC** fragments tends to be planar approaching the shape of the initial free **TTC** molecule. The deviation from planarity of the **COT** core is about 5° which is significantly smaller compared to the previously discussed directly fused **TTC**-structures.

The structure of the **TTC** ribbons fused through a four-membered ring (the third type) adopts linear topology in which alternating **TTC** macrocycles and biphenylene fragments can be distinguished. Moreover, the biphenylene fragments are strictly planar while the **TTC** fragments adopt a slightly corrugated structure with deviation from planarity ≈5°. The S--S distances between adjacent thiophene rings are ~3.96 Å that is larger compared to that for directly fused **TTC**-structures.
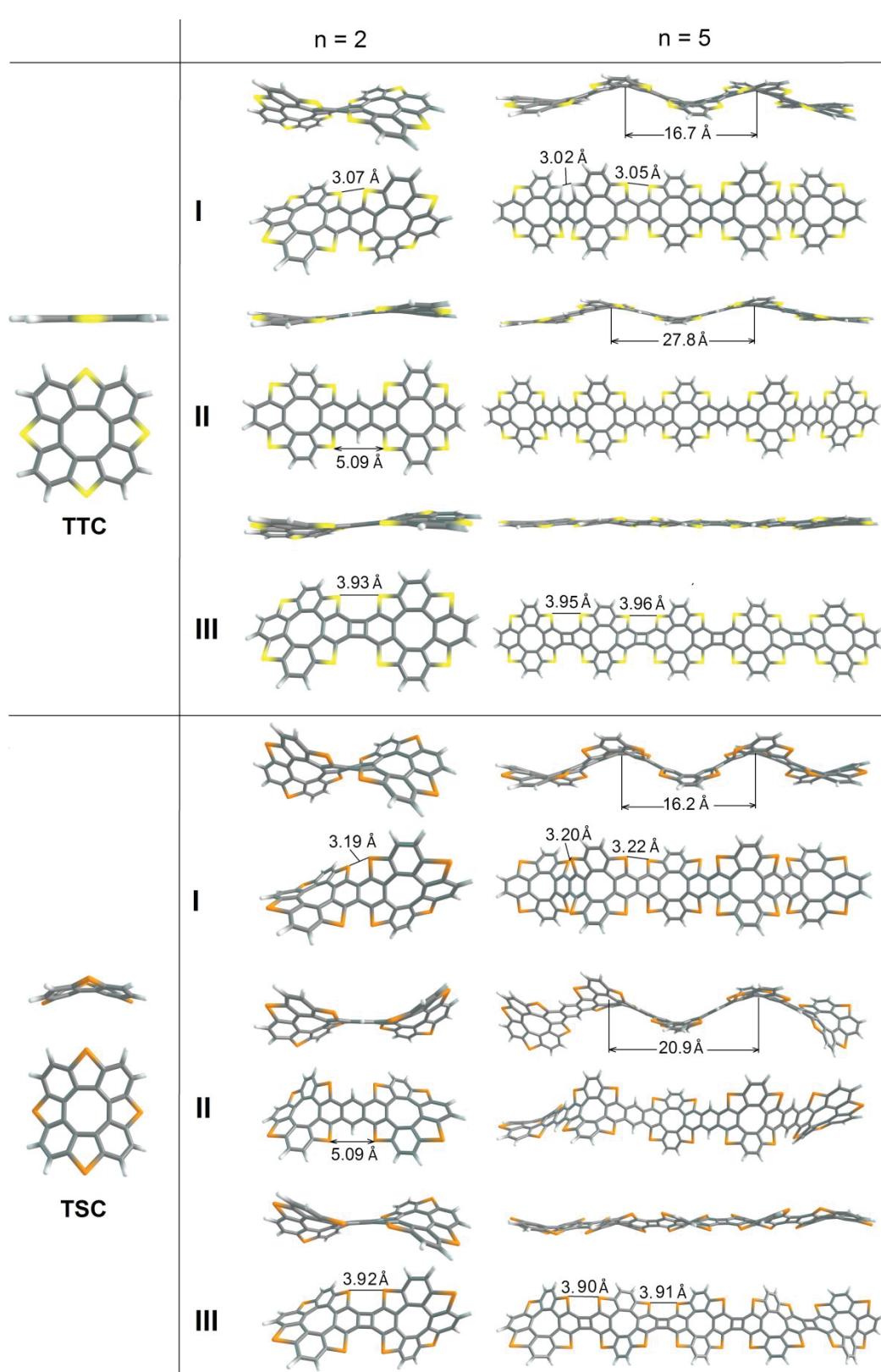
Fig. 2 Molecular representations of the **TTC** and **TSC** structures with n=2 and n = 5 (side and top view).

Similar to **TTC**-structures, the directly fused **TSC**-based ribbons possess a specific wave-like topology with distances between adjacent ridges of ~16.2 Å. It

should be noted that the direct fusion of the **TSC** monomers provides a more pronounced twist-type distortion of the **TSC** building units compared to the free **TSC** molecule and appearance of the saddle-shaped conformation with deviation from planarity of the COT core $\approx 25°$. The distances between selenium atoms of adjacent selenophene rings reach up to 3.22 Å along the **TSC** ribbons.

Table 1 The general size parameters of the **TTC**- and **TSC**-based ribbons designed by the B3LYP/6-31G(d) computations

TTC-based compounds	a, nm*	b, nm**	Empirical formula	TSC-based compounds	a, nm*	b, nm**	Empirical formula
Type **I**				Type **I**			
n = 2	1.04	1.90	$C_{46}H_{12}S_8$	n = 2	1.04	1.90	$C_{46}H_{12}Se_8$
n = 3	1.02	2.71	$C_{68}H_{16}S_{12}$	n = 3	1.00	2.63	$C_{68}H_{16}Se_{12}$
n = 4	1.02	3.55	$C_{90}H_{20}S_{16}$	n = 4	1.00	3.44	$C_{90}H_{20}Se_{16}$
n = 5	1.02	4.38	$C_{112}H_{24}S_{20}$	n = 5	1.00	4.25	$C_{112}H_{24}Se_{20}$
Type **II**				Type **II**			
n = 2	1.04	2.14	$C_{50}H_{14}S_8$	n = 2	1.04	2.12	$C_{50}H_{14}Se_8$
n = 3	1.04	3.22	$C_{76}H_{20}S_{12}$	n = 3	1.04	3.09	$C_{76}H_{20}Se_{12}$
n = 4	1.04	4.25	$C_{102}H_{26}S_{16}$	n = 4	1.04	4.14	$C_{102}H_{26}Se_{16}$
n = 5	1.04	5.41	$C_{128}H_{32}S_{20}$	n = 5	1.04	5.11	$C_{128}H_{32}Se_{20}$
Type **III**				Type **III**			
n = 2	1.04	2.05	$C_{48}H_{12}S_8$	n = 2	1.04	2.04	$C_{48}H_{12}Se_8$
n = 3	1.04	3.05	$C_{72}H_{16}S_{12}$	n = 3	1.04	3.02	$C_{72}H_{16}Se_{12}$
n = 4	1.04	4.05	$C_{96}H_{20}S_{16}$	n = 4	1.04	4.01	$C_{96}H_{20}Se_{16}$
n = 5	1.04	5.05	$C_{120}H_{24}S_{20}$	n = 5	1.04	5.00	$C_{120}H_{24}Se_{20}$
TTC	0.87	0.87	$C_{24}H_8S_4$	**TSC**	0.85	0.85	$C_{24}H_8Se_4$

*a or**b – width or length of the corresponding **TTC**- and **TSC**-based structures.

Insertion of the benzene-core linker into the structure of the **TSC** ribbons bent them in such a way that the formed aromatic acene fragments become planar. In this case, the **TSC** ribbons with n = 2–3 possess a specific curved structure, which adopts a regular wave-like topology with wavelength of 20.9 Å (Fig. 2). As for **TTC**, the third fusion type through four-membered rings adopts linear topology with planar biphenylene fragments and oppositely arranged saddle-shaped **TSC** fragments (Fig. 2).

3.2. Electronic absorption spectra

The calculated electronic absorption spectra of the **TTC**- and **TSC**-based ribbons are presented in Fig. 3. The electronic structure and UV-vis spectra of the methoxy-substituted **TTC** and **TSC** molecules have been previously studied in detail both experimentally and theoretically. [41] In particular, both methoxy-substituted **TTC** and **TSC** molecules show a long-wavelength absorption band in the region of 320–450 nm. The first $S_0 \rightarrow S_1$ electronic transition calculated at 414 and 442 nm for **TTC** and **TSC**, respectively, is symmetry allowed with very low intensity, providing a weak fluorescence.[41] For the unsubstituted **TTC** and **TSC** molecules, the electronic transitions into the S_1 excited state of the $X^1A \rightarrow {}^1A_2$ symmetry are forbidden (f=0, see ESI, Tables S1 and S2†) in the electric-dipole approximation but allowed as magnetic-dipole transitions with relatively large magnetic moments $(\mu_z) \approx 3.4\mu_B$. The transitions into the S_2 excited state are strongly symmetry forbidden in both electric-dipole and magnetic-dipole approximations (see ESI, Tables S1 and S2†). The third and fourth electronic transitions into the double degenerate ^1E excited state (see ESI, Tables S1 and S2†) provide strong bands at 382 and 415 nm for **TTC** and **TSC** molecules, respectively.

The first $S_0 \rightarrow S_1$ electronic transition is allowed for most of the **TTC** and **TSC** ribbons in the calculated absorption spectra of the designed **TTC** and **TSC** species (see ESI, Tables S1 and S2†). In particular, for the **TTC** ribbons of the first fusion type (n=2–5) the first broad band has a high intensity and takes place in the region of 430–550 nm (Fig. 3a). This band corresponds to the electronic transitions into the S_1 excited state resulting from the main contribution of the HOMO→LUMO configuration (Fig. 4). The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of the **TTC** compounds of the first fusion type are mainly localized over the naphthalene moieties (HOMO) and central COT core (LUMO) along the whole backbone (Fig. 4). Moreover, the first band intensity is characterized by high oscillator strength values which correlates well with the **TTC** ribbon length and continues to

increase linearly with increasing conjugation plane (for the **TTC** with n=2 $f = 0.48$; with n=3 $f = 1.02$; with n=4 $f = 1.62$; with n=5 $f = 2.26$ see ESI, Table S1†). The second band is more intense and takes place in a near UV range of 320–400 nm for short oligomers with n=2 and n=3; this band tends to shift to the visible region with the growth of the ribbon size (Fig. 3a).
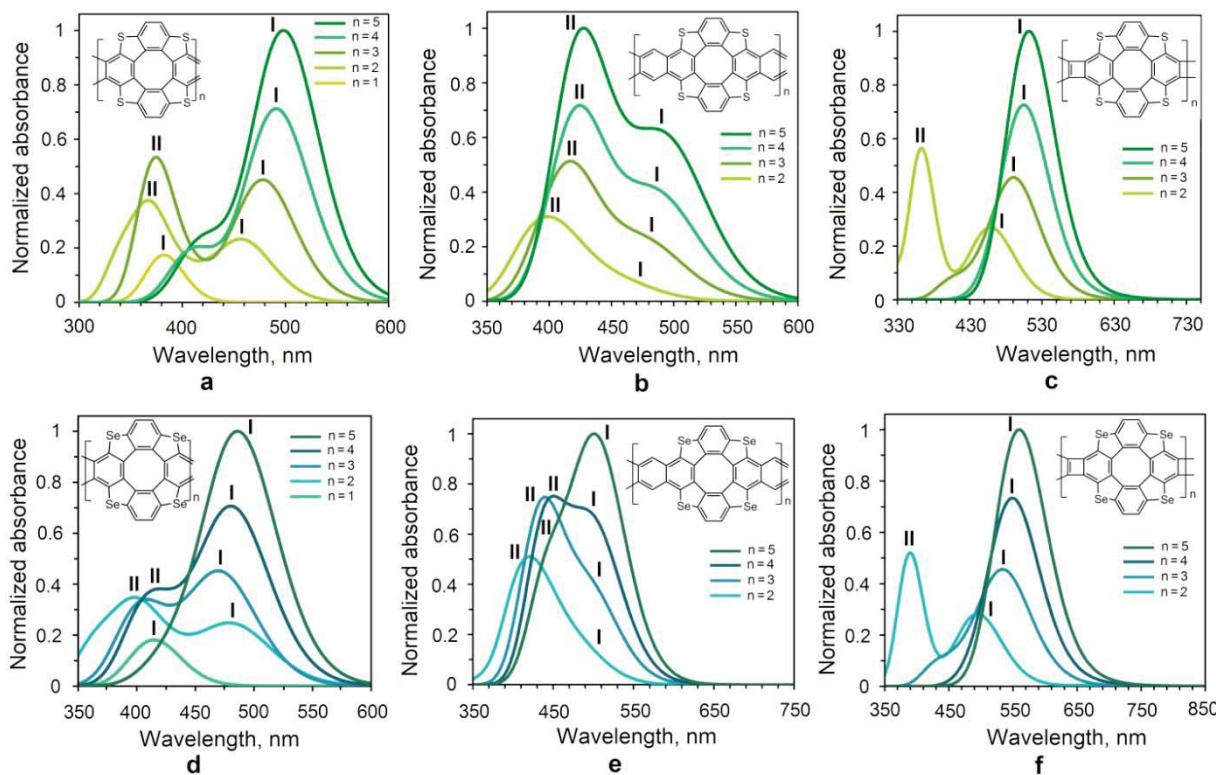
Fig. 3 Electronic absorption spectra of the **TTC**- and **TSC**-based ribbons calculated by the TD DFT/B3LYP/6-31G(d) method; **I** and **II** denote the first and second absorption bands (band half-width 3000 cm^{-1}, Gaussian distribution function).

TTC ribbons fused *via* a benzene-core linker (the second fusion type) possess the first band appearing in the range 450–500 nm (Fig. 3b) which are clearly visible for the large ribbons (n=4 and n=5) because the corresponding electronic transitions into S_2 and/or S_3 states become more intense (the oscillator strength values increase up to 3.00). The nature of these transitions can be interpreted as a mixture of the following configurations HOMO → LUMO+1, HOMO-1 → LUMO, and HOMO → LUMO+2 (see ESI, Figs. S1–S12†). The first $S_0 \rightarrow S_1$ electronic transition corresponding to the HOMO→LUMO configuration is

allowed only for the ribbon with n=2, but it is forbidden for the remaining ribbons (n=3–5). The second broad and much intense absorption band in the spectra of the **TTC** ribbons of this fusion type is predicted in the range of 380–440 nm which intensity proportionally increases with the growth of the ribbon length (Fig. 3b).
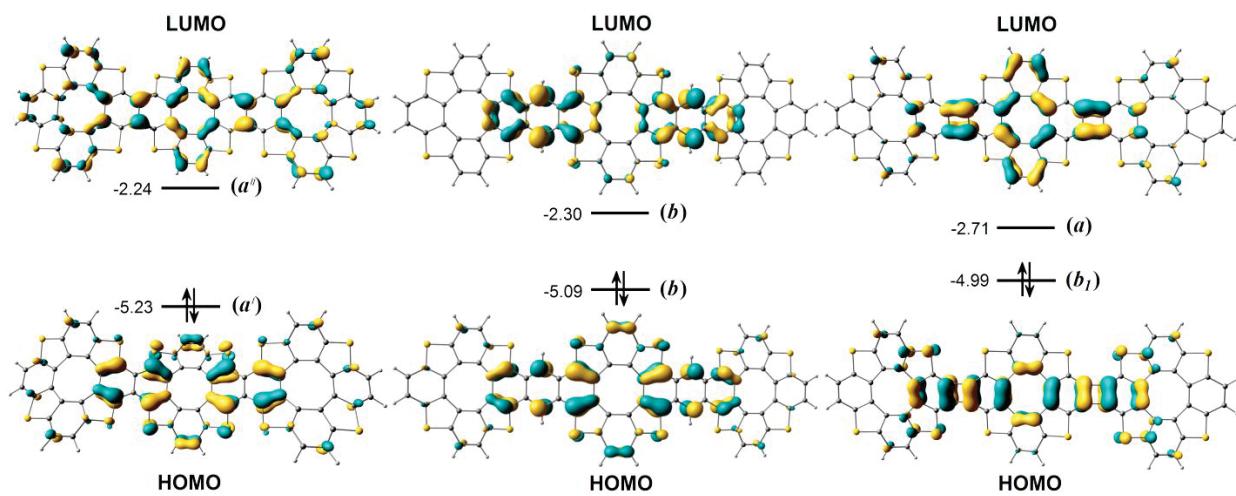
Fig. 4 Simplified molecular orbital energy diagram for the **TTC** ribbons of different fusion types with n = 3. (For the **TSC** ribbons with n=3 the MOs are identical). With increasing **TTC/TSC** units (n) MOs have the same nature for the corresponding **TTC/TSC** ribbon type.

From Fig. 4 one can see that the HOMO-LUMO transition is mainly localized being close to the central part of the ribbon with some admixtures from the terminal moiety. The same trend is seen in the longer oligomers and polymers, thus showing the local exciton nature of photoconductivity and other optoelectronics properties. The $S_0 \rightarrow S_1$ electronic transition corresponding to the HOMO→LUMO configuration was calculated in the range of 630–700 nm for the **TTC** ribbons of the third fusion type (n=2–5). However, it demonstrates a very weak intensity (f = 0.001–0.0001) being practically negligible, therefore, no absorption is visible in this region of spectra (Fig. 3c). The first high-intensity band takes place in the range of 430–550 nm (Fig. 3c), depending on the ribbon length that is similar to the previously discussed **TTC** ribbons (type **I**). A similar trend has also been

observed in the conjugated porphyrins. [59] The second more intense absorption band takes place in the UV region for the short oligomer with n=2.

The absorption spectra of the designed **TSC** compounds represent a similar shape of bands and orbital nature of the corresponding electronic transitions, but the replacement of sulfur with selenium heteroatoms strongly affects the bands positions, *i.e.* the electronic transition energies (see ESI, Tables S1 and S2,† and Fig. 3). Similar to the **TTC** ribbons, the absorption spectra of the **TSC** compounds are also characterized by an intense size-dependent absorption in a wide visible range for the first band and in the UV-vis region for the second band. This indicates that π-conjugation in the macrocyclic system plays a key role, defining the increase of the absorption intensity with the ribbon size growth. The same phenomenon is characteristic and typical for other strongly conjugated systems such as polyenes, polyacenes and recently studied related **TOC** ribbons. [59].

As one can see from Fig. 3d, for the **TSC** ribbons (type **I**) the first absorption band ($S_0 \rightarrow S_1$ transition) takes place in a narrow range 450–530 nm and reaches a maximum at $\approx$485 nm, while for the **TTC** compounds of the same fusion type, the absorption maximum of the first band tends to be slightly shifted to a longer wavelength up to $\approx$498 nm (Fig. 3a). Similar to **TTC** (type **I**) the HOMO$\rightarrow$LUMO configuration provided the dominant contribution to the $S_0 \rightarrow S_1$ transition for **TSC** compounds of the same fusion type. The **TSC** ribbons of the second type exhibit weak absorption calculated as a shoulder in the 485–540 nm region (the first band) and a strong long-wave shifted absorption in the range of 380–470 nm (the second band) (Fig. 3e). In the case of the third type of **TSC** ribbons the first red-shifted band is calculated in the range of 460–630 nm (Fig. 3f). The $S_0 \rightarrow S_1$ transition due to the HOMO$\rightarrow$LUMO configuration is forbidden for the **TSC** ribbons of both **II** and **III** fusion types beginning with n=3–5 (Fig. 4). The detailed orbital nature interpretation of the absorption spectra for **TSC** compounds n=2–5 is presented in the ESI.†

3.3. Band-gap engineering

Band-gap engineering [60,61] represents an attractive research area of computational materials design which allows tuning the band gap in order to achieve desired electronic and optical properties. It was shown previously that the HOMO-LUMO gap (HLG) depends on the 1D oligomer length and can be controlled by reducing or increasing the number of repeated molecular units. [62, 63] Moreover, the HLG value can be more precisely adjusted by the choice of the monomer coupling in the oligomeric system, *i.e.* the conjugation pathways. Here we deal with three different coupling types of monomers in the 1D **TTC/TSC** structures. Fig. 5 exhibits the HLG as a function of oligomer size (1/n) for all of the studied **TTC** and **TSC**-based 1D conjugated structures with n =1–5. As expected, the HLG diminishes with increasing number of repeated units (n) in the corresponding oligomer. This general tendency is clearly reflected in all presented series of the 1D structures with different coupling types. An interesting feature for both **TTC** and **TSC** series is that the HLG gradually decreases when we move from the ribbons with the first coupling type to the ribbons containing the conjugated anthracene system and then to the ribbons fused through four-membered rings.

For the **TTC** structures of the first fusion type, the HLG values shrink very slowly up to 2.87 eV for oligomers with n = 5. The inclusion of the benzene-core linker into the **TTC** structure leads to a faster decrease of the HLG up to 2.68 eV for **TTC** with n=5. This fact can be explained by an expansion of the π-conjugation system due to the formation of the cyclic anthracene structure. The HOMO and LUMO are primarily localized over the anthracene moieties along the whole backbone (Fig. 4). For the **TTC**s linked through a four-membered ring, the HLG decreases up to 2.16 eV because of the enhancement of π-conjugation in the macrocyclic system. In this case, the **TTC** monomers are fused with the formation of biphenylene fragments, which subsequently couple with each other through the –C–C– bridges of the central COT core forming a strongly π-conjugated chain.

The corresponding HOMO and LUMO are localized over the biphenylene and COT core continuously along the whole **TTC** backbone (Fig. 4).
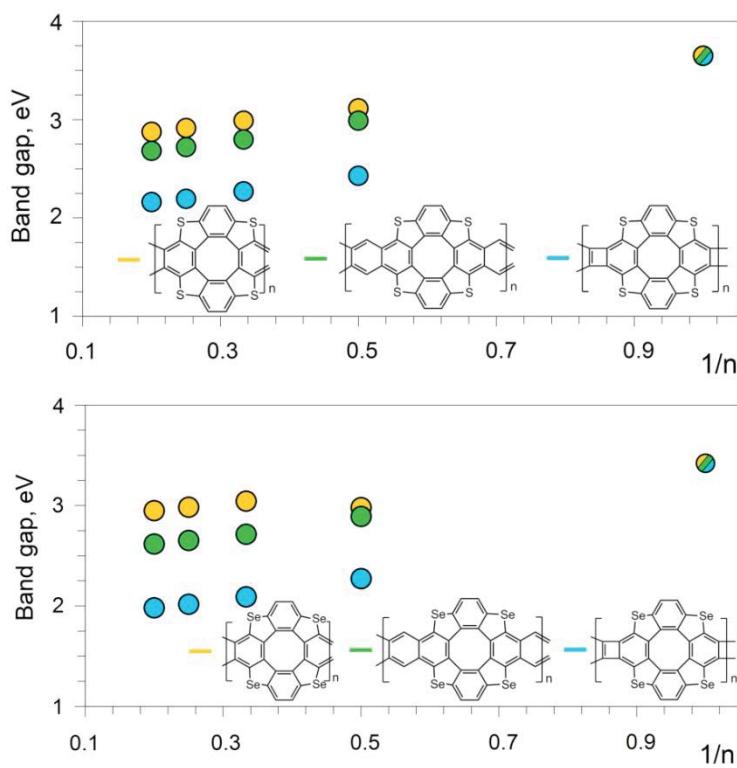
Fig. 5 The length dependence behaviour of the band gap for the **TTC**- and **TSC**-based 1D oligomers (n denote the numbers of the **TTC** and **TSC** monomers). Yellow, green and blue colors correspond to **I**, **II** and **III** types of ribbons.

The same tendency is observed for the **TSC** structures with different fusion types. In particular, replacing sulfur with selenium heteroatoms leads to a slower decrease in the band gap values (up to 2.95 eV) for the **TSC**s (n=5) of the first fusion type compared to those for **TTC**s. This is due to weakening of the π-conjugation because of steric complications in **TSC** ribbons of this type (see Structural part). In the case of **TSC** of the second type, the HLG decreases up to 2.62 eV with n = 5 similar to the corresponding **TTC**s. The **TSC** of the third type demonstrates HLG reduction up to 1.98 eV. We have neglected spin-orbit coupling [64] throughout all DFT calculations. Thus, we have to mention that some heavy atom effect [65] could be additionally expected in the **TTC** and **TSC** types of ribbons, while it will influence mostly the singlet-triplet transitions, which have not been considered in the present paper.

3.4. Structure and electronic properties of the infinite nanoribbons

Having the repeated units with certain wavelengths from finite structures calculations, we designed periodic nanoribbons of type **I** and type **II**. The relaxed structures demonstrate the lattice parameters a=16.51 (16.70) and 21.10 (19.9) Å for S(Se) type **I** and type **II** nanoribbons, respectively, that is slightly different from the respective oligomers. At the same time, the general features of the geometry are preserved. The decrease in wavelength parameter for the Se type **II** nanoribbons results from higher Gaussian curvature of the ribbons. The type **III** structure was not considered in the periodic approximation due to the absence of dependence on the number of monomers. This means that increasing oligomer length from 2 up to 5 units leads to a new structure with no periodicity at every step. The lack of periodicity for type **III** ribbons is likely caused by the close-lying energy minima for the possible twisting configurations of **TTC** and **TSC** moieties relative to the linking four-membered ring. As a result, type **III** ribbons are predicted to be conformationally soft through the small inter-monomer distortions leading to the formally non-periodic infinite structures. However, it may be possible that type **III** ribbons demonstrate periodicity with the larger size of the unit cell.
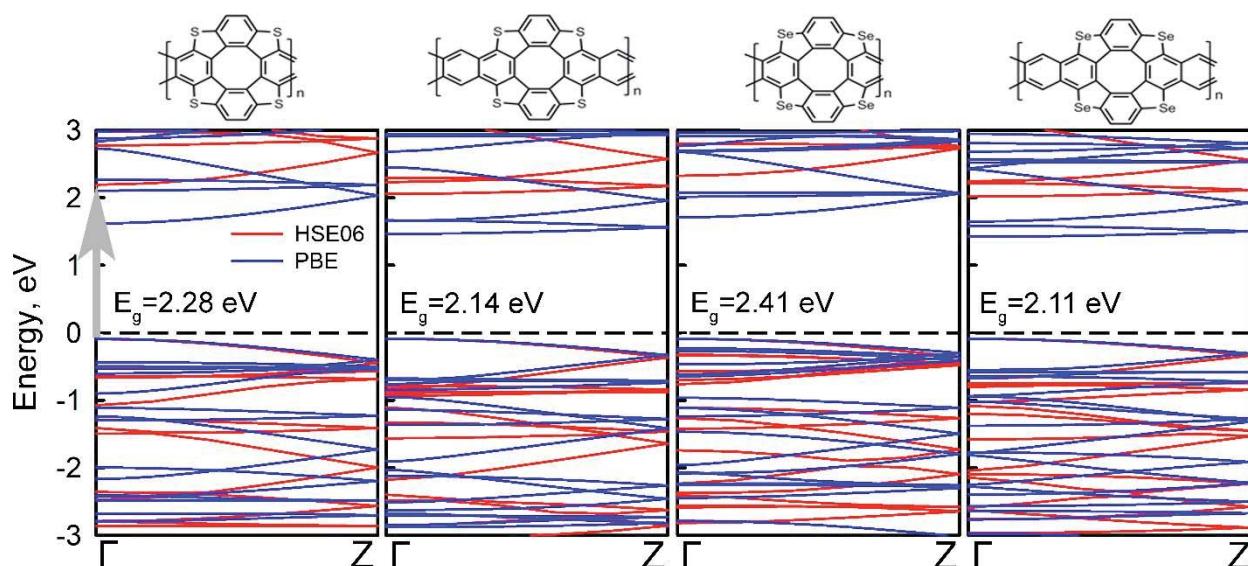
Fig. 6 Band structures of the **TTC**- and **TSC**-based 1D polymers calculated at the PBE (blue) and HSE06 (red) levels of theory. The Fermi level is set to 0 eV.

Band structure calculations (Fig. 6) for type **I** and **II** ribbons reveal 2.11-2.41 eV band gaps calculated at the HSE06 level of theory that depend on the fusion type and composition. These gaps are generally ~0.6 eV larger compared to those calculated within the PBE functional. While direct fusion reveals a minor increase in band gap width with replacement of S by Se, the second type nanoribbons demonstrate almost the same gaps for the infinite ribbons. As for finite oligomers, the inclusion of the benzene-core linker into the **TTC** and **TSC** structures leads to a faster decrease of the HLG. It is important to note that the molecular nanoribbons possess direct band gaps of a size that are promising for optoelectronic applications. It is notable that the studied nanostructures have elastic constants in the periodic direction predicted to be 10-30 GPa, something that reflects their softness and makes them possible candidates to piezo- and thermoelectric materials.[58]

4. Conclusions

In this paper, we have presented a comprehensive DFT study of the electronic structure and spectral properties for the two series of novel one-dimensional tetrathia[8]circulene and tetraselena[8]circulene-based nanostructures with different fusion types. The directly fused (type **I**) and fused *via* benzene-core linker (type **II**) monomers in tetrathia[8]circulene and tetraselena[8]circulene ribbons form wave-like structures while ribbons fused through a four-membered ring (type **III**) adopt a linear topology with slight rotation of the monomers. All the studied 1D tetrathia[8]circulene and tetraselena[8]circulene compounds demonstrate a strong size-dependent visible absorption in the electronic spectra due to specific π-conjugation in the **TTC**- and **TSC**-based systems. The materials possess variable middle-range direct band gaps, making them attractive candidates for solar cell technology and optoelectronic applications.

Conflicts of interest

There are no conflicts to declare.

Acknowledgements

References

1. X. Guo, M. Baumgarten and K. Müllen, *Progress in Polymer Science*, 2013, **38**, 1832.

2. G. M. Mamardashvili, N. Zh. Mamardashvili and O. I. Koifman, *Russ. Chem. Rev.*, 2008, **77**, 59.

3. C. J. Medforth, Z. Wang, K. E. Martin, Y. Song, J. L. Jacobsenc and J. A. Shelnutt, *Chem. Commun.*, 2009, 7261.

4. C. M. Drain, A. Varotto and I. Radivojevic, *Chem. Rev.*, 2009, **109**, 1630.

5. M. Abel, S.Clair, O.Ourdjini, M.Mossoyan and L. Porte, *J. Am. Chem. Soc.*, 2011, **133**, 1203.

6. L. Latos-Grazynski, in The Porphyrin Handbook, ed. K. M. Kadish, K. M. Smith and R. Guilard, *Academic Press*, New York, 2000, **2**, 361.

7. N. Zhang, L. Wang, H. Wang, R. Cao, J. Wang, F. Bai and H. Fan, *Nano Lett.*, 2018, **18**, 1560.

8. N. Aratani, D. Kim and A. Osuka, *Acc. Chem. Res.*, 2009, **42**, 1922.

9. Y. Nakamura, N. Aratani, H. Shinokubo, A. Takagi, T. Kawai, T. Matsumoto, Z. S. Yoon, D. Y. Kim, T. K. Ahn, D. Kim, A. Muranaka, N. Kobayashi and A. Osuka, *J. Am. Chem. Soc.*, 2006, **128**, 4119.

10. Y. Nakamura, N. Aratani, K. Furukawa and A. Osuka, *Tetrahedron*, 2008, **64**, 11433.

11. C. G. Claessens, U. Hahn and T. Torres, *Chem Rec.*, 2008, **8**, 75.

12. M. Abel, S. Clair, O. Ourdjini, M. Mossoyan and L. Porte, *J. Am. Chem. Soc.*, 2011, **133**, 1203.

13. M. Urbani, G. de la Torre, M. K. Nazeeruddin and T. Torres, *Chem. Soc. Rev.*, 2019, **48**, 2738.

14. J. R. Darwent, I. Mc Cubbin and G. Porter, *J. Chem. Soc.*, *Farad. Trans.*, 1982, **2**, 903.

15. J. R. Darwent, P. Douglas, A. Harriman, G. Porter and M.-C. Richoux, *Coor. Chem. Rev.*, 1982, **44**, 83.

16. G. Di Carlo, A. O. Biroli, F. Tessore, S. Caramori and M. Pizzotti, *Coord. Chem. Rev.*, 2018, **358**, 153.

17. M. Urbani, M.-E. Ragoussia, M. K. Nazeeruddin and T. Torres, *Coord. Chem. Rev.*, 2019, **381**, 1.

18. G. V. Baryshnikov, B. F. Minaev and V. A. Minaeva, *Russ. Chem. Rev.*, 2015, **84**, 455.

19. T. Hensel, N. N. Andersen, M. Plesner and M. Pittelkow, *Synlett.*, 2016, 498.

20. N. N. Karaush, G. V. Baryshnikov, V. A. Minaeva, H. Ågren and B. F. Minaev, *Mol. Phys.*, 2017, **115**, 2218.

21. N. N. Karaush-Karmazin, G. V. Baryshnikov, H. Agren and B. F. Minaev, In Reference Module in Chemistry, Molecular Sciences and Chemical Engineering, ed. H. N. C. Wong, Chapter Furans and Their Benzo Derivatives: Structure, *Elsevier*, 2019, 1.

22. G. V. Baryshnikov, R. R. Valiev, B. F. Minaev, H. Ågren, *New J. Chem.*, 2017, **41**, 2717.

23. V. A Minaeva, N. N. Karaush, B. F. Minaev, G. V. Baryshnikov, F. Chen, T. Tanaka and A. Osuka, *Opt. Spectrosc.*, 2017, **122**, 523.

24. N. N. Karaush, G. V. Baryshnikov, H. Ågren and B. F. Minaev, *New J. Chem.*, 2018, **42**, 11493.

25. R. R. Valiev, V. N. Cherepanov, G. V. Baryshnikov and D. Sundholm, *Phys. Chem. Chem. Phys.*, 2018, **20**, 6121.

26. V. Minaeva, N. Karaush-Karmazin, G. Baryshnikov and B. Minaev, *Vib. Spectrosc.*, 2019, **100**, 107.

27. G. Baryshnikov, R. R. Valiev, V. N. Cherepanov, N. N. Karaush-Karmazin, V. A. Minaeva, B. F. Minaev, H. Ågren, *Phys. Chem. Chem. Phys.*, 2019, **21**, 9246.

28. C. B. Nielsen, T. Brock-Nannestad, T. K. Reenberg, P. Hammershøj, J. B. Christensen, J. W. Stouwdam and M. Pittelkow, *Chem. Eur. J.*, 2010, **16**, 13030.

29. G. V. Baryshnikov, R. R. Valiev, N. N. Karaush, V. A. Minaeva, A. N. Sinelnikov, S. K. Pedersen, M. Pittelkow, B. F. Minaev and H. Ågren, *Phys. Chem. Chem. Phys.*, 2016, **18**, 28040.

30. K. B. Ivaniuk, G. V. Baryshnikov, P. Y. Stakhira, S. K. Pedersen, M. Pittelkow, A. Lazauskas, D. Volyniuk, J. V. Grazulevicius, B. F. Minaev and H. Ågren, *J. Mater. Chem. C*, 2017, **5**, 4123.

31. T. Fujimoto, M. M. Matsushita and K. Awaga, *J. Phys. Chem. C*, 2012, **116**, 5240.

32. T. Fujimoto, M. M. Matsushita and K. Awaga, *Appl. Phys. Lett.*, 2010, **97**, 123303.

33. A. Dadvand, F. Cicoira, K. Yu. Chernichenko, E. S. Balenkova, R. M. Osuna, F. Rosei, V. G. Nenajdenko and D. F. Perepichka, *Chem. Commun.*, 2008, 5354.

34. G. Baryshnikov, B. Minaev, N. Karaush and V. Minaeva, *Phys. Chem. Chem. Phys.*, 2014, **16**, 6555.

35. G. Baryshnikov, B. Minaev, N. Karaush and V. Minaeva, *RSC Adv.*, 2014, **4**, 25843.

36. J. Yu, Q. Sun, Y. Kawazoe and P. Jena, *Nanoscale*, 2014, **6**, 14962.

37. A. V. Kuklin, G. V. Baryshnikov, B. F. Minaev, N. Ignatova and H. Ågren, *J. Phys. Chem. C*, 2018, **122**, 22216.

38. N. N. Karaush, G. V. Baryshnikov and B. F. Minaev, *RSC Adv.*, 2015, **5**, 24299.

39. N. N. Karaush, G. V. Baryshnikov, B. A. Minaeva and B. F. Minaev, *New J. Chem.*, 2015, **39**, 7815.

40. X. Xiong, C.-L. Deng, B. F. Minaev, G. V. Baryshnikov, X.-S. Peng and H. N. C. Wong, *Chem. Asian. J.*, 2015, **10**, 969.

41. V. A. Minaeva, G. V. Baryshnikov, B. F. Minaev, N. N. Karaush, X.-D. Xiong, M.-D. Li, D. L. Phillips and H. N. C. Wong, *Spectrochim. Acta A Mol. Biomol. Spectrosc.*, 2015, **151**, 247.

42. G. V. Baryshnikov, N. N. Karaush, R. R. Valiev, B. F. Minaev, *J. Mol. Model.*, 2015, **21**, 136.

43. V. T. T. Huong, T. B. Tai and M. T. Nguyen, *RSC Adv.*, 2015, **5**, 24167.

44. S. Kato, S. Akahori, Y. Serizawa, X. Lin, M. Yamauchi, S. Yagai, T. Sakurai, W. Matsuda, S. Seki, H. Shinokubo and Y. Miyake, *J. Org. Chem.*, 2020, **85**, 62.

45. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.

46. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.

47. M. S. Gordon, J. S. Binkley, J. A. Pople, W. J. Pietro and W. J. Hehre, *J. Am. Chem. Soc.*, 1982, **104**, 2797.

48. M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, D. J. DeFrees, J. A. Pople and M. S. Gordon, *J. Chem. Phys.*, 1982, **77**, 3654.

49. R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650.

50. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng,J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K.

Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O.Ë. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 16, Rev. A. 03*, Gaussian, Inc., Wallingford, CT, 2016.

51. E. Runge and E. K. U. Gross, *Phys. Rev. Lett.*, 1984, **52**, 997.

52. G. Kresse and J. Furthmüller, *Phys. Rev. B*, 1996, **54**, 11169.

53. G. Kresse and J. Hafner, *Phys. Rev. B*, 1993, **47**, 558.

54. P. E. Blöchl, *Phys. Rev. B*, 1994, **50**, 17953.

55. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865.

56. J. Heyd, G. E. Scuseria and M. Ernzerhof, *J. Chem.Phys.*, 2003, **118**, 8207.

57. H. J. Monkhorst and J. D. Pack, *Phys. Rev. B*, 1976, **13**, 5188.

58. J. Yu, Q. Sun, P. Jena, *J. Phys. Chem. C*, 2016, **120**, 49, 27829.

59. A. Tsuda and A. Osuka, *Science*, 2001, **293**, 79.

60. L. Liua and Z. Shen, *Appl. Phys. Lett.*, 2009, **95**, 252104.

61. P. Ruffieux, J. Cai, N. C. Plumb, L. Patthey, D. Prezzi, A. Ferretti, E. Molinari, X. Feng, K. Müllen, C. A. Pignedoli and R. Fasel, *ACS Nano*, 2012, **6**, 6930.

62. N. N. Karaush, S. V. Bondarchuk, G. V. Baryshnikov, V. A. Minaeva, W.-H. Sun and B. F. Minaev, *RSC Adv.*, 2016, **6**, 49505.

63. R. Gutzler and D. F. Perepichka, *J. Am. Chem. Soc.*, 2013, **135**, 16585.

64. O. Loboda, I. Tunell, B. Minaev and H. Ågren, *Chem. Phys.*, 2005, **312**, 299.

65. B. F. Minaev, S. Knuts and H. Ågren, *Chem. Phys.*, 1994, **181**, 15.
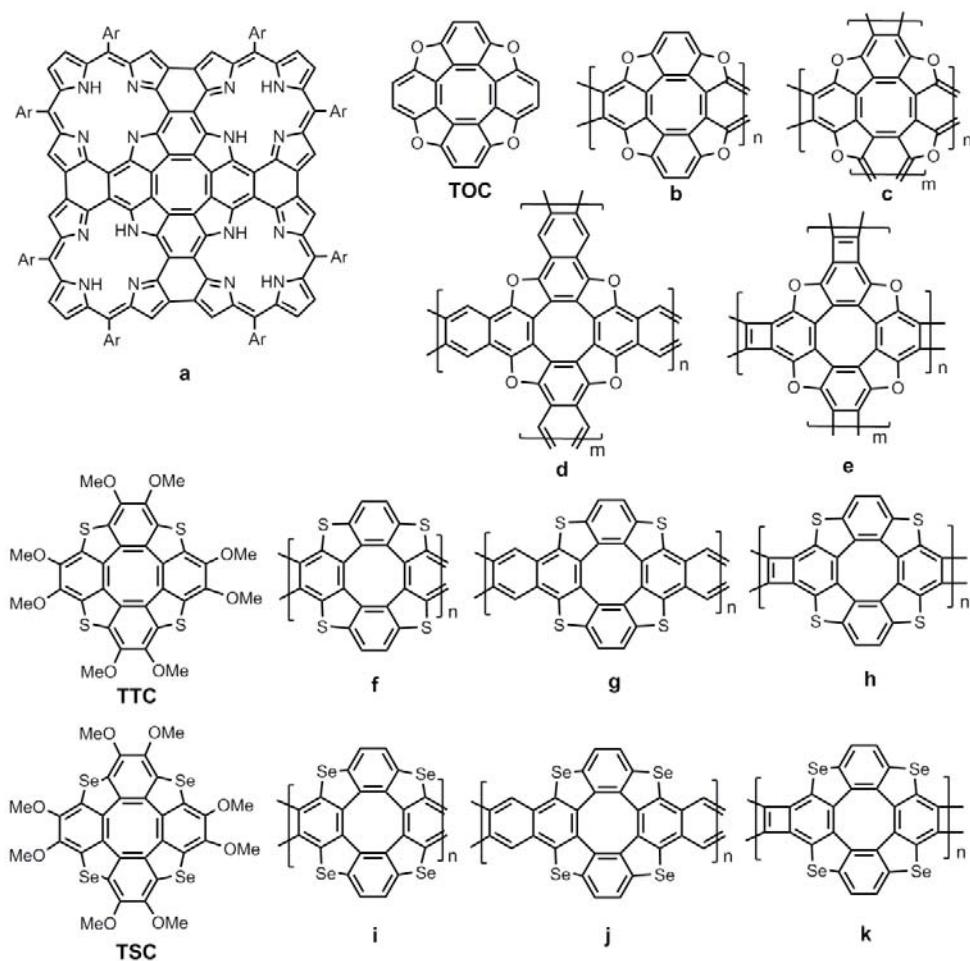
Some examples of the 1D and 2D polymers containing porphyrin (a),9, 10 tetraoxa[8]circulene (b–e),34−37 tetrathia[8]circulene (f–h) and tetraselena[8]circulene (i–k) monomers studied in this paper.

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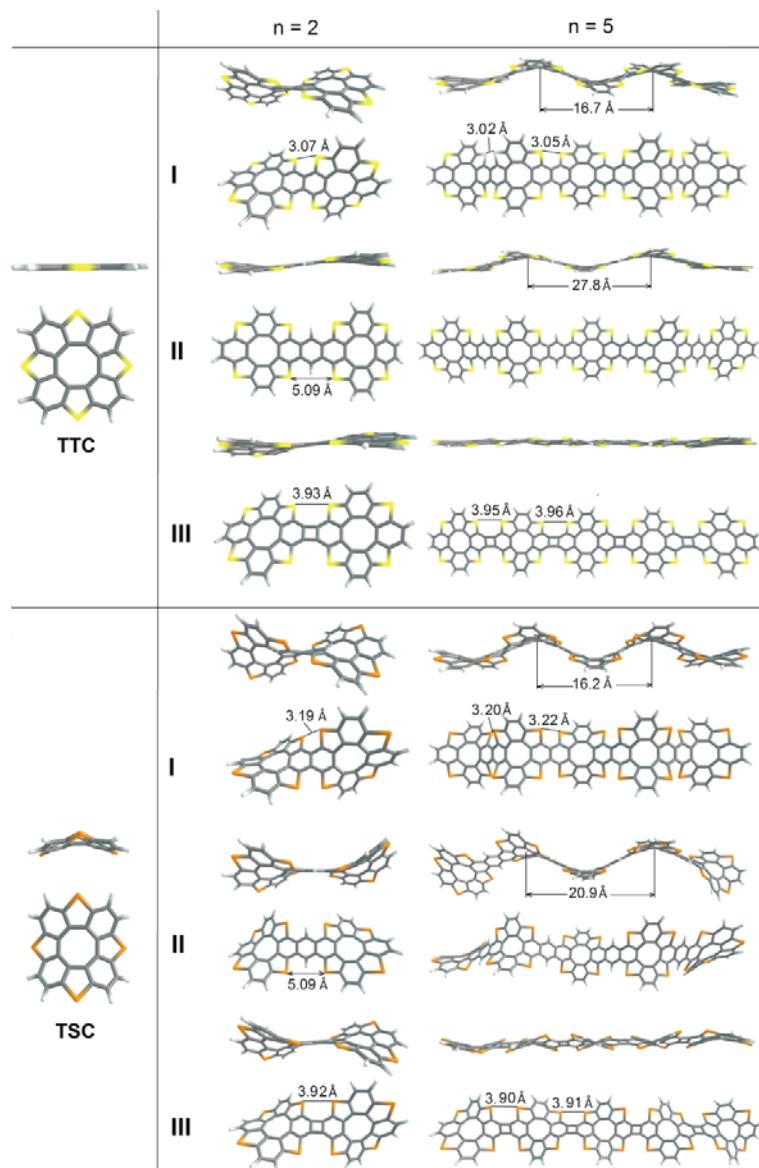
Molecular representations of the TTC and TSC structures with n=2 and n = 5 (side and top view).

189x293mm (300 x 300 DPI)

Electronic absorption spectra of the TTC- and TSC-based ribbons calculated by the TD DFT/B3LYP/6-31G(d) method; I and II denote the first and second absorption bands (band half-width 3000 cm−1, Gaussian distribution function).

Simplified molecular orbital energy diagram for the TTC ribbons of different fusion types with n = 3. (For the TSC ribbons with n=3 the MOs are identical). With increasing TTC/TSC units (n) MOs have the same nature for the corresponding TTC/TSC ribbon type.

The length dependence behaviour of the band gap for the TTC- and TSC-based 1D oligomers (n denote the numbers of the TTC and TSC monomers). Yellow, green and blue colors correspond to I, II and III types of ribbons.

Band structures of the TTC- and TSC-based 1D polymers calculated at the PBE (blue) and HSE06 (red) levels of theory. The Fermi level is set to 0 eV.

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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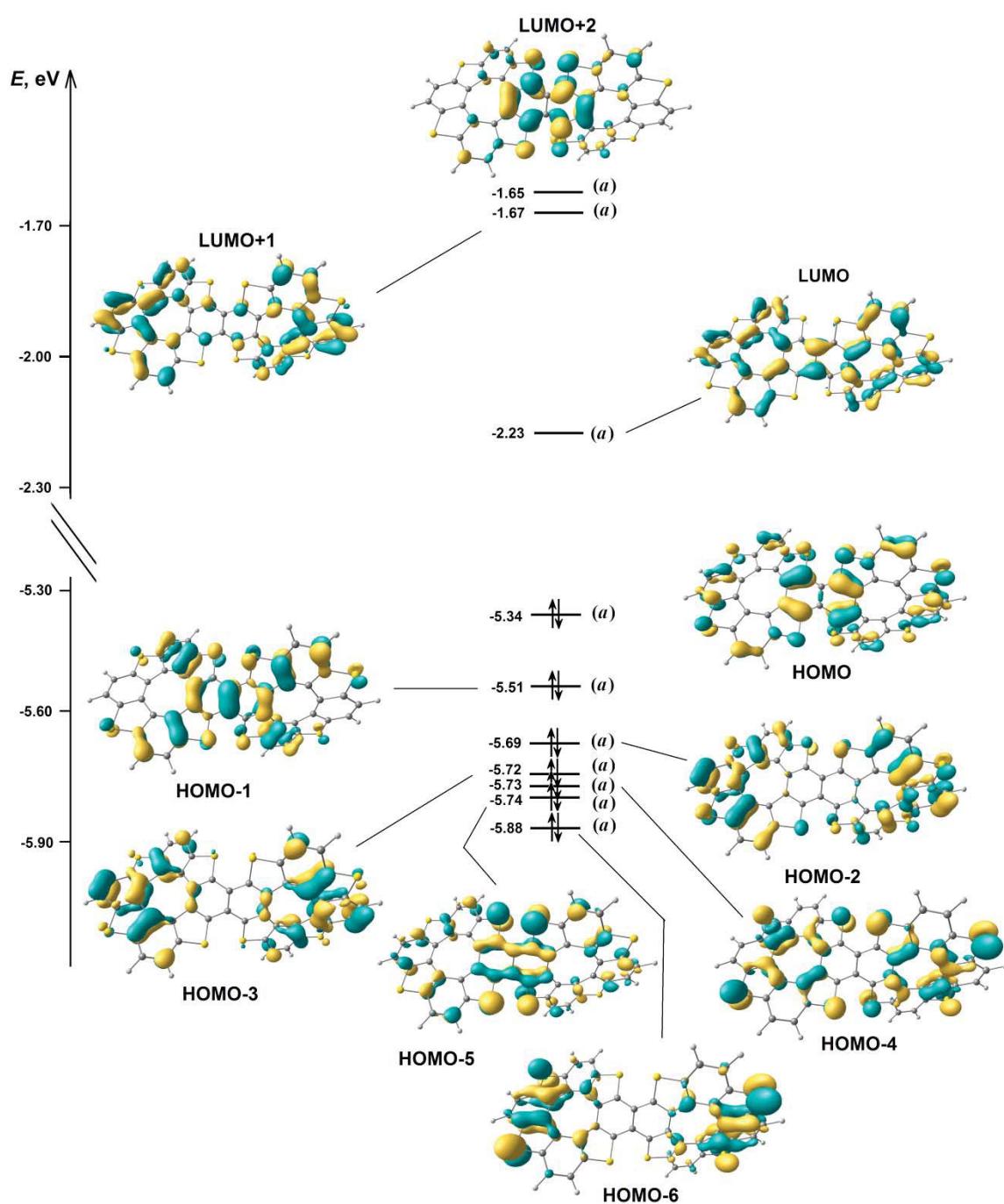
Figure S1. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=2 (type **I**) calculated at the B3LYP/6-31G(d) level of theory.
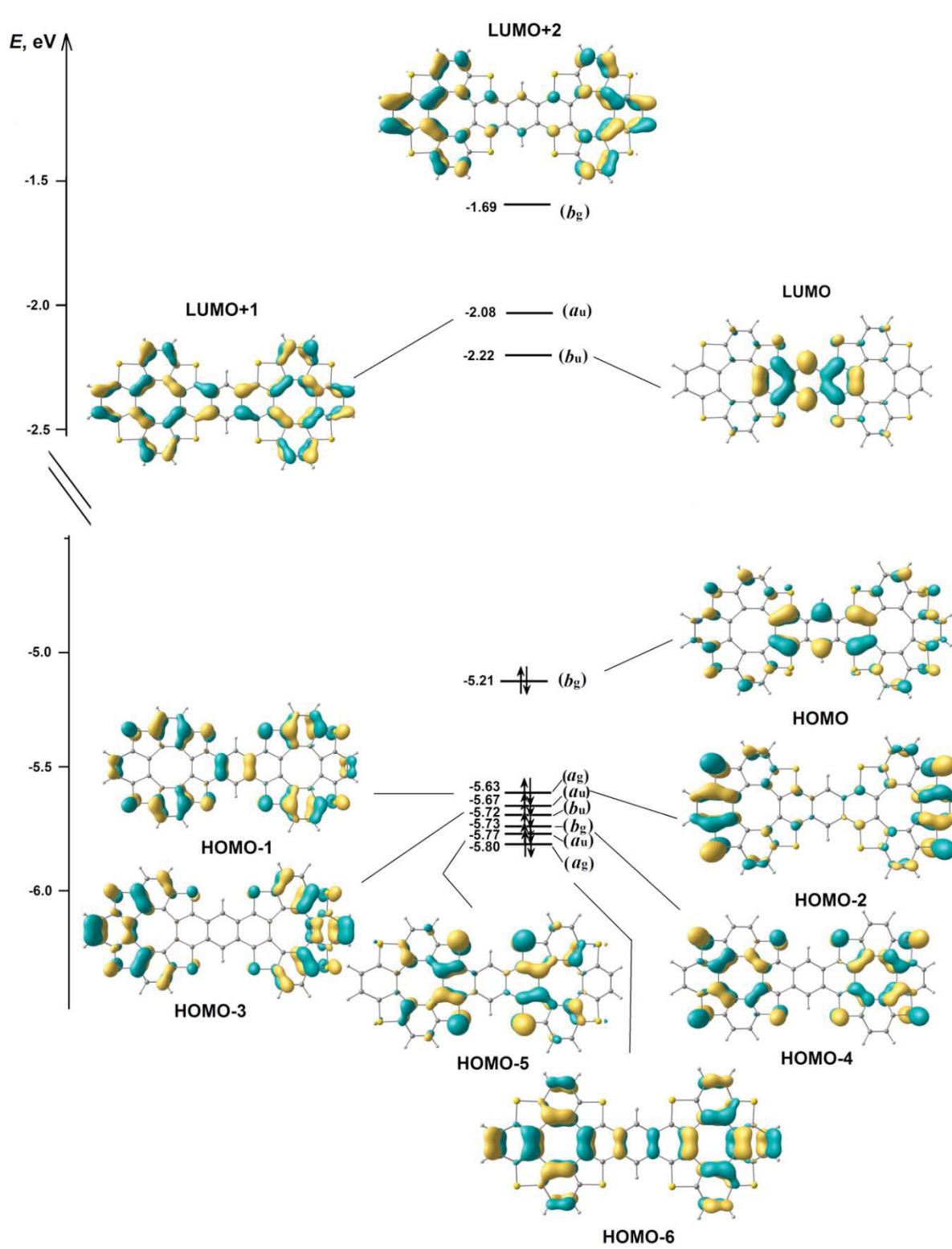
Figure S2. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=2 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.
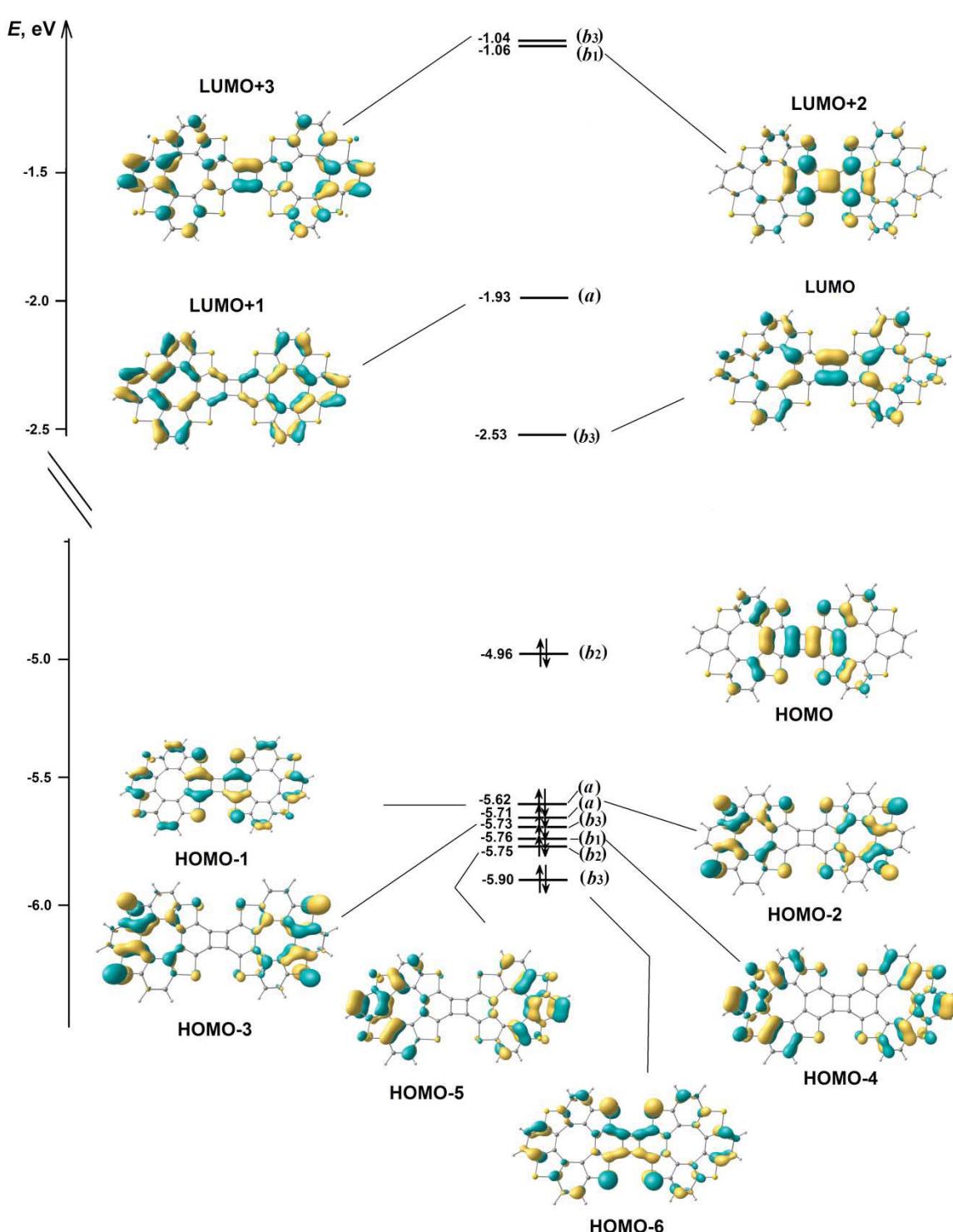
Figure S3. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=2 (type **III**) calculated at the B3LYP/6-31G(d) level of theory.
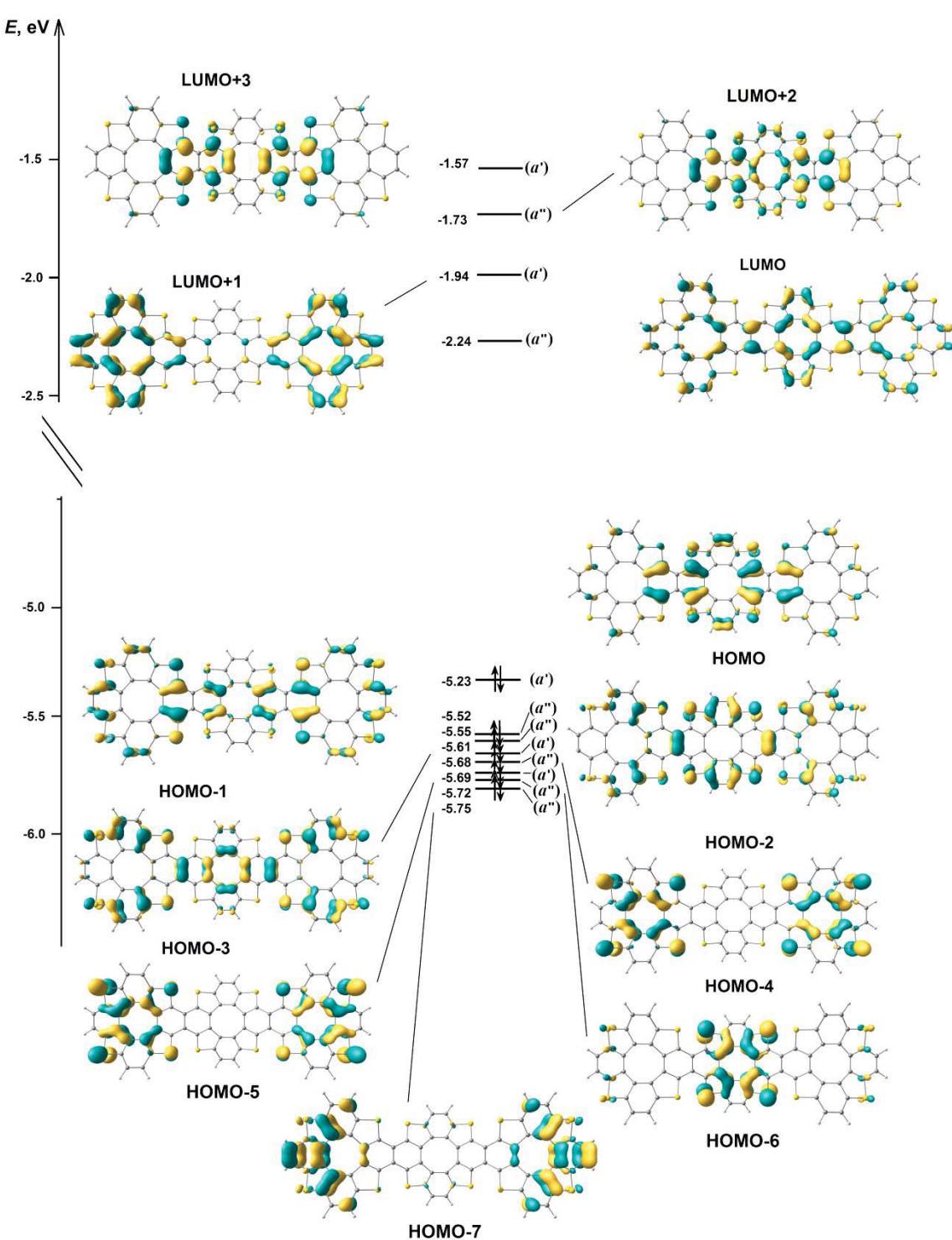
Figure S4. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=3 (type **I**) calculated at the B3LYP/6-31G(d) level of theory.
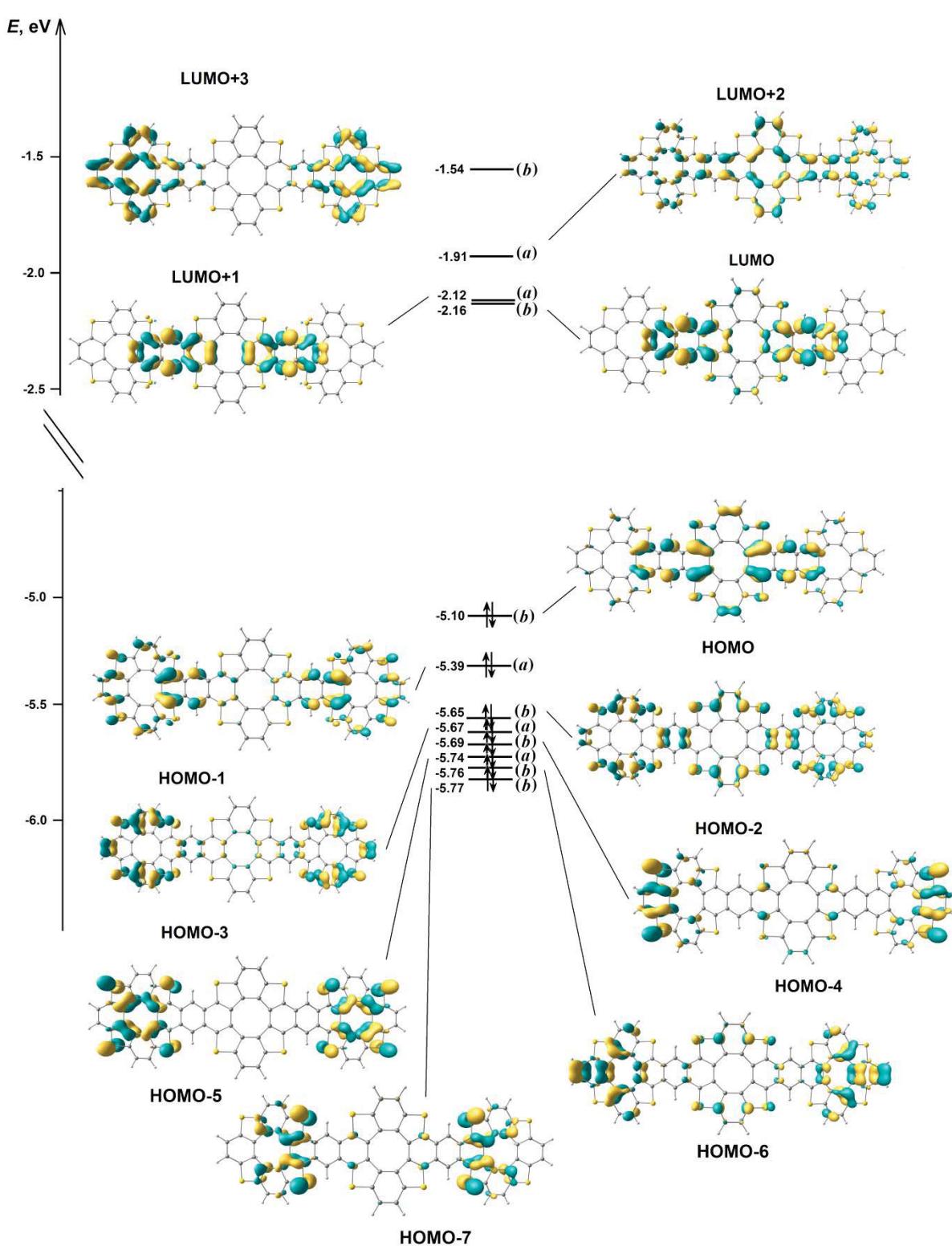
Figure S5. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=3 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.
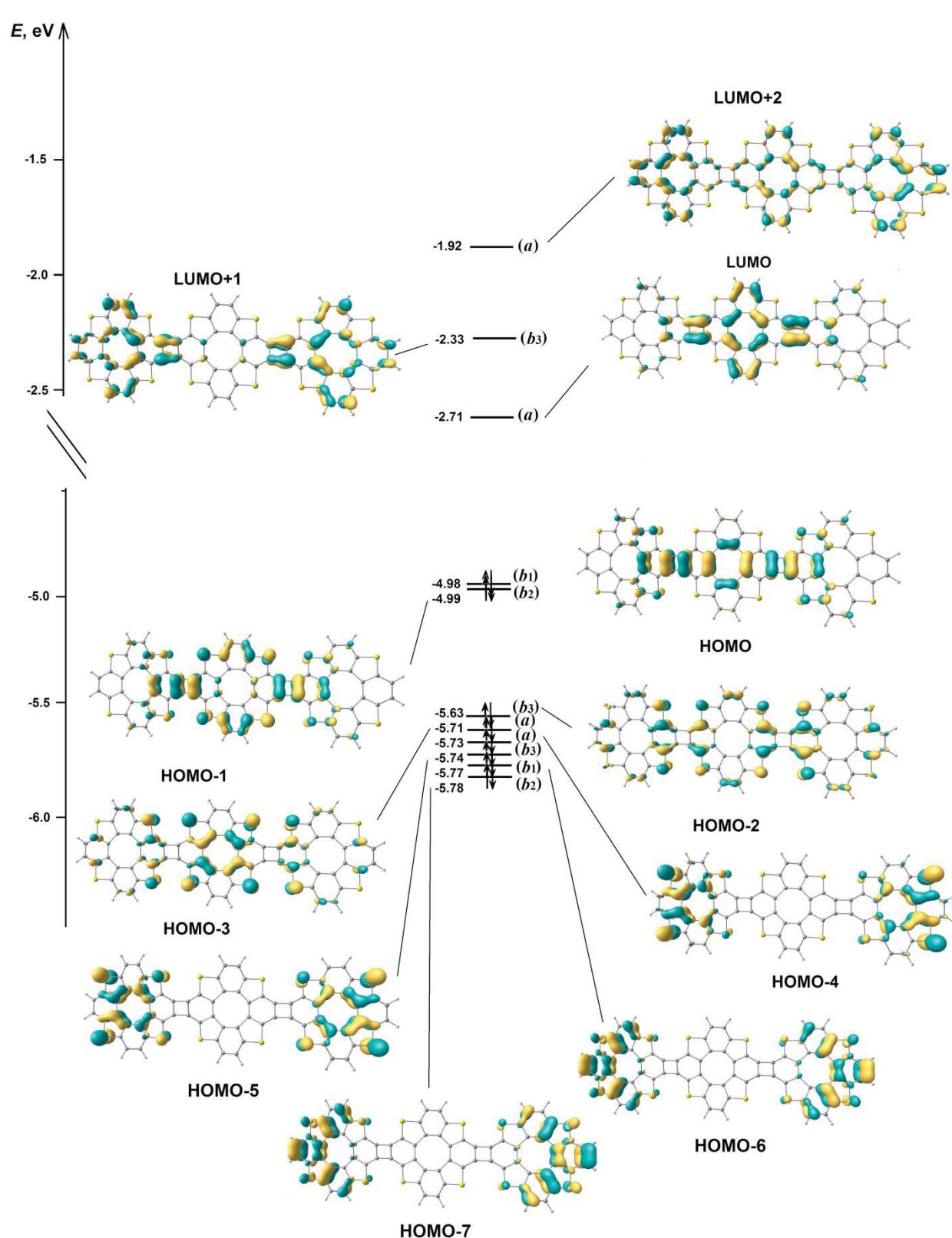
Figure S6. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=3 (type **III**) calculated at the B3LYP/6-31G(d) level of theory.

7
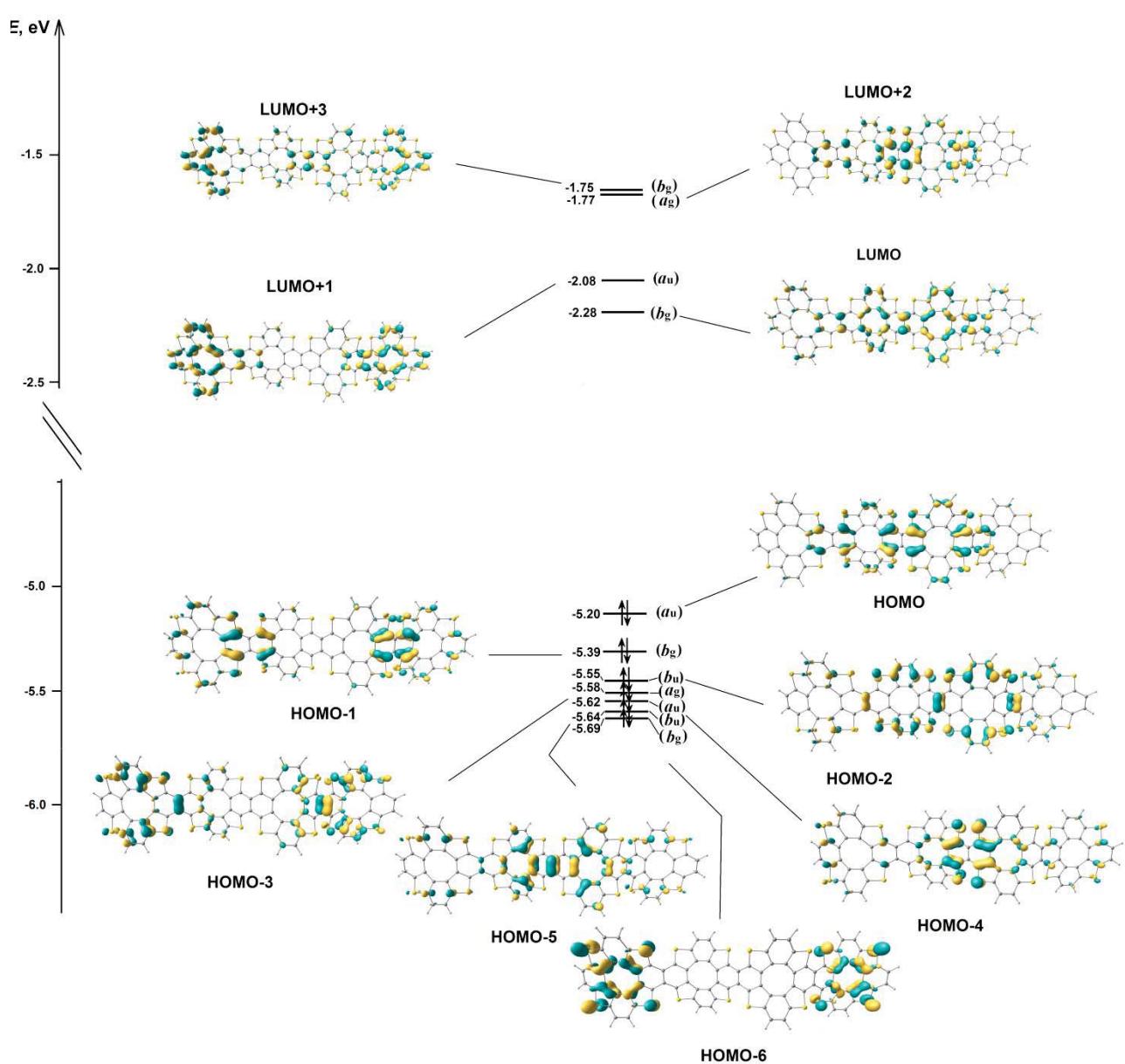
Figure S7. Molecular orbital diagram of the tetrathia[8]circulene-based compound <u>with n=4</u> (<u>type **I**</u>) calculated at the B3LYP/6-31G(d) level of theory.

LUMO

-2.33 ——— (a)

-5.06 ⇅ (a)

HOMO
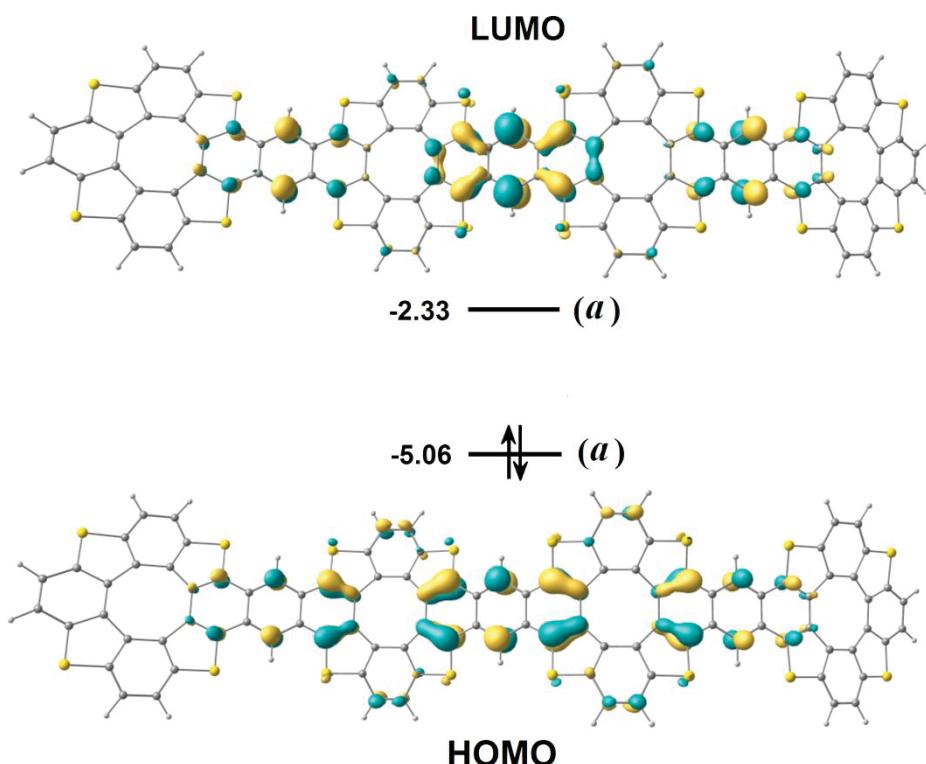
Figure S8. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=4 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.
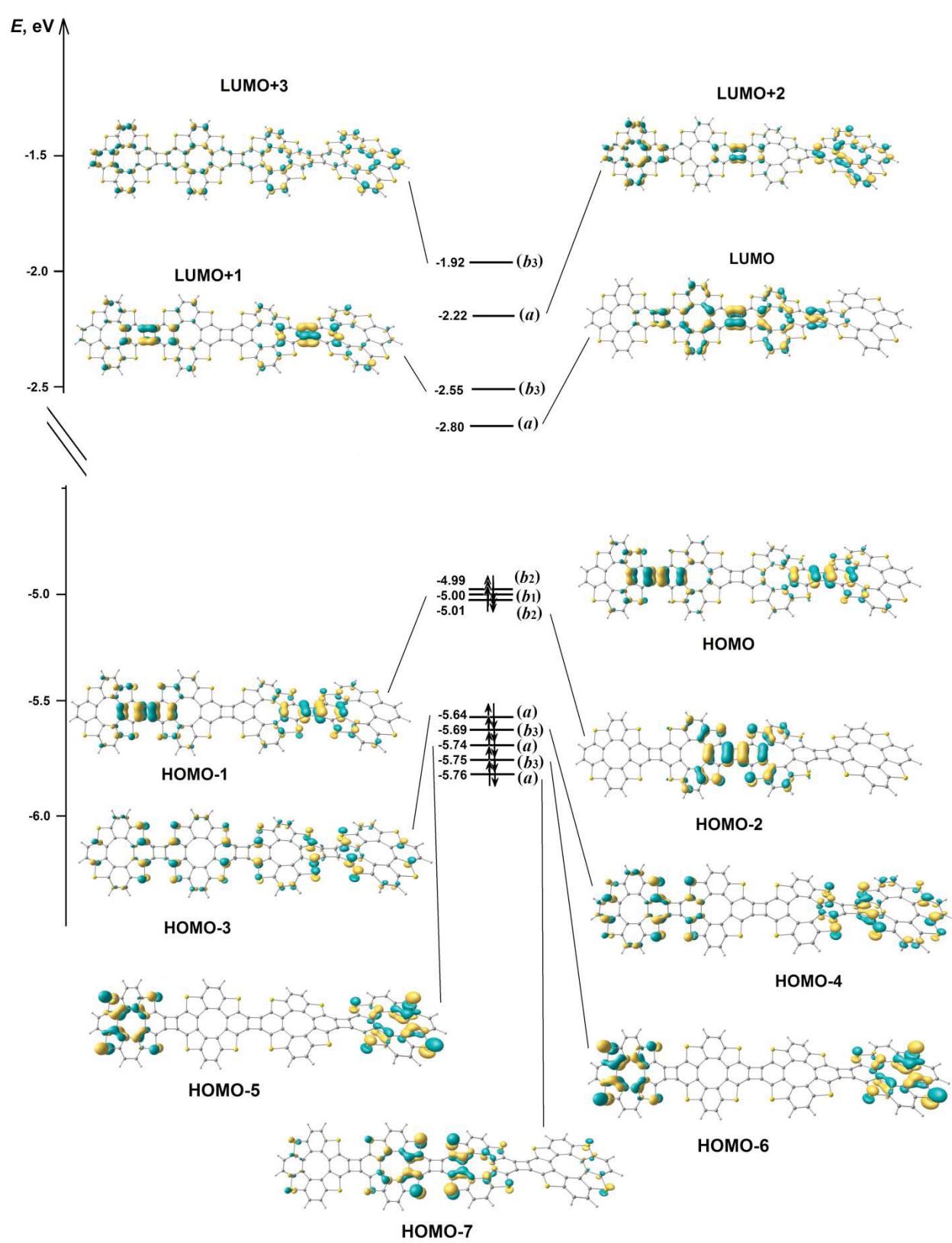
Figure S9. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=4 (type **III**) calculated at the B3LYP/6-31G(d) level of theory.

LUMO

-2.30 ——— (a_2)

-5.18 ⇅ (b_2)

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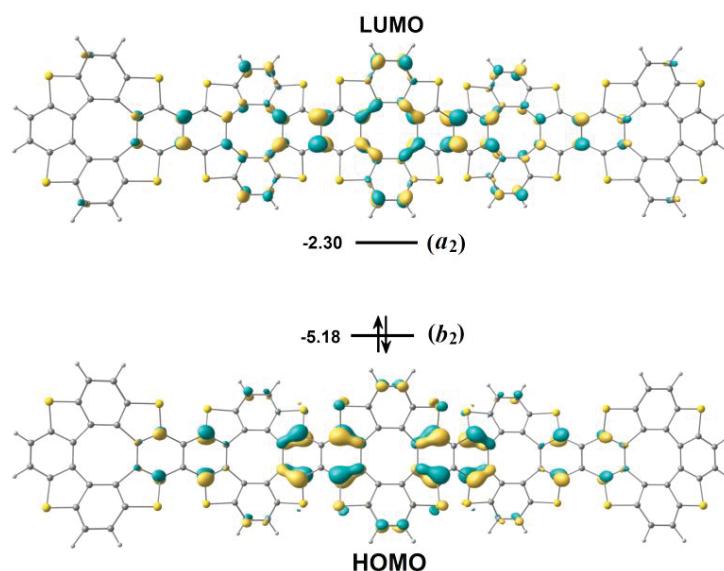
Figure S10. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=5 (type **I**) calculated at the B3LYP/6-31G(d) level of theory.

LUMO

-2.35 ——— (b_1)

-5.03 ⇅ (b_2)

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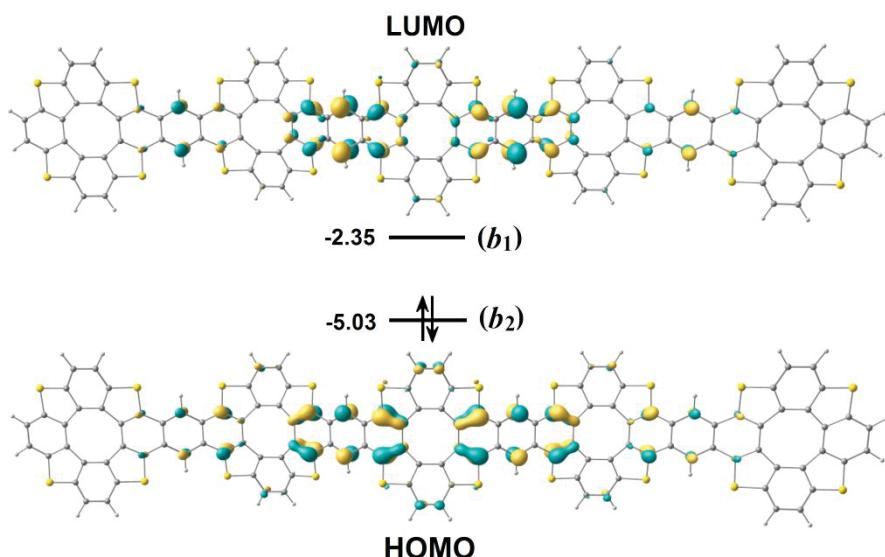
Figure S11. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=5 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.

11
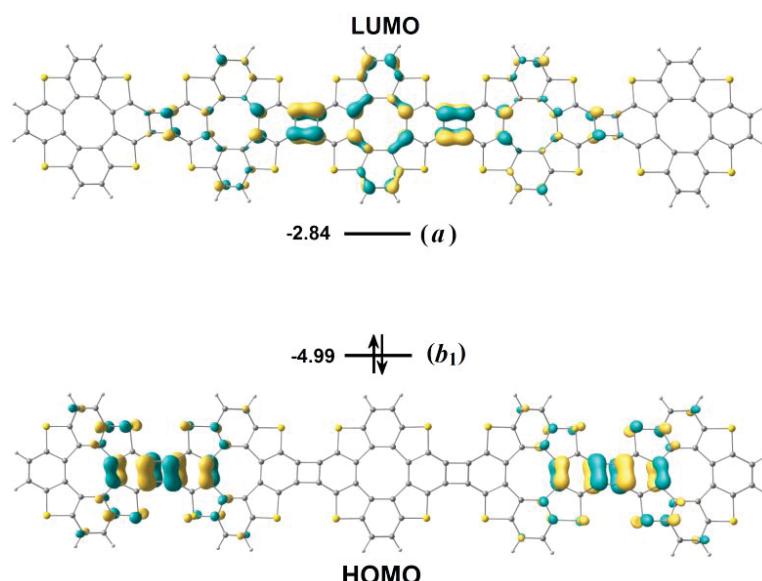
Figure S12. Molecular orbital diagram of the tetrathia[8]circulene-based compound with n=5 (type **III**) calculated at the B3LYP/6-31G(d) level of theory.

LUMO

-2.25 ——— (*a*)

-5.23 ⇵ (*a*)

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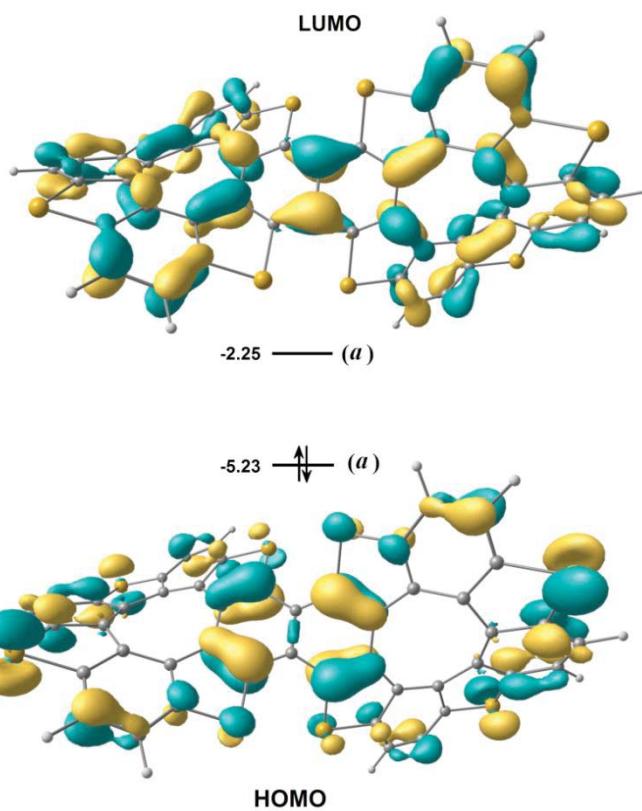
Figure S13. Molecular orbital diagram of the tetraselena[8]circulene-based compound <u>with n=2</u> (<u>type **I**</u>) calculated at the B3LYP/6-31G(d) level of theory.

LUMO

-2.23 ——— (*a*)

-5.12 ⇵ (*a*)

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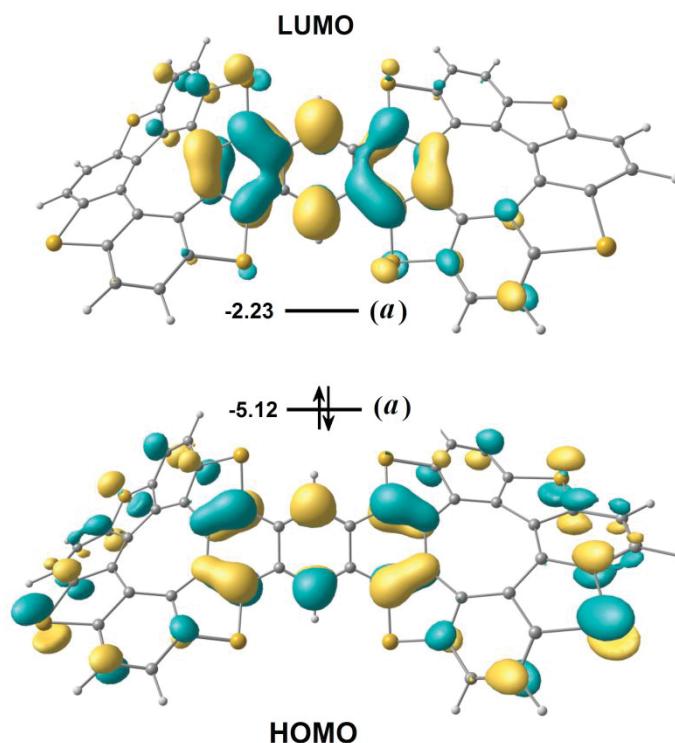
Figure S14. Molecular orbital diagram of the tetraselena[8]circulene-based compound <u>with n=2</u> (<u>type **II**</u>) calculated at the B3LYP/6-31G(d) level of theory.

13
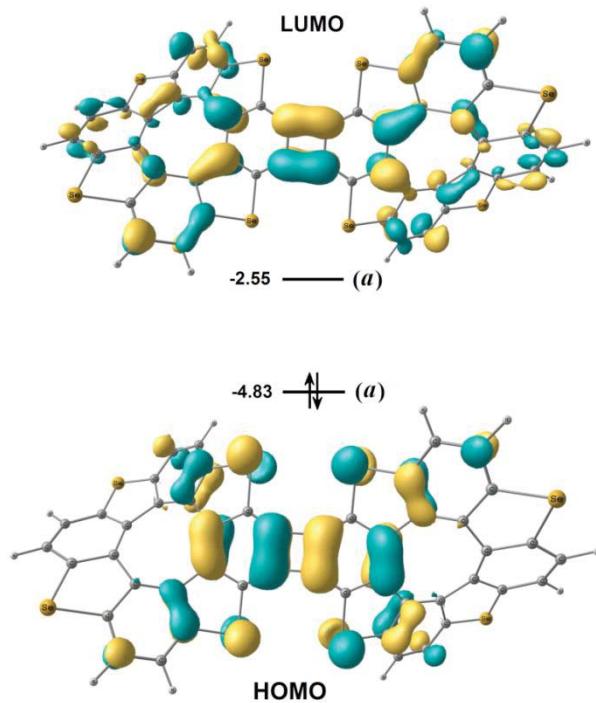
Figure S15. Molecular orbital diagram of the tetraselena[8]circulene-based compound <u>with n=2</u> (<u>type **III**</u>) calculated at the B3LYP/6-31G(d) level of theory.
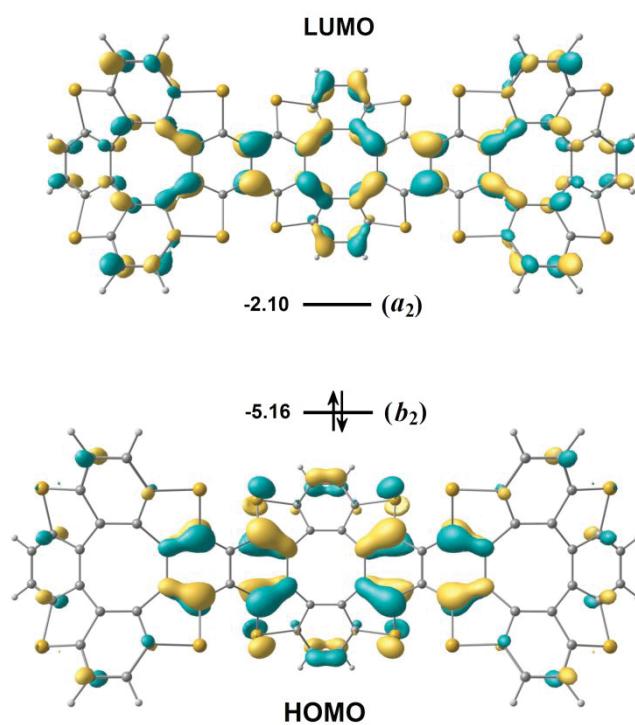
Figure S16. Molecular orbital diagram of the tetraselena[8]circulene-based compound <u>with n=3</u> (<u>type **II**</u>) calculated at the B3LYP/6-31G(d) level of theory.

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LUMO

-2.29 ——— (**b**)

-5.00 ⇅ (**b**)

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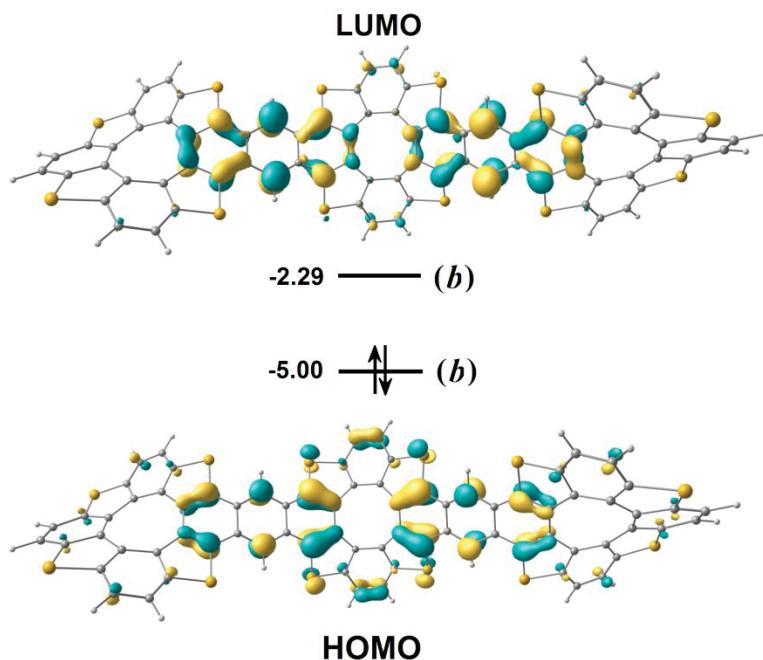
Figure S17. Molecular orbital diagram of the tetraselena[8]circulene-based compound with n=3 (type **II**) calculated at the B3LYP/6-31G(d) level of theory.

LUMO

-2.73 ——— (**a**)

-4.82 ⇅ (**b**)

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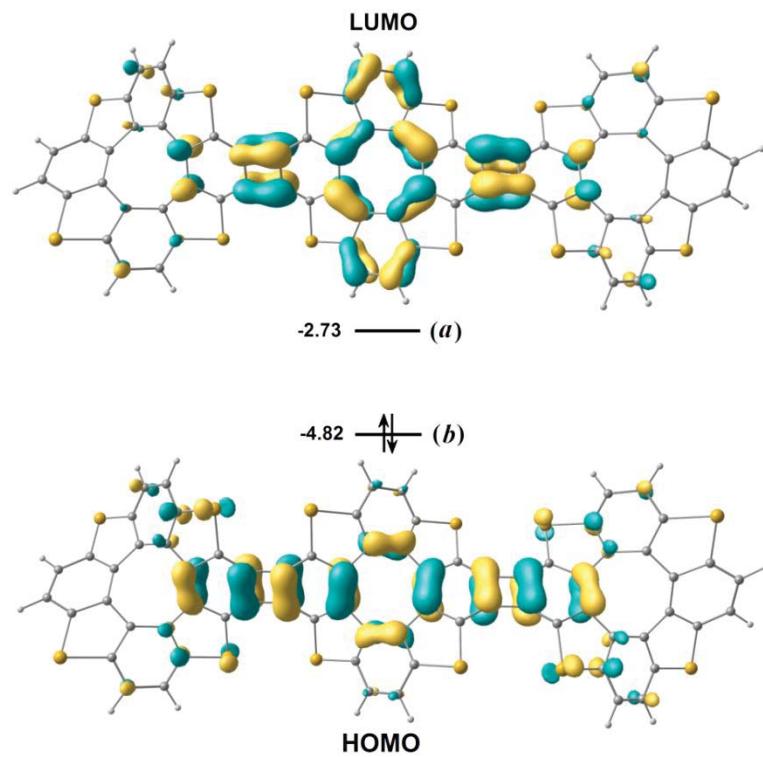
Figure S18. Molecular orbital diagram of the tetraselena[8]circulene-based compound with n=3 (type **III**) calculated at the B3LYP/6-31G(d) level of theory.

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

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

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					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%)

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					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%)

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

	State	Transition	λ nm	f	Assignment
					HOMO→LUMO+1 (11%)
					HOMO-1→LUMO (9%)
	S_7	$X^1A \to 4^1B_1$	593	0.0002	HOMO-1→LUMO+1 (48%)
					HOMO→LUMO (26%)
					HOMO→LUMO+2 (12%)
					HOMO-3→LUMO+1 (9%)
	S_{10}	$X^1A \to 5^1B_2$	536	0.0264	HOMO-1→LUMO+2 (65%)
					HOMO→LUMO+1 (17%)
					HOMO→LUMO+3 (13%)
	S_{12}	$X^1A \to 6^1B_2$	531	0.0160	HOMO-3→LUMO+2 (90%)
	S_{13}	$X^1A \to 1^1B_3$	512	2.0862	HOMO-4→LUMO (73%)
					HOMO-5→LUMO+1 (9%)
					HOMO-8→LUMO (7%)
	S_{16}	$X^1A \to 2^1B_3$	490	0.0554	HOMO-6→LUMO (51%)
					HOMO-8→LUMO (11%)
					HOMO-5→LUMO+1 (11%)
					HOMO-7→LUMO+1 (6%)
	S_{17}	$X^1A \to 7^1B_2$	484	0.0155	HOMO→LUMO+3 (56%)
					HOMO-1→LUMO+4 (12%)
					HOMO-1→LUMO+2 (12%)
					HOMO-2→LUMO+3 (10%)
	S_{19}	$X^1A \to 8^1B_2$	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	$X^1A \to 1^1A_2$	429	0	HOMO-3→LUMO (99%)
	S_2	$X^1A \to 1^1A_1$	420	0	HOMO-2→LUMO (98%)
	$S_{3(4)}$	$X^1A \to 1^1E$	415	0.1749	HOMO→LUMO (95%) (HOMO-1→LUMO (95%))
TSCs (Type **I**)					
n=2 (C_1 symmetry point group)	S_1	$X^1A \to 1^1A$	485	0.4157	HOMO→LUMO (91%)
	S_2	$X^1A \to 2^1A$	476	0.0238	HOMO-1→LUMO (80%) HOMO-5→LUMO (14%)
	S_3	$X^1A \to 3^1A$	441	0.0354	HOMO-2→LUMO (91%)
	S_4	$X^1A \to 4^1A$	437	0.0642	HOMO-5→LUMO (80%) HOMO-1→LUMO (14%)
	S_5	$X^1A \to 5^1A$	431	0.0750	HOMO-4→LUMO (80%) HOMO-6→LUMO (16%)
	S_{10}	$X^1A \to 19^1A$	399	0.5084	HOMO-1→LUMO+2 (86%)
n=3 (C_{2v} symmetry point group)	S_1	$X^1A_1 \to 1^1B_1$	473	0.8103	HOMO→LUMO (93%)
	S_2	$X^1A_1 \to 1^1A_1$	445	0.0004	HOMO-2→LUMO (93%)
	S_3	$X^1A_1 \to 1^1B_2$	439	0.0905	HOMO-1→LUMO (84%)
	S_4	$X^1A_1 \to 2^1A_1$	436	0.0036	HOMO-3→LUMO (45%) HOMO→LUMO+1 (26%) HOMO-6→LUMO (10%)
	S_6	$X^1A_1 \to 2^1B_1$	430	0.0119	HOMO-4→LUMO (76%) HOMO-2→LUMO+1 (15%)
	S_7	$X^1A_1 \to 3^1A_1$	418	0.0121	HOMO-6→LUMO (62%) HOMO-4→LUMO+1 (13%) HOMO→LUMO+1 (9%)

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	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%)

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	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%)

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point group)					
	S_2	$X^1A \rightarrow 2^1A$	528	0.0343	HOMO$\rightarrow$LUMO+1 (89%) HOMO-5$\rightarrow$LUMO (6%)
	S_3	$X^1A \rightarrow 3^1A$	508	0.2631	HOMO-1$\rightarrow$LUMO (79%) HOMO-2$\rightarrow$LUMO (16%)
	S_4	$X^1A \rightarrow 4^1A$	487	0.0090	HOMO-4$\rightarrow$LUMO (94%)
	S_5	$X^1A \rightarrow 5^1A$	482	0.2060	HOMO-2$\rightarrow$LUMO (80%) HOMO-1$\rightarrow$LUMO (16%)
	S_7	$X^1A \rightarrow 7^1A$	479	0.0732	HOMO-5$\rightarrow$LUMO (79%) HOMO$\rightarrow$LUMO+1 (9%)
	S_9	$X^1A \rightarrow 9^1A$	441	0.0401	HOMO-7$\rightarrow$LUMO (82%) HOMO-5$\rightarrow$LUMO (10%)
	S_{11}	$X^1A \rightarrow 11^1A$	395	0.3739	HOMO-3$\rightarrow$LUMO+1 (61%) HOMO$\rightarrow$LUMO+2 (33%)
	S_{13}	$X^1A \rightarrow 13^1A$	388	0.0220	HOMO-5$\rightarrow$LUMO+1 (74%) HOMO$\rightarrow$LUMO+3 (20%)
	S_{14}	$X^1A \rightarrow 14^1A$	388	0.0676	HOMO-4$\rightarrow$LUMO+1 (84%) HOMO-7$\rightarrow$LUMO (6%)
	S_{15}	$X^1A \rightarrow 15^1A$	387	0.5168	HOMO$\rightarrow$LUMO+2 (54%) HOMO-3$\rightarrow$LUMO+1 (30%) HOMO-6$\rightarrow$LUMO+1 (9%)
	S_{17}	$X^1A \rightarrow 17^1A$	383	0.0109	HOMO$\rightarrow$LUMO+4 (91%)
	S_{18}	$X^1A \rightarrow 18^1A$	374	0.0020	HOMO-6$\rightarrow$LUMO+1 (87%)
	S_{19}	$X^1A \rightarrow 19^1A$	365	0.0107	HOMO-7$\rightarrow$LUMO+1 (64%) HOMO$\rightarrow$LUMO+3 (25%)
n=3 (C_2 symmetry point group)	S_1	$X^1A \rightarrow 1^1B$	779	0	HOMO$\rightarrow$LUMO (95%)
	S_2	$X^1A \rightarrow 1^1A$	718	0.0004	HOMO-1$\rightarrow$LUMO (94%)
	S_3	$X^1A \rightarrow 2^1A$	595	0.0359	HOMO$\rightarrow$LUMO+1 (89%)
	S_4	$X^1A \rightarrow 2^1B$	586	0.0003	HOMO-1$\rightarrow$LUMO+1 (88%) HOMO$\rightarrow$LUMO+2 (8%)
	S_5	$X^1A \rightarrow 3^1B$	540	0.7386	HOMO-2$\rightarrow$LUMO (91%)
	S_8	$X^1A \rightarrow 4^1A$	499	0.0056	HOMO-7$\rightarrow$LUMO (67%) HOMO-1$\rightarrow$LUMO+2 (14%) HOMO-6$\rightarrow$LUMO+1 (12%)
	S_{10}	$X^1A \rightarrow 6^1B$	497	0.1529	HOMO-5$\rightarrow$LUMO (84%) HOMO-4$\rightarrow$LUMO+1 (7%)
	S_{12}	$X^1A \rightarrow 6^1A$	486	0.0821	HOMO-1$\rightarrow$LUMO+2 (78%) HOMO-7$\rightarrow$LUMO (13%)
	S_{15}	$X^1A \rightarrow 8^1A$	454	0.0703	HOMO-10$\rightarrow$LUMO (83%) HOMO-7$\rightarrow$LUMO (6%)
	S_{20}	$X^1A \rightarrow 10^1B$	429	0.1344	HOMO-4$\rightarrow$LUMO+1 (80%) HOMO-5$\rightarrow$LUMO+2 (7%) HOMO-5$\rightarrow$LUMO (7%)
n=4 (C_1 symmetry point group)	S_1	$X^1A \rightarrow 1^1A$	805	0.0008	HOMO$\rightarrow$LUMO (80%) HOMO-2$\rightarrow$LUMO (10%) HOMO-1$\rightarrow$LUMO+1 (7%)
	S_2	$X^1A \rightarrow 2^1A$	759	0.0001	HOMO-1$\rightarrow$LUMO (77%) HOMO$\rightarrow$LUMO+1 (20%)
	S_3	$X^1A \rightarrow 3^1A$	721	0.0037	HOMO-2$\rightarrow$LUMO (84%) HOMO-1$\rightarrow$LUMO+1 (9%)
	S_4	$X^1A \rightarrow 4^1A$	641	0.0188	HOMO$\rightarrow$LUMO+1 (63%) HOMO-2$\rightarrow$LUMO+1 (17%) HOMO-1$\rightarrow$LUMO (15%)
	S_5	$X^1A \rightarrow 5^1A$	625	0.0026	HOMO-1$\rightarrow$LUMO+1 (72%) HOMO$\rightarrow$LUMO (11%) HOMO$\rightarrow$LUMO+2 (8%)
	S_7	$X^1A \rightarrow 7^1A$	553	0.0095	HOMO$\rightarrow$LUMO+2 (75%) HOMO-1$\rightarrow$LUMO+3 (11%) HOMO-1$\rightarrow$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	S_1	$X^1A \rightarrow 1^1B_1$	818	0	HOMO→LUMO (68%)
(D_2 symmetry					HOMO-2→LUMO (15%)
point group)					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%)

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Table S3. 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    Atomic          Coordinates (Angstroms)
Number    Number        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 S4. 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    Atomic          Coordinates (Angstroms)
Number    Number        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
```

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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 S5. 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   Atomic        Coordinates (Angstroms)
Number   Number      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 S6. 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      Atomic            Coordinates (Angstroms)
Number      Number         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
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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
--------------------------------------------------------
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Table S7. 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

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--------------------------------------------------------
Center     Atomic            Coordinates (Angstroms)
Number     Number         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
```

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2	5	6	6.624095	0.722895	0.916276
3	6	6	-9.096319	1.697519	1.306694
4	7	6	7.653579	1.698857	1.309433
5	8	6	-14.981884	0.725740	-0.511938
6	9	6	1.750654	0.723185	-0.401812
7	10	6	18.495933	0.719643	-0.771702
8	11	6	-9.096319	-1.697519	1.306694
9	12	6	7.653579	-1.698857	1.309433
10	13	6	-14.981884	-0.725740	-0.511938
11	14	6	1.750654	-0.723185	-0.401812
12	15	6	18.495933	-0.719643	-0.771702
13	16	6	-16.002580	-1.731110	-0.881047
14	17	6	0.721493	-1.702609	-0.789603
15	18	6	17.445612	-1.739352	-0.956291
16	19	6	-10.123428	-0.722955	0.902190
17	20	6	6.624095	-0.722895	0.916276
18	21	6	-17.445612	-1.739352	-0.956291
19	22	6	-0.721493	-1.702609	-0.789603
20	23	6	16.002580	-1.731110	-0.881047
21	24	6	-6.624095	-0.722895	0.916276
22	25	6	10.123428	-0.722955	0.902190
23	26	6	-7.653579	-1.698857	1.309433
24	27	6	9.096319	-1.697519	1.306694
25	28	6	-18.495933	-0.719643	-0.771702
26	29	6	-1.750654	-0.723185	-0.401812
27	30	6	14.981884	-0.725740	-0.511938
28	31	6	-7.653579	1.698857	1.309433
29	32	6	9.096319	1.697519	1.306694
30	33	6	-18.495933	0.719643	-0.771702
31	34	6	-1.750654	0.723185	-0.401812
32	35	6	14.981884	0.725740	-0.511938
33	36	6	-17.445612	1.739352	-0.956291
34	37	6	-0.721493	1.702609	-0.789603
35	38	6	16.002580	1.731110	-0.881047
36	39	6	-6.624095	0.722895	0.916276
37	40	6	10.123428	0.722955	0.902190
38	41	6	-15.378499	-2.993593	-1.078065
39	42	6	1.335499	-2.950053	-1.082301
40	43	6	18.044545	-3.016409	-1.167326
41	44	6	-5.372048	1.352015	0.716488
42	45	6	11.374087	1.352350	0.692767
43	46	6	-9.711973	-2.940515	1.610789
44	47	6	7.040478	-2.944377	1.610947
45	48	6	-19.778384	1.337776	-0.699060
46	49	6	-3.003288	1.351398	-0.200258
47	50	6	13.730224	1.347472	-0.264396
48	51	6	-9.711973	2.940515	1.610789
49	52	6	7.040478	2.944377	1.610947
50	53	6	-19.778384	-1.337776	-0.699060
51	54	6	-3.003288	-1.351398	-0.200258
52	55	6	13.730224	-1.347472	-0.264396
53	56	6	-15.378499	2.993593	-1.078065
54	57	6	1.335499	2.950053	-1.082301
55	58	6	18.044545	3.016409	-1.167326
56	59	6	-5.372048	-1.352015	0.716488
57	60	6	11.374087	-1.352350	0.692767
58	61	6	-18.044545	3.016409	-1.167326
59	62	6	-1.335499	2.950053	-1.082301
60	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

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Table S8. 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     Atomic            Coordinates (Angstroms)
Number     Number         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
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       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 S9. 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    Atomic           Coordinates (Angstroms)
Number    Number          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
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    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
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Table S10. 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

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  Center    Atomic         Coordinates (Angstroms)
  Number    Number         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 S11. 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

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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

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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
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Table S12. 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

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  ------------------------------------------------------------
  Center    Atomic            Coordinates (Angstroms)
  Number    Number         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
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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
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Table S13. 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

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 Center     Atomic             Coordinates (Angstroms)
 Number     Number          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
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Center	Atomic	X	Y	Z
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 S14. 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

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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

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 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 S15. 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    Atomic          Coordinates (Angstroms)
     Number    Number        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
```

1				
2	29	6	9.340537	4.286013	0.151843
3	30	6	19.357191	4.264744	-0.561132
4	31	6	-24.323432	-0.683168	0.002699
5	32	6	-14.254611	-0.678663	-0.155410
6	33	6	-4.249215	-0.679352	0.152026
7	34	6	5.756816	-0.679383	-0.152050
8	35	6	15.762326	-0.677828	0.155720
9	36	6	-15.762326	0.677828	0.155720
10	37	6	-5.756816	0.679383	-0.152050
11	38	6	4.249215	0.679352	0.152026
12	39	6	14.254611	0.678663	-0.155410
13	40	6	24.323432	0.683168	0.002699
14	41	6	-21.793962	0.722179	0.030170
15	42	6	-11.777500	0.712629	0.103009
16	43	6	-1.772035	0.712972	-0.100691
17	44	6	8.233822	0.713004	0.100343
18	45	6	18.243945	0.709589	-0.132257
19	46	6	-18.243945	-0.709589	-0.132257
20	47	6	-8.233822	-0.713004	0.100343
21	48	6	1.772035	-0.712972	-0.100691
22	49	6	11.777500	-0.712629	0.103009
23	50	6	21.793962	-0.722179	0.030170
24	51	6	-20.744638	-1.762840	-0.147136
25	52	6	-10.722881	-1.758115	-0.105174
26	53	6	-0.717330	-1.758534	0.101399
27	54	6	9.288544	-1.758522	-0.099460
28	55	6	19.299315	-1.751961	0.249906
29	56	6	-19.299315	1.751961	0.249906
30	57	6	-9.288544	1.758522	-0.099460
31	58	6	0.717330	1.758534	0.101399
32	59	6	10.722881	1.758115	-0.105174
33	60	6	20.744638	1.762840	-0.147136
34	61	6	-21.793962	-0.722179	-0.030170
35	62	6	-11.777500	-0.712629	-0.103009
36	63	6	-1.772035	-0.712972	0.100691
37	64	6	8.233822	-0.713004	-0.100343
38	65	6	18.243945	-0.709589	0.132257
39	66	6	-18.243945	0.709589	0.132257
40	67	6	-8.233822	0.713004	-0.100343
41	68	6	1.772035	0.712972	0.100691
42	69	6	11.777500	0.712629	-0.103009
43	70	6	21.793962	0.722179	-0.030170
44	71	6	-20.744638	1.762840	0.147136
45	72	6	-10.722881	1.758115	0.105174
46	73	6	-0.717330	1.758534	-0.101399
47	74	6	9.288544	1.758522	0.099460
48	75	6	19.299315	1.751961	-0.249906
49	76	6	-19.299315	-1.751961	-0.249906
50	77	6	-9.288544	-1.758522	0.099460
51	78	6	0.717330	-1.758534	-0.101399
52	79	6	10.722881	-1.758115	0.105174
53	80	6	20.744638	-1.762840	0.147136
54	81	6	-23.084899	1.332051	0.016869
55	82	6	-13.070671	1.355897	0.271988
56	83	6	-3.065419	1.356987	-0.266492
57	84	6	6.940537	1.357133	0.266386
58	85	6	16.945994	1.350088	-0.291304
59	86	6	-16.945994	-1.350088	-0.291304
60	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 S16. 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    Atomic         Coordinates (Angstroms)
Number    Number       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 S17. 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    Atomic          Coordinates (Angstroms)
    Number    Number        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 S18. 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

Center Number	Atomic Number	X	Y	Z
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 S19. 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

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         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
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Table S20. 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

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        ----------------------------------------------------------
        Center    Atomic         Coordinates (Angstroms)
        Number    Number        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
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2	21	6	-16.952197	-1.722873	-1.159909
3	22	6	-0.720396	-1.692146	-1.181136
4	23	6	15.508882	-1.713637	-1.163101
5	24	6	-6.394911	-0.725776	1.169561
6	25	6	9.828145	-0.725832	1.164099
7	26	6	-7.391881	-1.689780	1.687060
8	27	6	8.832462	-1.688906	1.686731
9	28	6	-17.970135	-0.721086	-0.755236
10	29	6	-1.717460	-0.725941	-0.666862
11	30	6	14.508416	-0.727433	-0.681636
12	31	6	-7.391881	1.689780	1.687060
13	32	6	8.832462	1.688906	1.686731
14	33	6	-17.970135	0.721086	-0.755236
15	34	6	-1.717460	0.725941	-0.666862
16	35	6	14.508416	0.727433	-0.681636
17	36	6	-16.952197	1.722873	-1.159909
18	37	6	-0.720396	1.692146	-1.181136
19	38	6	15.508882	1.713637	-1.163101
20	39	6	-6.394911	0.725776	1.169561
21	40	6	9.828145	0.725832	1.164099
22	41	6	-14.883600	-2.940118	-1.520990
23	42	6	1.339502	-2.910123	-1.571704
24	43	6	17.554484	-2.977741	-1.464895
25	44	6	-5.166563	1.345958	0.857415
26	45	6	11.055355	1.346718	0.848046
27	46	6	-9.452806	-2.903609	2.083942
28	47	6	6.773134	-2.906355	2.081946
29	48	6	-19.225552	1.336567	-0.480854
30	49	6	-2.946255	1.345503	-0.354315
31	50	6	13.274112	1.340935	-0.369927
32	51	6	-9.452806	2.903609	2.083942
33	52	6	6.773134	2.906355	2.081946
34	53	6	-19.225552	-1.336567	-0.480854
35	54	6	-2.946255	-1.345503	-0.354315
36	55	6	13.274112	-1.340935	-0.369927
37	56	6	-14.883600	2.940118	-1.520990
38	57	6	1.339502	2.910123	-1.571704
39	58	6	17.554484	2.977741	-1.464895
40	59	6	-5.166563	-1.345958	0.857415
41	60	6	11.055355	-1.346718	0.848046
42	61	6	-17.554484	2.977741	-1.464895
43	62	6	-1.339502	2.910123	-1.571704
44	63	6	14.883600	2.940118	-1.520990
45	64	6	-11.055355	-1.346718	0.848046
46	65	6	5.166563	-1.345958	0.857415
47	66	6	-6.773134	2.906355	2.081946
48	67	6	9.452806	2.903609	2.083942
49	68	6	-13.274112	-1.340935	-0.369927
50	69	6	2.946255	-1.345503	-0.354315
51	70	6	19.225552	-1.336567	-0.480854
52	71	6	-6.773134	-2.906355	2.081946
53	72	6	9.452806	-2.903609	2.083942
54	73	6	-13.274112	1.340935	-0.369927
55	74	6	2.946255	1.345503	-0.354315
56	75	6	19.225552	1.336567	-0.480854
57	76	6	-17.554484	-2.977741	-1.464895
58	77	6	-1.339502	-2.910123	-1.571704
59	78	6	14.883600	-2.940118	-1.520990
60	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

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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 S21. 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

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-----------------------------------------------------------
Center    Atomic           Coordinates (Angstroms)
Number    Number        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 S22. 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

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Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

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      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
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  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
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Table S23. 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

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 ----------------------------------------------------------
 Center     Atomic           Coordinates (Angstroms)
 Number     Number         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
```

1				
2	35	6	3.299280	0.835765	1.761884
3	36	6	13.955398	0.640740	0.119376
4	37	6	-13.817788	-0.799827	0.159374
5	38	6	-3.292904	-0.625631	-1.784031
6	39	6	6.727963	-0.654650	2.210591
7	40	6	16.895266	-0.601799	-1.859950
8	41	6	-15.751778	-1.551480	1.867179
9	42	6	-5.662511	-1.617775	-2.564314
10	43	6	4.229355	-1.620832	2.358689
11	44	6	14.619240	-1.732129	-0.982209
12	45	6	-15.150153	1.508688	-0.234166
13	46	6	-4.263579	1.837078	-2.296403
14	47	6	5.698578	1.823319	2.446384
15	48	6	16.562467	1.308882	-0.002566
16	49	6	-16.893275	-0.605652	1.864819
17	50	6	-6.728836	-0.648826	-2.215372
18	51	6	3.292704	-0.632503	1.772484
19	52	6	13.820332	-0.798943	-0.153844
20	53	6	-13.955274	0.639191	-0.116114
21	54	6	-3.301874	0.842521	-1.763625
22	55	6	6.741297	0.812472	2.148938
23	56	6	17.308054	0.427986	-0.933866
24	57	6	-16.563383	1.303029	0.005045
25	58	6	-5.701373	1.830561	-2.447218
26	59	6	4.260441	1.828668	2.298714
27	60	6	15.148975	1.512083	0.237251
28	61	6	-14.614166	-1.732445	0.990798
29	62	6	-4.229557	-1.612044	-2.373431
30	63	6	5.661635	-1.625341	2.554649
31	64	6	15.756438	-1.550867	-1.859065
32	65	6	-18.689304	0.769317	0.994098
33	66	6	-8.009584	1.408521	-1.988633
34	67	6	2.103419	1.446052	1.341809
35	68	6	12.779822	1.292531	0.531351
36	69	6	-12.650826	-1.404293	-0.343264
37	70	6	-2.097223	-1.233435	-1.360561
38	71	6	7.984750	-1.278447	2.114114
39	72	6	17.835214	-0.911168	-2.886529
40	73	6	-15.912517	-2.557329	2.864804
41	74	6	-6.215580	-2.854262	-3.009821
42	75	6	3.572600	-2.858942	2.621383
43	76	6	14.020046	-3.024514	-1.029979
44	77	6	-14.814092	2.770733	-0.805500
45	78	6	-3.629508	3.092761	-2.529297
46	79	6	6.281839	3.077263	2.793889
47	80	6	17.427060	2.251156	0.628000
48	81	6	-17.833250	-0.915234	2.891288
49	82	6	-7.984692	-1.274035	-2.116298
50	83	6	2.098744	-1.239514	1.343110
51	84	6	12.654009	-1.404395	0.349116
52	85	6	-12.780878	1.292240	-0.529465
53	86	6	-2.107504	1.452022	-1.338282
54	87	6	8.006790	1.404070	1.985043
55	88	6	18.688544	0.779483	-0.993604
56	89	6	-17.429371	2.243288	-0.626610
57	90	6	-6.285337	3.084752	-2.792619
58	91	6	3.625132	3.082262	2.539336
59	92	6	14.810941	2.773700	0.808383
60	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 S24. 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

1					
2	34	6	0.228417	-6.338312	-0.842856
3	35	6	0.802580	-16.823978	-0.394628
	36	6	-0.802580	16.823978	-0.394628
4	37	6	-0.228417	6.338312	-0.842856
5	38	6	1.298179	-3.976109	0.268397
6	39	6	2.196122	-14.391524	-0.728546
	40	6	1.973101	-24.711579	2.969328
7	41	6	-1.285491	22.648646	1.085715
8	42	6	-0.873341	12.119635	-1.969157
9	43	6	0.483914	1.811784	1.052289
	44	6	1.998655	-8.530311	-1.561481
10	45	6	1.957323	-18.965552	1.205957
11	46	6	-1.957323	18.965552	1.205957
12	47	6	-1.998655	8.530311	-1.561481
	48	6	-0.483914	-1.811784	1.052289
13	49	6	0.873341	-12.119635	-1.969157
14	50	6	1.285491	-22.648646	1.085715
15	51	6	-2.245405	20.986114	2.965978
	52	6	-3.248425	10.896521	-1.673301
16	53	6	-1.803966	0.473526	1.549883
17	54	6	-0.246931	-9.729251	-2.423317
18	55	6	0.154885	-20.507820	-0.084871
	56	6	-0.154885	20.507820	-0.084871
19	57	6	0.246931	9.729251	-2.423317
20	58	6	1.803966	-0.473526	1.549883
21	59	6	3.248425	-10.896521	-1.673301
	60	6	2.245405	-20.986114	2.965978
22	61	6	-1.788269	22.272847	2.387212
23	62	6	-2.259243	11.986768	-1.502155
24	63	6	-0.970151	1.616241	1.107362
	64	6	0.550156	-8.673600	-1.754589
25	65	6	0.794640	-19.244280	0.348743
26	66	6	-0.794640	19.244280	0.348743
27	67	6	-0.550156	8.673600	-1.754589
	68	6	0.970151	-1.616241	1.107362
28	69	6	2.259243	-11.986768	-1.502155
29	70	6	1.788269	-22.272847	2.387212
30	71	6	-0.528789	21.898371	0.055445
	72	6	0.074043	11.156335	-2.577567
31	73	6	1.610518	0.958084	1.498556
32	74	6	3.133600	-9.458979	-1.774210
33	75	6	2.501381	-19.686537	2.381196
	76	6	-2.501381	19.686537	2.381196
34	77	6	-3.133600	9.458979	-1.774210
35	78	6	-1.610518	-0.958084	1.498556
36	79	6	-0.074043	-11.156335	-2.577567
	80	6	0.528789	-21.898371	0.055445
37	81	6	-1.335619	24.042202	0.789511
38	82	6	-0.360288	13.429929	-1.980168
39	83	6	0.912511	3.111887	0.730396
	84	6	2.442388	-7.233652	-1.242443
40	85	6	2.544735	-17.699415	1.040078
41	86	6	-2.544735	17.699415	1.040078
42	87	6	-2.442388	7.233652	-1.242443
	88	6	-0.912511	-3.111887	0.730396
43	89	6	0.360288	-13.429929	-1.980168
44	90	6	1.335619	-24.042202	0.789511
45	91	6	-2.696698	21.148965	4.308321
	92	6	-4.581746	11.397559	-1.605616
46	93	6	-3.113300	0.902144	1.916499
47	94	6	-1.485877	-9.210805	-2.902237
48	95	6	-0.938433	-20.260544	-0.964759
	96	6	0.938433	20.260544	-0.964759
49	97	6	1.485877	9.210805	-2.902237
50	98	6	3.113300	-0.902144	1.916499
51	99	6	4.581746	-11.397559	-1.605616
	100	6	2.696698	-21.148965	4.308321
52	101	6	-1.994990	23.354919	3.292100
53	102	6	-2.859095	13.165296	-1.025889
54	103	6	-1.747311	2.764931	0.871301
	104	6	-0.217488	-7.524581	-1.495845
55	105	6	0.217488	-18.121148	-0.271827
56	106	6	-0.217488	18.121148	-0.271827
57	107	6	0.217488	7.524581	-1.495845
	108	6	1.747311	-2.764931	0.871301
58	109	6	2.859095	-13.165296	-1.025889
59	110	6	1.994990	-23.354919	3.292100
60	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 S25. 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

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Center     Atomic            Coordinates (Angstroms)
Number     Number          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
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Table S26. 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

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Center    Atomic          Coordinates (Angstroms)
Number    Number       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 S27. 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

1				
2	33	6	-16.615072	0.710724	0.131567
3	34	6	-6.696876	0.535793	0.482206
	35	6	3.209731	0.712811	-0.104378
4	36	6	13.121040	0.533480	-0.485818
5	37	6	-13.121040	-0.533483	-0.485817
6	38	6	-3.209731	-0.712807	-0.104382
7	39	6	6.696876	-0.535790	0.482210
	40	6	16.615072	-0.710728	0.131565
8	41	6	-15.564901	-1.652213	-0.595231
9	42	6	-5.645378	-1.486985	-0.930852
10	43	6	4.260138	-1.665653	0.551393
11	44	6	14.172932	-1.476897	0.951749
	45	6	-14.172932	1.476894	0.951750
12	46	6	-4.260138	1.665656	0.551388
13	47	6	5.645379	1.486988	-0.930847
14	48	6	15.564902	1.652210	-0.595233
15	49	6	-16.615072	-0.710727	-0.131560
16	50	6	-6.696876	-0.535789	-0.482213
	51	6	3.209730	-0.712808	0.104377
17	52	6	13.121040	-0.533483	0.485820
18	53	6	-13.121040	0.533481	0.485821
19	54	6	-3.209731	0.712811	0.104373
20	55	6	6.696876	0.535792	-0.482210
	56	6	16.615072	0.710723	-0.131562
21	57	6	-15.564901	1.652210	0.595238
22	58	6	-5.645378	1.486989	0.930843
23	59	6	4.260138	1.665655	-0.551393
24	60	6	14.172933	1.476894	-0.951746
25	61	6	-14.172932	-1.476897	-0.951745
	62	6	-4.260138	-1.665652	-0.551398
26	63	6	5.645378	-1.486986	0.930847
27	64	6	15.564901	-1.652214	0.595236
28	65	6	-17.895517	1.334316	0.094328
29	66	6	-7.981953	0.926521	1.031897
	67	6	1.924528	1.385554	-0.056267
30	68	6	11.833563	0.923720	-1.033681
31	69	6	-11.833563	-0.923720	-1.033681
32	70	6	-1.924528	-1.385551	-0.056269
33	71	6	7.981953	-0.926520	1.031900
	72	6	17.895516	-1.334320	0.094326
34	73	6	-16.110294	-2.937932	-0.879306
35	74	6	-6.178369	-2.506766	-1.774410
36	75	6	3.724269	-2.964277	0.802293
	76	6	13.637084	-2.492610	1.799339
37	77	6	-13.637085	2.492606	1.799341
38	78	6	-3.724270	2.964281	0.802288
39	79	6	6.178370	2.506770	-1.774405
40	80	6	16.110295	2.937929	-0.879307
	81	6	-17.895517	-1.334319	-0.094321
41	82	6	-7.981954	-0.926519	-1.031902
42	83	6	1.924527	-1.385551	0.056264
43	84	6	11.833562	-0.923720	1.033683
44	85	6	-11.833562	0.923719	1.033684
	86	6	-1.924528	1.385554	0.056262
45	87	6	7.981954	0.926521	-1.031899
46	88	6	17.895517	1.334315	-0.094322
47	89	6	-16.110295	2.937929	0.879314
48	90	6	-6.178369	2.506771	1.774400
	91	6	3.724271	2.964280	-0.802294
49	92	6	13.637086	2.492607	-1.799336
50	93	6	-13.637085	-2.492610	-1.799335
51	94	6	-3.724270	-2.964276	-0.802299
52	95	6	6.178368	-2.506767	1.774405
53	96	6	16.110294	-2.937933	0.879311
	97	34	-11.855938	2.255350	2.333843
54	98	34	-1.953217	3.237370	0.243787
55	99	34	7.954043	2.264034	-2.326721
56	100	34	17.891244	3.178529	-0.376188
57	101	34	-17.891243	-3.178533	-0.376187
	102	34	-7.954043	-2.264031	-2.326725
58	103	34	1.953217	-3.237366	0.243790
59	104	34	11.855937	-2.255351	2.333842
60	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

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  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
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Table S28. 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

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  ---------------------------------------------------------
  Center    Atomic         Coordinates (Angstroms)
  Number    Number        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
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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

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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
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