

The art of the possible: computational design of the 1D and 2D materials based on the tetraoxa[8]circulene monomer

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Electronic Supplementary Information

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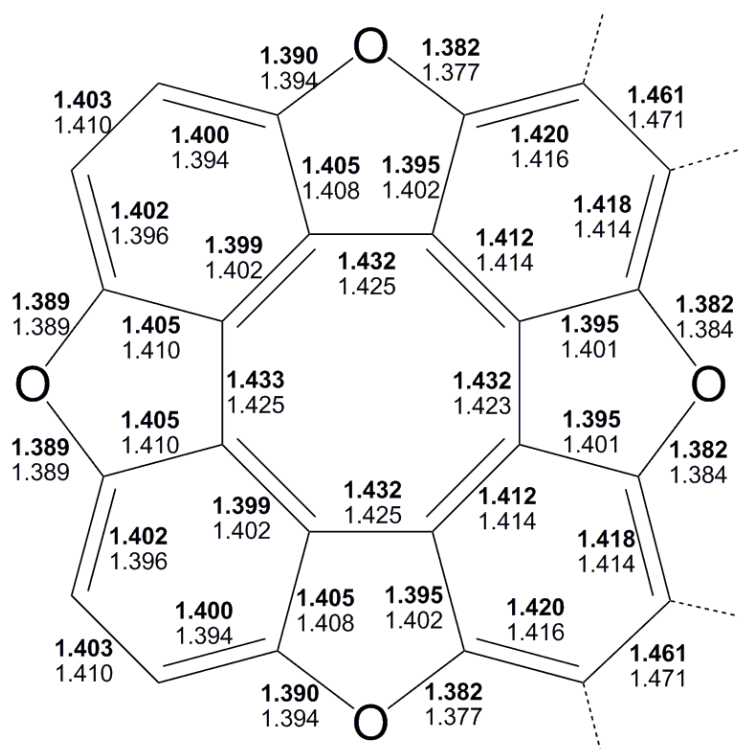


Figure S1. The bond lengths for the S₀ (in bold) and T₁ states (top) for the main fragment of the compound **1** calculated at the B3LYP/6-21G(d) theory level.*

* The 6-21G(d) double-valence split basis set affords us to optimize all studied systems which consist at the most of 432 atoms (compounds **4** and **5**). The extension of the chosen basis set prevents optimization of all studied molecules at the uniform level of accuracy. For comparison we have optimized the sheet **1** with the 6-31G(d) basis set. The calculated deviations in the structural parameters are negligible (no more than 0.004 Å for the bond lengths) and all conclusions remain. Thus, the choice of the 6-21G(d) basis set is quite justified by a very big size of the studied systems.

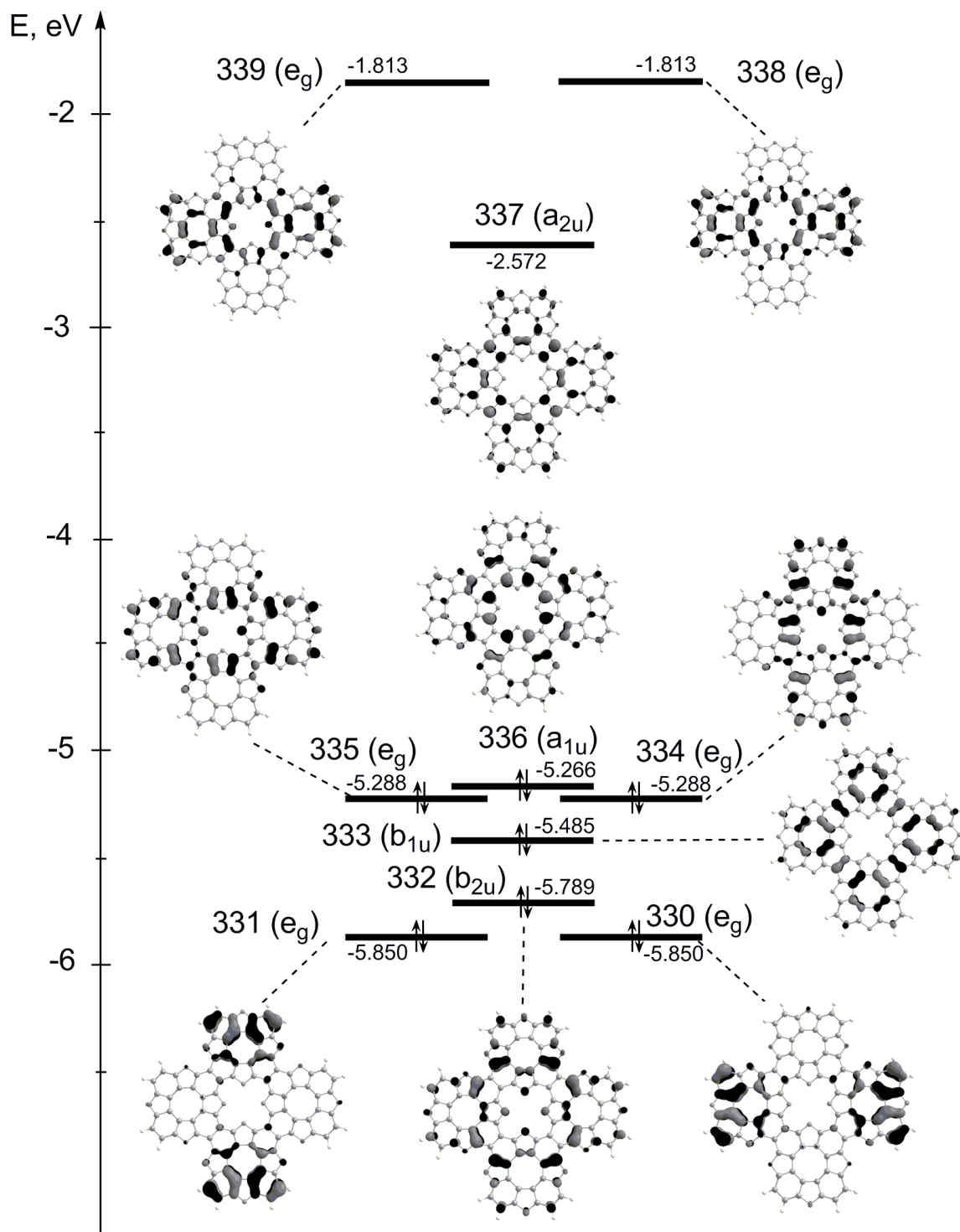


Figure S2. Molecular orbital diagram of the compound **1** calculated at the B3LYP/6-21G(d) level of theory. The highest occupied and lowest empty MO are numerated and their symmetry in the D_{4h} point group are given in parenthesis.

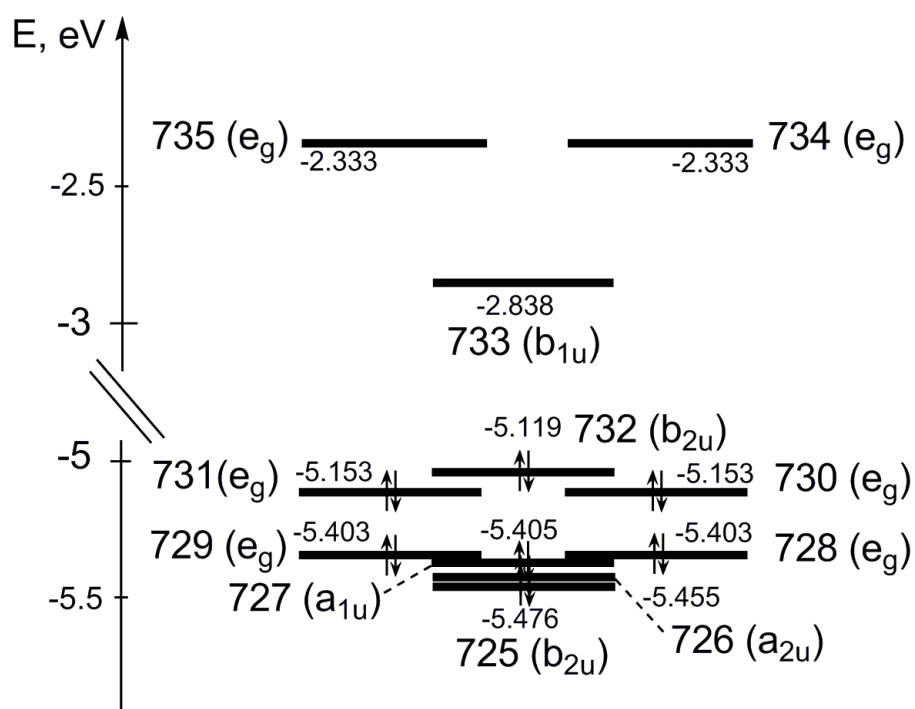


Figure S3. Molecular orbital energy diagram of the compound **2** calculated at the B3LYP/6-21G(d) level of theory

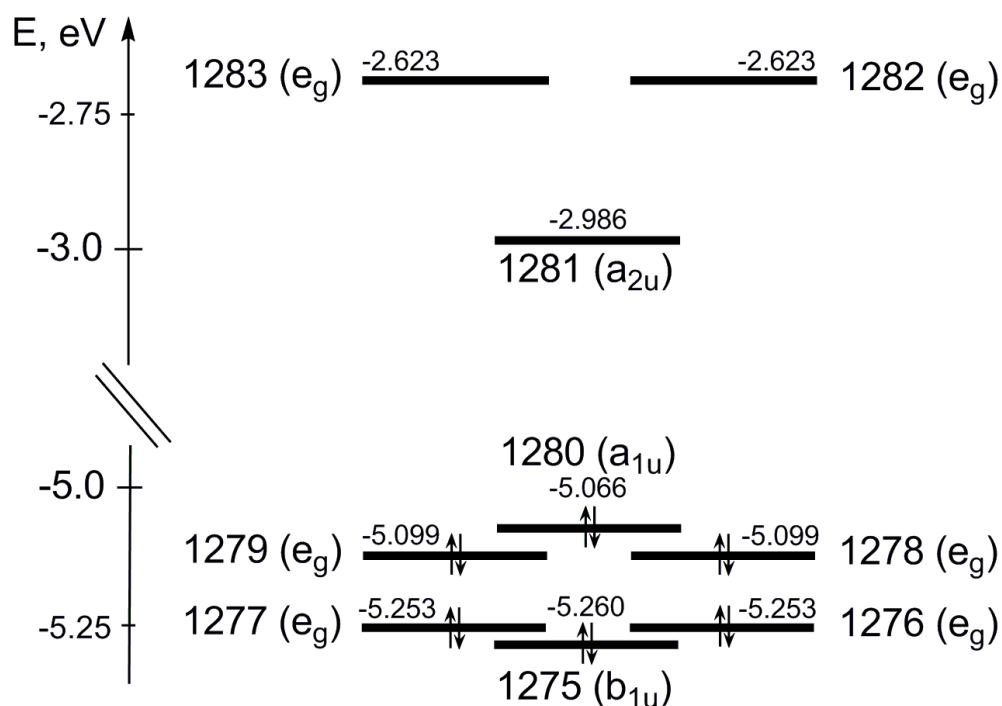


Figure S4. Molecular orbital energy diagram of the compound **3** calculated at the B3LYP/6-21G(d) level of theory

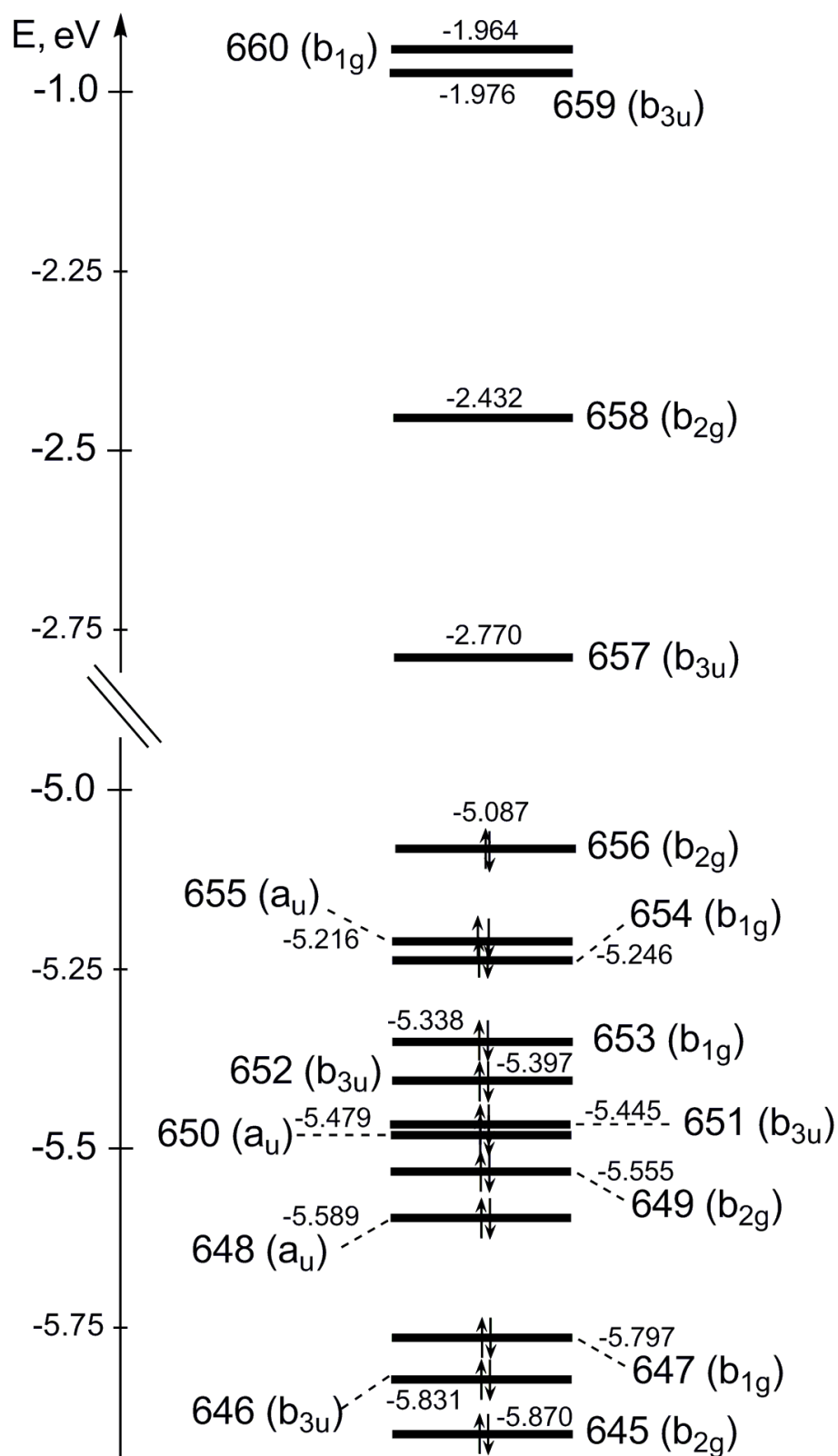


Figure S5. Molecular orbital energy diagram of the compound **4** calculated at the B3LYP/6-21G(d) level of theory

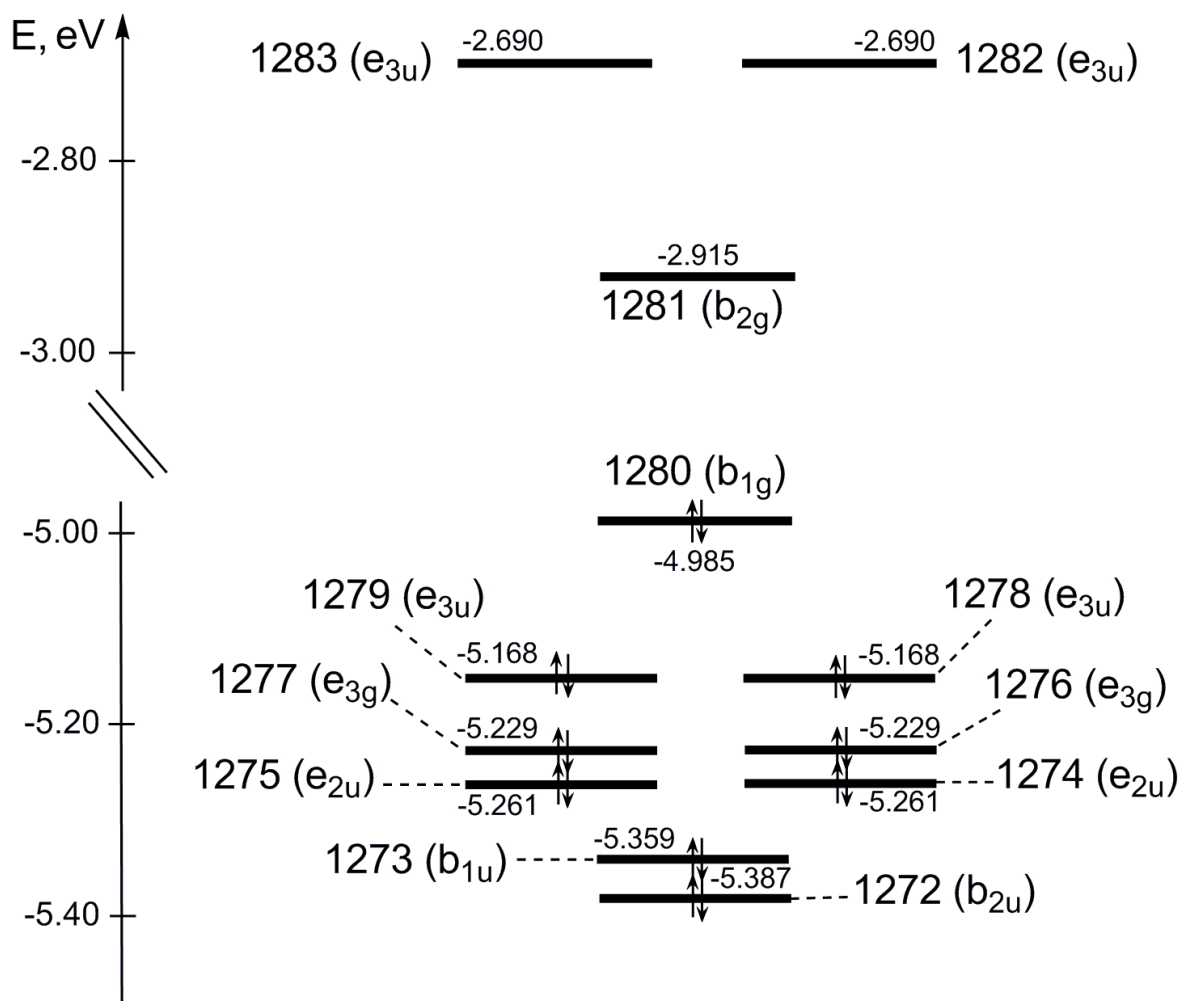


Figure S6. Molecular orbital energy diagram of the compound **5** calculated at the B3LYP/6-21G(d) level of theory

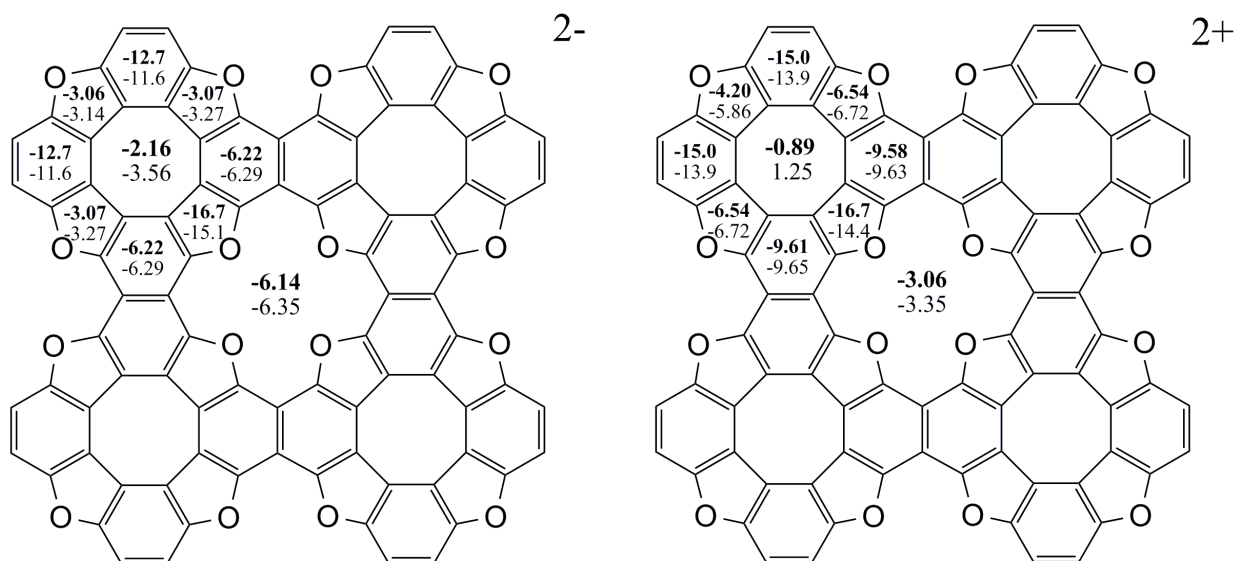


Figure S7. The NICS(0) (bold type in top) and NICS (1) (bottom) indexes calculated at the GIAO B3LYP/6-311++G(d,p) level of theory for the dicationic and dianionic forms of the compound **1**.

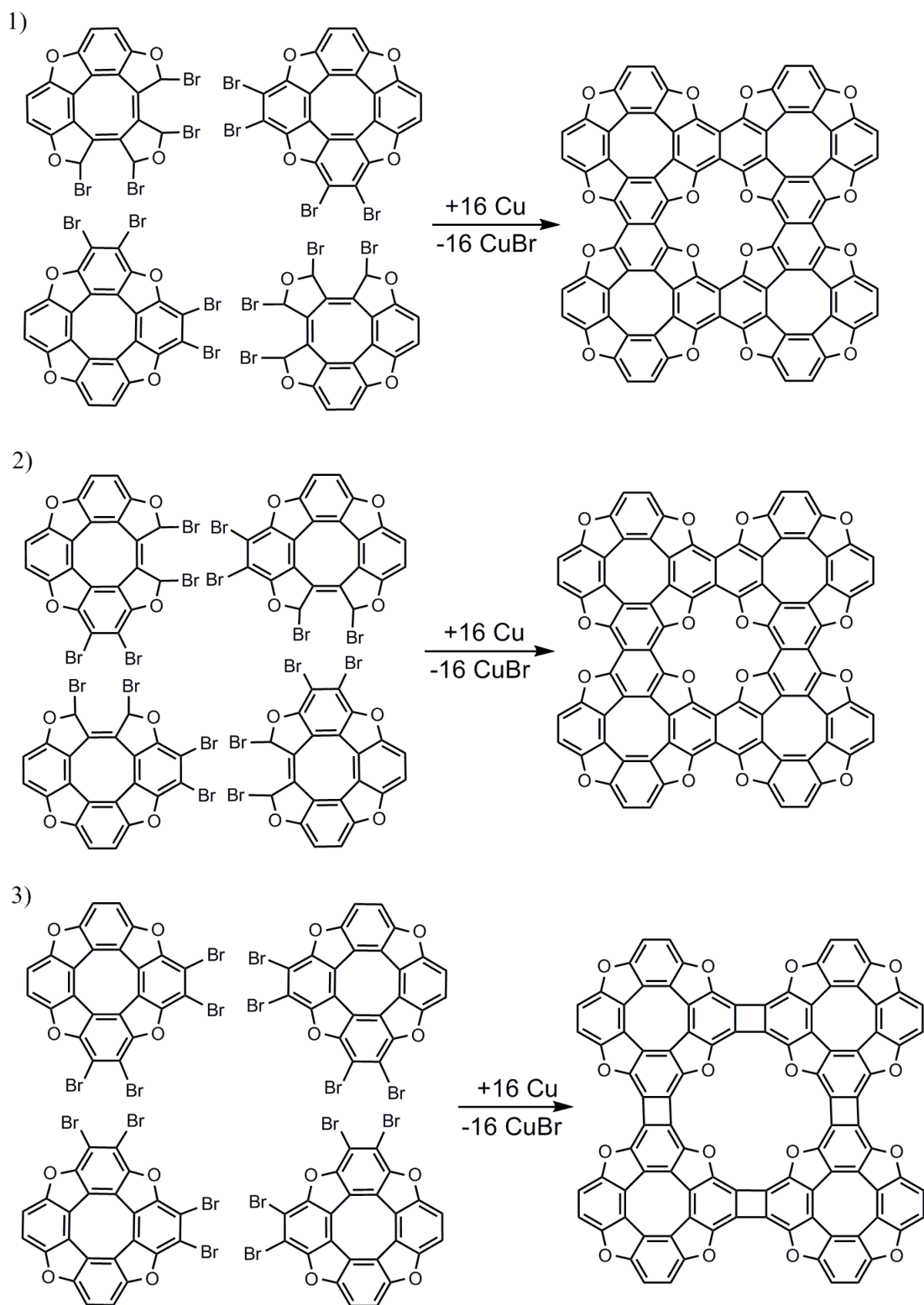


Figure S8. The Ullman-type polymerization as the possible route to synthesize the TOC-based sheets.

Table S1. Calculated parameters and assignment of the vertical electronic transitions in the electronic absorption spectrum of the compounds **1–5** at the B3LYP/3–21G Level

State	Transition	λ , nm	M_{xy} , a.u.	μ_z, β	f	Assignment (in vacuum approximation)
Compound 1						
T ₁₍₂₎	X ¹ A _{1g} →1 ³ E _u	567	0	0	0.000	0.47(335, 334→337) + 0.46[(335→337) – (334→337)]
T ₃	X ¹ A _{1g} →1 ³ A _{2g}	561	0	0	0.000	0.66(336→337) – 0.11[(335→338) – (334→339)]
S ₁	X ¹ A _{1g} →1 ¹ A _{2g}	519	0	6.22	0.000	0.70(336→337)
S ₂₍₃₎	X ¹ A _{1g} →1 ¹ E _u	482	3.40	0	0.730	0.70(335, 334→337)
S ₄	X ¹ A _{1g} →1 ¹ B _{2g}	475	0	0	0.000	0.70(333→337)
S ₅₍₆₎	X ¹ A _{1g} →2 ¹ E _u	417	0.66	0	0.031	0.50(330, 331→337) + 0.45[(330→337) – (331→337)] + 0.12[(333→338) – (333→339)] + 0.11(333→338, 339)
S ₇	X ¹ A _{1g} →1 ¹ B _{1g}	411	0	0	0.000	0.67(332→337)
S ₈	X ¹ A _{1g} →2 ¹ A _{2g}	395	0	2.74	0.000	0.49[(335→339) + (334→338)]
S ₉	X ¹ A _{1g} →2 ¹ B _{1g}	388	0	0	0.000	0.47[(335→338) + (334→339)] + 0.17(332→337)
S ₁₀	X ¹ A _{1g} →3 ¹ A _{2g}	384	0	0	0.000	0.49[(334→338) – (335→339)]
S ₁₁₍₁₂₎	X ¹ A _{1g} →3 ¹ E _u	382	1.66	0	0.219	0.48[(335→338) – (334→339)] + 0.46(334→339) – 0.47(336→339)
S ₁₃	X ¹ A _{1g} →4 ¹ A _{2g}	379	0	0	0.000	0.50(329→337) + 0.34[(334→338) – (335→339)]
S ₁₄	X ¹ A _{1g} →5 ¹ A _{2g}	371	0	0	0.000	0.48(329→337) + 0.34[(335→339) – (334→338)]
S ₁₅	X ¹ A _{1g} →2 ¹ B _{2g}	370	0	0	0.000	0.69(328→337) – 0.12 (336→340)
S ₁₆₍₁₇₎	X ¹ A _{1g} →4 ¹ E _u	369	1.00	0	0.082	0.64(333→338,339) – 0.15[(331→337) + (330→337)] – 0.11(325,327→337)
S ₁₈	X ¹ A _{1g} →3 ¹ B _{1g}	365	0	0	0.000	0.69(327→337)
S ₁₉₍₂₀₎	X ¹ A _{1g} →5 ¹ E _u	363	0.99	0	0.082	0.66(325,326→337) – 0.16[(325→337) + (326→337)] + 0.11(333→338,339)
Compound 2						
T ₁₍₂₎	X ¹ A _{1g} →1 ³ E _u	630	0	0	0.000	0.60(730,731→733) + 0.27[(731→733) – (730→733)]
T ₃	X ¹ A _{1g} →1 ³ A _{2g}	629	0	0	0.000	0.64(732→733) + 0.12[(731→734) – (730→735)]
S ₁	X ¹ A _{1g} →1 ¹ A _{2g}	592	0	10.69	0.000	0.69(732→733)
S ₂₍₃₎	X ¹ A _{1g} →1 ¹ E _u	561	0.89	0	1.158	0.67(730,731→733) + 0.16[(729→733) – (728→733)]
S ₄	X ¹ A _{1g} →1 ¹ B _{1g}	522	0	0.001	0.000	0.67(727→733)
S ₅₍₆₎	X ¹ A _{1g} →2 ¹ E _u	520	2.49	0	0.362	0.65(728,729→733) + 0.18[(731→733) – (730→733)] – 0.16(732→734, 735)
S ₇	X ¹ A _{1g} →2 ¹ A _{2g}	512	0	0.51	0.000	0.69(725→733)
S ₈	X ¹ A _{1g} →1 ¹ B _{2g}	493	0	0	0.000	0.69(726→733)
S ₉₍₁₀₎	X ¹ A _{1g} →3 ¹ E _u	472	0.84	0	0.046	0.64(724→733) + 0.14(725, 732→734) + (727→735)]

Compound 3						
T ₁₍₂₎	X ¹ A _{1g} →1 ³ E _u	667	0	0	0.000	0.56(1278, 1279→1281) + 0.33[(1279→1281) – (1278→1281)]
T ₃	X ¹ A _{1g} →1 ³ A _{2g}	666	0	0	0.000	0.63(1280→1281) – 0.12(1278→1282) – (1279→1283) – (1277→1283) – (1276→1282)]
S ₁	X ¹ A _{1g} →1 ¹ A _{2g}	635	0	15.62	0.000	0.68(1280→1281)
S ₂₍₃₎	X ¹ A _{1g} →1 ¹ E _u	610	5.69	0	1.605	0.66(1278,1279→1281) – 0.21(1276,1277→1281)
S ₄	X ¹ A _{1g} →1 ¹ B _{2g}	578	0	0	0.000	0.66(1275→1281)
S ₅₍₆₎	X ¹ A _{1g} →2 ¹ E _u	576	3.87	0	0.788	0.59(1276, 1277→1281) + 0.22(1278,1279→1281) – 0.21[(1276→1281) + (1277→1281)] – 0.16(1280→1282,1283)
Compound 4						
T ₁	X ¹ A _g →1 ³ B _{1u}	632	0	0	0.000	0.66(656→657) + 0.14(652→658)
T ₂	X ¹ A _g →1 ³ B _{3g}	594	0	0	0.000	0.62(655→657) – 0.22(653→658) + 0.10(656→660)
T ₃	X ¹ A _g →1 ³ B _{2u}	592	0	0	0.000	0.64(654→657) – 0.15(650→658)
S ₁	X ¹ A _g →1 ¹ B _{1u}	562	6.52	0	2.296	0.70(656→657)
S ₂	X ¹ A _g →1 ¹ B _{3g}	552	0	9.29	0.000	0.68(655→657) – 0.11[(653→658) + (648→657)]
S ₃	X ¹ A _g →1 ¹ B _{2u}	545	0.90	0	0.045	0.64(654→657) – 0.20(653→657) + 0.15(655→658) – 0.12(650→658)
S ₄	X ¹ A _g →2 ¹ B _{3g}	506	0	4.46	0.000	0.60(650→657) – 0.30(654→658) + 0.12[(648→657 – (653→658)]
S ₅	X ¹ A _g →1 ¹ A _g	501	0	0	0.000	0.66(651→657) – 0.18(652→657) – 0.12(649→658)
S ₆	X ¹ A _g →2 ¹ B _{2u}	500	3.47	0	0.732	0.66(653→657) + 0.22(654→657)
S ₇	X ¹ A _g →2 ¹ A _g	490	0	0	0.000	0.65(652→657) + 0.18(656→658) – 0.17(651→657)
S ₈	X ¹ A _g →3 ¹ A _g	481	0	0	0.000	0.67(656→658) – 0.19(652→657)
S ₉	X ¹ A _g →3 ¹ B _{1u}	479	0.32	0	0.006	0.66(649→657) + 0.22(651→658)
S ₁₀	X ¹ A _g →3 ¹ B _{3g}	462	0	0.42	0.000	0.65(648→657) + 0.15(654→658) – 0.11(655→657) + 0.10(653→658)
S ₁₁	X ¹ A _g →2 ¹ B _{2u}	459	2.48	0	0.407	0.67(655→658) – 0.12[(654→657) + (653→657)]
S ₁₂	X ¹ A _g →4 ¹ B _{3g}	458	0	0	0.000	0.61(654→658) + 0.33(650→657) – 0.10(648→657)
S ₁₃	X ¹ A _g →3 ¹ B _{2u}	444	0.33	0	0.007	0.48(647→657) + 0.44(650→658) + 0.14(644→657)]
S ₁₄	X ¹ A _g →5 ¹ B _{3g}	443	0	7.29	0.000	0.62(653→658) – 0.23(656→660) + 0.14(655→657) – 0.11[(650→657) – (655→659)]
S ₁₅	X ¹ A _g →4 ¹ A _g	436	0	0	0.000	0.59(646→657) – 0.31(649→658) – 0.12(651→659)
S ₁₆	X ¹ A _g →4 ¹ B _{1u}	435	2.52	0	0.443	0.59(652→658) + 0.31(651→658) + 0.15(645→657)
S ₁₇	X ¹ A _g →5 ¹ B _{1u}	430	0.39	0	0.150	0.53(651→658) – 0.32(652→658) – 0.23(649→657) + 0.17(645→657) + 0.11(649→659)
S ₁₈	X ¹ A _g →6 ¹ B _{3g}	427	0	1.80	0.000	0.63(656→660) + 0.22(653→658) – 0.14(648→657)
S ₁₉	X ¹ A _g →4 ¹ B _{2u}	423	0.45	0	0.015	0.48[(647→657) – (650→658)] – 0.10(656→661)
S ₂₀	X ¹ A _g →6 ¹ B _{1u}	419	0.42	0	0.013	0.60(645→657) – 0.26(656→659) – 0.22(651→658)

S ₂₁	X ¹ A _g →5 ¹ B _{2u}	418	0.85	0	0.053	0.58(644→657) + 0.28(648→658) – 0.13(656→661) – – 0.11(647→657) – 0.10(650→658)
S ₂₂	X ¹ A _g →5 ¹ A _g	416	0	0	0.000	0.57(649→658) + 0.33(646→657) – 0.16(651→657)
S ₂₃	X ¹ A _g →7 ¹ B _{1u}	414	0.26	0	0.005	0.60(656→659) + 0.23(645→657) – 0.17(643→657) + + 0.11(655→660) – 0.10(646→658)
S ₂₄	X ¹ A _g →6 ¹ B _{2u}	409	0.24	0	0.005	0.59(656→661) – 0.21(652→660) + 0.18(648→658) – – 0.15(650→658) + 0.13(653→659)
S ₂₅	X ¹ A _g →8 ¹ B _{1u}	408	1.90	0	0.270	0.52(643→657) + 0.25(646→658) – 0.23(655→660) + + 0.20(656→659)
S ₂₆	X ¹ A _g →7 ¹ B _{2u}	406	1.15	0	0.100	0.54(648→658) – 0.32(644→657) – 0.19(656→661) + + 0.14(653→659) + 0.11(654→659) + 0.10(655→662)
S ₂₇	X ¹ A _g →7 ¹ B _{3g}	405	0	0.36	0.000	0.55(655→659) + 0.19[(647→658) – (642→657)] – – 0.16(640→657) + 0.14(650→659)
S ₂₈	X ¹ A _g →9 ¹ B _{1u}	400	2.57	0	0.501	0.62(655→660) + 0.23(643→657) + 0.12(653→661)
S ₂₉	X ¹ A _g →6 ¹ A _g	399	0	0	0.000	0.61(654→660) – 0.18(656→662) – 0.15(655→661) – – 0.13(641→657)
S ₃₀	X ¹ A _g →8 ¹ B _{3g}	398	0	2.26	0.000	0.35(642→657) – 0.32(647→658) + 0.29(656→663) + + 0.28(655→659) + 0.15(640→657)
Compound 5						
T ₁	X ¹ A _{1g} →1 ³ A _{2g}	674	0	0	0.000	0.62(1280→1281) + 0.21[(1278→1282) + + (1279→1283)]
T ₂₍₃₎	X ¹ A _{1g} →1 ³ E _{2u}	640	0	0	0.000	0.42(1278,1279→1281) + 0.37(1280→1282,1283) + + 0.25[(1279→1281) – (1278→1281)] + + 0.22[(1280→1283) – (1280→1282)]
S ₁	X ¹ A _{1g} →1 ¹ A _{2g}	641	0	15.61	0.000	0.67(1280→1281) + 0.15[(1278→1282) + + (1279→1283)]
S ₂₍₃₎	X ¹ A _{1g} →1 ¹ E _{2u}	569	5.73	0	1.757	0.62(1278,1279→1281) + 0.33(1280→1282,1283)]
S ₄₍₅₎	X ¹ A _{1g} →1 ¹ E _{1g}	568	0	10.00	0.000	0.60(1276,1277→1281) – 0.25[(1277→1281) + + (1276→1281)] + 0.14[(1272→1283) – – (1272→1282)] + 0.13[(1274→1283) – – (1274→1282) – (1275→1282,1283)]

μ_z – magnetic dipole moment along the x axis (β – Bohr magneton);

M_{xy} – electric dipole moment along the xy plane;

λ – wavelength;

f_{vac} – oscillator strength, calculating in the vacuum.

Table S2. Calculated parameters and assignment of the vertical electronic transitions in the electronic absorption spectrum of the **1D ribbons** at the B3LYP/3–21G Level

1D ribbons	State	Transition	λ , nm	M_x , a.u.	μ_z , β	f	Assignment (in vacuum approximation)
n = 2	T ₁	X ¹ A _g →1 ³ B _{1u}	446	0	0	0.000	0.60(173→177) + 0.29(174→178) – 0.10(175→180)
	T ₂	X ¹ A _g →1 ³ A _g	424	0	0	0.000	0.47(176→178) + 0.44(172→177) + 0.15(170→177)
	S ₁	X ¹ A _g →1 ¹ B _{2u}	433	3.40	0	0.809	0.69(176→177) + 0.14(175→179)
	S ₂	X ¹ A _g →1 ¹ B _{1u}	430	0.44	0	0.014	0.69(175→177) + 0.11(174→178) + 0.10(173→177)
	S ₃	X ¹ A _g →1 ¹ B _{3g}	394	0	4.03	0.000	0.68(174→177) + 0.13(175→178)
	S ₄	X ¹ A _g →2 ¹ B _{1u}	371	1.60	0	0.210	0.69(173→177)
	S ₅	X ¹ A _g →1 ¹ A _g	352	0	0	0.000	0.56(172→177) – 0.42(176→178)
	S ₆	X ¹ A _g →2 ¹ B _{2u}	349	0.93	0	0.076	0.69(171→177)
	S ₇	X ¹ A _g →2 ¹ A _g	346	0	0	0.000	0.56(176→178) + 0.38(172→177) – 0.17(170→177)
	S ₈	X ¹ A _g →2 ¹ B _{3g}	345	0	2.23	0.000	0.66(175→178) + 0.18(169→177) – 0.15(174→177)
	S ₉	X ¹ A _g →3 ¹ A _g	331	0	0	0.000	0.66(170→177) + 0.15(172→177) + 0.11(174→179)
	S ₁₀	X ¹ A _g →3 ¹ B _{3g}	317	0	0.27	0.000	0.66(169→177) + 0.15(173→178) – 0.19(175→178)
	S ₁₁	X ¹ A _g →3 ¹ B _{1u}	313	0.13	0	0.002	0.67(176→179) + 0.18(174→178)
	S ₁₂	X ¹ A _g →4 ¹ B _{1u}	309	1.48	0	0.215	0.66(174→178) – 0.16(176→179) – 0.11(175→177)
	S ₁₃	X ¹ A _g →3 ¹ B _{2u}	305	3.25	0	1.050	0.56(175→179) + 0.23(168→177) + 0.16(176→180) – 0.13(173→179) – 0.12[(176→177) – (172→178)]
S ₁₄	X ¹ A _g →4 ¹ B _{3g}	304	0	2.40	0.000	0.68(173→178) – 0.13(169→177)	
S ₁₅	X ¹ A _g →4 ¹ B _{2u}	298	1.08	0	0.119	0.63(168→177) – 0.17(176→180) – 0.21(175→179)	
n = 3	T ₁	X ¹ A _g →1 ³ A _g	491	0	0	0.000	0.52(258→261) + 0.44(260→262)
	T ₂	X ¹ A _g →1 ³ B _{3g}	467	0	0	0.000	0.48(256→261) – 0.30(255→262) – 0.24(257→262) + 0.18(259→263) – 0.16(256→263)
	S ₁	X ¹ A _g →1 ¹ B _{1u}	474	4.94	0	1.563	0.70(260→261)
	S ₂	X ¹ A _g →1 ¹ B _{3g}	443	0	0.13	0.000	0.69(259→261) + 0.13(257→262)
	S ₃	X ¹ A _g →1 ¹ B _{2u}	419	0.59	0	0.025	0.65(257→261) + 0.18(259→262) – 0.14(256→262)
	S ₄	X ¹ A _g →1 ¹ A _g	406	0	0	0.000	0.68(258→261) + 0.11(259→265)
	S ₅	X ¹ A _g →2 ¹ A _g	400	0	0	0.000	0.70(260→262)
	S ₆	X ¹ A _g →2 ¹ B _{3g}	394	0	4.99	0.000	0.65(256→261) – 0.21(257→262) – 0.10(255→262)
	S ₇	X ¹ A _g →2 ¹ B _{2u}	382	1.40	0	0.155	0.60(255→261) + 0.28(259→262) – 0.19(257→261)
	S ₈	X ¹ A _g →3 ¹ B _{2u}	372	0.99	0	0.079	0.60(259→262) – 0.32(255→261) – 0.13(257→263) – 0.12(257→261)
S ₉	X ¹ A _g →2 ¹ B _{3g}	363	0	1.99	0.000	0.62(257→262) + 0.23(256→261) – 0.15(259→263) – 0.11[(259→261) – (250→261)]	
S ₁₀	X ¹ A _g →4 ¹ B _{1u}	355	0.14	0	0.002	0.54(254→261) + 0.39(258→262) – 0.16(253→262)	
n = 4	T ₁	X ¹ A _g →1 ³ A _g	526	0	0	0.000	0.50(343→345) + 0.44(344→346) – 0.13(339→346)

	T ₂	X ¹ A _g →1 ³ B _{1u}	499	0	0	0.000	0.49(340→345) + 0.29(341→346) + 0.22(342→347) + 0.14(338→346)
	S ₁	X ¹ A _g →1 ¹ B _{2u}	498	6.16	0	2.320	0.69(344→345) + 0.12(343→346)
	S ₂	X ¹ A _g →1 ¹ B _{1u}	449	0.15	0	0.002	0.67(342→345) - 0.18(341→346)
	S ₃	X ¹ A _g →1 ¹ A _g	437	0	0.50	0.000	0.62(343→345) + 0.30(344→346)
	S ₄	X ¹ A _g →1 ¹ B _{3g}	432	0	0	0.000	0.63(341→345) - 0.25(342→346) + 0.12(340→346)
	S ₅	X ¹ A _g →2 ¹ A _g	430	0	0	0.000	0.63(344→346) - 0.31(343→345)
	S ₆	X ¹ A _g →2 ¹ B _{1u}	411	0.72	0	0.038	0.62(340→345) + 0.23(341→346) + 0.16(338→346)
	S ₇	X ¹ A _g →2 ¹ B _{2u}	397	2.00	0	0.306	0.53(343→346) - 0.42(339→345) + 0.11(342→351)
	S ₈	X ¹ A _g →2 ¹ B _{3g}	393	0	5.23	0.000	0.54(338→345) - 0.28(342→346) + 0.19[(340→346) - (341→345)] - 0.16(337→346) - 0.15(341→347)
	S ₉	X ¹ A _g →3 ¹ B _{2u}	390	1.24	0	0.121	0.53(339→345) - 0.16(344→347) + 0.41(343→346)
	S ₁₀	X ¹ A _g →3 ¹ B _{3g}	389	0	3.03	0.000	0.57(342→346) + 0.27(338→345) + 0.23(340→346)
n = 9	T ₁	X ¹ A _g →1 ³ A _g	540	0	0	0.000	0.34(761→765) - 0.33(762→766) + 0.28(764→768) - 0.31(764→768)
	T ₂	X ¹ A _g →1 ³ B _{1u}	517	0	0	0.000	0.30[(757→765) + (762→767) - (761→766)] - 0.27(763→768) - 0.23(764→769)
	S ₁	X ¹ A _g →1 ¹ B _{1u}	534	10.6	0	6.340	0.62(764→765) + 0.27(763→766) + 0.14(762→767)
	S ₂	X ¹ A _g →1 ¹ A _g	506	0	0	0.000	0.50(763→765) + 0.44(764→766) + 0.15(762→766)
	S ₃	X ¹ A _g →2 ¹ B _{1u}	479	3.11	0	0.612	0.45(763→766) + 0.41(762→765) + 0.29(764→767)
	S ₄	X ¹ A _g →2 ¹ A _g	473	0	0	0.000	0.50(764→766) - 0.44(763→765) + 0.14(763→767) - 0.12(762→766)
	S ₅	X ¹ A _g →3 ¹ B _{1u}	458	1.58	0	0.166	0.53(762→765) - 0.30(763→766) + 0.21(764→765) - 0.20(764→767) - 0.13(761→766)
	S ₆	X ¹ A _g →1 ¹ B _{3g}	456	0	0.20	0.000	0.54(760→765) - 0.28(759→766) + 0.23(758→765) - 0.18(758→767) + 0.12(756→766)
	S ₇	X ¹ A _g →3 ¹ A _g	455	0	0	0.000	0.47(762→766) - 0.30(761→765) + 0.35(763→767) - 0.15(764→768) - 0.10(763→765)
	S ₈	X ¹ A _g →4 ¹ B _{1u}	453	1.47	0	0.146	0.58(764→767) - 0.29(763→766) + 0.22(764→765) - 0.14(763→768)
	S ₉	X ¹ A _g →1 ¹ B _{2u}	452	0.09	0	0.001	0.46(759→765) - 0.40(760→766) + 0.16(759→767) - 0.18(756→765) + 0.12(758→766)
	S ₁₀	X ¹ A _g →2 ¹ B _{3g}	445	0	0.70	0.000	0.47(758→765) + 0.35(759→766) - 0.26(760→767) + 0.15(755→765) + 0.13(756→766)
n=16	T ₁	X ¹ A _g →1 ³ A _g	591	0	0	0.000	0.36(1352→1354) - 0.35(1351→1353) + 0.19(1351→1355) - 0.17(1350→1354) - 0.14(1350→1356) + 0.13(1349→1355) + 0.12(1349→1353) + 0.11(1349→1357)
	T ₂	X ¹ A _g →1 ³ B _{2u}	585	0	0	0.000	0.32(1350→1353) + 0.32(1353→1355) + 0.28(1351→1354) + 0.15(1351→1356) +

							$+ 0.14(1349 \rightarrow 1354) + 0.11[(1348 \rightarrow 1355) - (1350 \rightarrow 1357) + (1348 \rightarrow 1353)]$
S ₁	X ¹ A _g → 1 ¹ B _{2u}	543	14.7 6	0	12.18 9		$0.51(1352 \rightarrow 1353) - 0.32(1351 \rightarrow 1354) + 0.23(1350 \rightarrow 1355) - 0.16(1349 \rightarrow 1356) - 0.11(1348 \rightarrow 1357) + 0.10(1350 \rightarrow 1353)$
S ₂	X ¹ A _g → 1 ¹ A _g	530	4.06	0	0.000		$0.40[(1351 \rightarrow 1353) - (1352 \rightarrow 1354)] - 0.21(1351 \rightarrow 1355) + 0.19(1350 \rightarrow 1354) + 0.13(1350 \rightarrow 1356) - 0.12(1349 \rightarrow 1355)$
S ₃	X ¹ A _g → 2 ¹ B _{2u}	514	0	0	0.974		$0.38(1350 \rightarrow 1353) + 0.32(1351 \rightarrow 1354) + 0.35(1352 \rightarrow 1355) + 0.15(1349 \rightarrow 1354) + 0.14(1351 \rightarrow 1356) + 0.11[(1352 \rightarrow 1353) - (1350 \rightarrow 1355)]$
S ₄	X ¹ A _g → 2 ¹ A _g	499	0	0	0.000		$0.34(1349 \rightarrow 1353) + 0.33(1350 \rightarrow 1354) - 0.30(1351 \rightarrow 1355) - 0.28(1352 \rightarrow 1356) - 0.12(1348 \rightarrow 1354) - 0.11(1351 \rightarrow 1353)$
S ₅	X ¹ A _g → 3 ¹ B _{2u}	485	2.45	0	0.376		$0.33(1350 \rightarrow 1355) - 0.32(1349 \rightarrow 1354) + 0.33(1350 \rightarrow 1355) - 0.27(1351 \rightarrow 1356) - 0.21(1352 \rightarrow 1357) + 0.11(1351 \rightarrow 1354)$
S ₆	X ¹ A _g → 3 ¹ A _g	481	0	0	0.000		$0.43[(1352 \rightarrow 1354) + (1351 \rightarrow 1353)] + 0.21(1350 \rightarrow 1354) + 0.20(1351 \rightarrow 1355) - 0.11(1350 \rightarrow 1356) + 0.10(1349 \rightarrow 1355)$
S ₇	X ¹ A _g → 4 ¹ B _{2u}	476	0.86	0	0.047		$0.47(1350 \rightarrow 1353) - 0.37(1352 \rightarrow 1355) + 0.21(1349 \rightarrow 1354) - 0.19(1352 \rightarrow 1353) - 0.14(1351 \rightarrow 1354) - 0.13(1351 \rightarrow 1356) + 0.10(1348 \rightarrow 1355)$

μ_z – magnetic dipole moment along the z axis (β – Bohr magneton);

M_x – electric dipole moment along the x axis;

λ – wavelength;

f_{vac} – oscillator strength, calculating in a vacuum.

Table S3. Total energy of the ground singlet state ($^1A_{1g}$) of the compounds **1–5** at the B3LYP/6–21G(d) level of theory

Compounds	n	$E_{tot}, a.u.$
1	4	–4563.5596
2	9	–10032.3719
3	16	–17625.8718
4	8	–8970.0279
5	8	–17625.6829
1D ribbons	2	–2360.3252
	3	–3501.2146
	4	–4642.1048
	9	–10346.5556
	16	–18332.7859

The 6-21G(d) double-valence split basis set affords us to optimize all studied systems which consist at the most of 486 atoms (TOC ribbon, n=16). The extension of the chosen basis set prevents optimization of all studied molecules at the uniform level of accuracy. For comparison we have optimized the sheet **1** with the 6-311++G(d,p) basis. The calculated deviations in the structural parameters are negligible (no more than 0.002 Å for the bond lengths) and all conclusions remain. Thus, the choice of the 6-21G(d) basis set is quite justified by a very big size of the studied systems.

Table S4. The optimized Cartesian coordinates of the compound **1** calculated at the B3LYP/6–21G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.694016	6.648979	-0.210859
2	6	0.710768	7.636484	-0.088471
3	6	-0.710768	7.636484	0.088471
4	6	-1.694016	6.648979	0.210859
5	6	-1.701891	5.216925	0.211839
6	6	-0.710724	4.218849	0.088466
7	6	0.710724	4.218849	-0.088466
8	6	1.701891	5.216925	-0.211839
9	6	1.091836	2.877940	-0.135904
10	6	-1.091836	2.877940	0.135904
11	6	-3.034449	4.839613	0.377706
12	6	-3.031207	7.048413	0.377302
13	6	-1.099016	8.986043	0.136797
14	6	1.099016	8.986043	-0.136797
15	6	3.031207	7.048413	-0.377302
16	6	3.034449	4.839613	-0.377706
17	8	0.000000	2.041179	0.000000
18	8	-3.864006	5.940194	0.480963
19	6	-3.419942	8.392929	0.425689
20	6	-2.433238	9.382426	0.302871
21	8	0.000000	9.824002	0.000000
22	6	2.433238	9.382426	-0.302871
23	6	3.419942	8.392929	-0.425689
24	8	3.864006	5.940194	-0.480963
25	1	-4.463562	8.663949	0.555591
26	1	-2.698177	10.435146	0.335849
27	1	2.698177	10.435146	-0.335849
28	1	4.463562	8.663949	-0.555591
29	6	-4.186542	0.716209	0.521110
30	6	-5.176974	1.715024	0.644391
31	6	-6.598062	1.707089	0.821278
32	6	-7.578005	0.716253	0.943254
33	6	-7.578005	-0.716253	0.943254
34	6	-6.598062	-1.707089	0.821278
35	6	-5.176974	-1.715024	0.644391
36	6	-4.186542	-0.716209	0.521110
37	6	-4.802552	-3.057866	0.597786
38	6	-6.994438	-3.054599	0.870616
39	6	-8.917229	-1.107497	1.109951
40	6	-8.917229	1.107497	1.109951
41	6	-6.994438	3.054599	0.870616
42	6	-4.802552	3.057866	0.597786
43	6	-2.855901	1.100261	0.355481
44	6	-2.855901	-1.100261	0.355481
45	6	-3.459239	-3.485933	0.430580
46	8	-5.894705	-3.893825	0.733729
47	6	-8.328658	-3.446334	1.036690
48	6	-9.310577	-2.452015	1.158912
49	8	-9.748772	0.000000	1.213455
50	6	-9.310577	2.452015	1.158912
51	6	-8.328658	3.446334	1.036690
52	8	-5.894705	3.893825	0.733729
53	6	-3.459239	3.485933	0.430580
54	6	-2.433819	2.452601	0.302944
55	8	-2.025548	0.000000	0.252125
56	1	-8.597602	-4.498008	1.070166
57	1	-10.355235	-2.718999	1.288943
58	1	-10.355235	2.718999	1.288943
59	1	-8.597602	4.498008	1.070166
60	6	7.578005	0.716253	-0.943254
61	6	6.598062	1.707089	-0.821278
62	6	5.176974	1.715024	-0.644391
63	6	4.186542	0.716209	-0.521110
64	6	4.186542	-0.716209	-0.521110
65	6	5.176974	-1.715024	-0.644391
66	6	6.598062	-1.707089	-0.821278
67	6	7.578005	-0.716253	-0.943254
68	6	6.994438	-3.054599	-0.870616
69	6	4.802552	-3.057866	-0.597786
70	6	2.855901	-1.100261	-0.355481

71	6	2.855901	1.100261	-0.355481
72	6	4.802552	3.057866	-0.597786
73	6	6.994438	3.054599	-0.870616
74	6	8.917229	1.107497	-1.109951
75	6	8.917229	-1.107497	-1.109951
76	6	9.310577	-2.452015	-1.158912
77	6	8.328658	-3.446334	-1.036690
78	8	5.894705	-3.893825	-0.733729
79	8	2.025548	0.000000	-0.252125
80	6	2.433819	2.452601	-0.302944
81	6	3.459239	3.485933	-0.430580
82	8	5.894705	3.893825	-0.733729
83	6	8.328658	3.446334	-1.036690
84	6	9.310577	2.452015	-1.158912
85	8	9.748772	0.000000	-1.213455
86	1	10.355235	-2.718999	-1.288943
87	1	8.597602	-4.498008	-1.070166
88	1	8.597602	4.498008	-1.070166
89	1	10.355235	2.718999	-1.288943
90	6	1.701891	-5.216925	-0.211839
91	6	0.710724	-4.218849	-0.088466
92	6	-0.710724	-4.218849	0.088466
93	6	-1.701891	-5.216925	0.211839
94	6	-1.694016	-6.648979	0.210859
95	6	-0.710768	-7.636484	0.088471
96	6	0.710768	-7.636484	-0.088471
97	6	1.694016	-6.648979	-0.210859
98	6	1.099016	-8.986043	-0.136797
99	6	-1.099016	-8.986043	0.136797
100	6	-3.031207	-7.048413	0.377302
101	6	-3.034449	-4.839613	0.377706
102	6	-1.091836	-2.877940	0.135904
103	6	1.091836	-2.877940	-0.135904
104	6	3.034449	-4.839613	-0.377706
105	6	3.031207	-7.048413	-0.377302
106	6	3.419942	-8.392929	-0.425689
107	6	2.433238	-9.382426	-0.302871
108	8	0.000000	-9.824002	0.000000
109	6	-2.433238	-9.382426	0.302871
110	6	-3.419942	-8.392929	0.425689
111	8	-3.864006	-5.940194	0.480963
112	6	-2.433819	-2.452601	0.302944
113	8	0.000000	-2.041179	0.000000
114	6	2.433819	-2.452601	-0.302944
115	6	3.459239	-3.485933	-0.430580
116	8	3.864006	-5.940194	-0.480963
117	1	4.463562	-8.663949	-0.555591
118	1	2.698177	-10.435146	-0.335849
119	1	-2.698177	-10.435146	0.335849
120	1	-4.463562	-8.663949	0.555591

Table S5. The optimized Cartesian coordinates of the compound **2** calculated at the B3LYP/6–21G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.924107	-10.003018	0.000000
2	6	1.410224	-8.624757	0.000000
3	6	8.827468	-12.755952	0.000000
4	6	7.822022	-0.933115	0.000000
5	6	9.153432	-1.402683	0.000000
6	6	9.763634	-2.697780	0.000000
7	6	9.298132	-4.018868	0.000000
8	6	8.010836	-4.645358	0.000000
9	6	6.679156	-4.176554	0.000000
10	6	6.061720	-2.885277	0.000000
11	6	6.531483	-1.552094	0.000000
12	6	4.685914	-3.117717	0.000000
13	6	5.635866	-5.102422	0.000000
14	6	8.249724	-6.019677	0.000000
15	6	10.240284	-5.062191	0.000000
16	6	11.151720	-2.475545	0.000000
17	6	10.201099	-0.481697	0.000000
18	6	7.589605	0.442264	0.000000
19	6	5.605298	-0.508518	0.000000
20	6	4.201355	-0.706399	0.000000
21	6	3.716142	-2.083428	0.000000
22	8	4.406313	-4.470763	0.000000
23	8	9.603804	-6.297215	0.000000
24	6	11.623120	-4.838943	0.000000
25	6	12.089146	-3.516366	0.000000
26	8	11.430059	-1.114326	0.000000
27	6	10.003018	0.924107	0.000000
28	6	8.624757	1.410224	0.000000
29	8	6.235670	0.720930	0.000000
30	6	5.031619	-8.848279	0.000000
31	6	6.364144	-9.316983	0.000000
32	6	6.975307	-10.612120	0.000000
33	6	6.507781	-11.930832	0.000000
34	6	5.215734	-12.549585	0.000000
35	6	3.895229	-12.087150	0.000000
36	6	3.269310	-10.799079	0.000000
37	6	3.739486	-9.467073	0.000000
38	6	1.895413	-11.038951	0.000000
39	6	2.852568	-13.029531	0.000000
40	6	5.445732	-13.935650	0.000000
41	6	7.443491	-12.978936	0.000000
42	6	8.363157	-10.390546	0.000000
43	6	7.412312	-8.396943	0.000000
44	6	2.814086	-8.423746	0.000000
45	8	1.617039	-12.392760	0.000000
46	6	3.080216	-14.411471	0.000000
47	6	4.404402	-14.874130	0.000000
48	8	6.806553	-14.213080	0.000000
49	6	9.297127	-11.434232	0.000000
50	8	8.641585	-9.028750	0.000000
51	6	7.214112	-6.990775	0.000000
52	8	3.444995	-7.193655	0.000000
53	1	2.248976	-15.110253	0.000000
54	1	4.618497	-15.938770	0.000000
55	6	14.411471	3.080216	0.000000
56	6	10.612120	6.975307	0.000000
57	6	11.930832	6.507781	0.000000
58	6	12.549585	5.215734	0.000000
59	6	12.087150	3.895229	0.000000
60	6	10.799079	3.269310	0.000000
61	6	9.467073	3.739486	0.000000
62	6	8.848279	5.031619	0.000000
63	6	9.316983	6.364144	0.000000
64	6	7.473241	4.798879	0.000000
65	6	8.423746	2.814086	0.000000
66	6	11.038951	1.895413	0.000000
67	6	13.029531	2.852568	0.000000
68	6	13.935650	5.445732	0.000000
69	6	12.978936	7.443491	0.000000
70	6	10.390546	8.363157	0.000000

71	6	8.396943	7.412312	0.000000
72	6	6.990775	7.214112	0.000000
73	6	6.505493	5.835556	0.000000
74	8	7.193655	3.444995	0.000000
75	8	12.392760	1.617039	0.000000
76	6	14.874130	4.404402	0.000000
77	8	14.213080	6.806553	0.000000
78	6	12.755952	8.827468	0.000000
79	6	11.434232	9.297127	0.000000
80	8	9.028750	8.641585	0.000000
81	6	4.798879	-7.473241	0.000000
82	6	5.835556	-6.505493	0.000000
83	6	-0.095447	1.855655	0.000000
84	6	1.237656	1.385920	0.000000
85	6	1.855655	0.095447	0.000000
86	6	1.385920	-1.237656	0.000000
87	6	0.095447	-1.855655	0.000000
88	6	-1.237656	-1.385920	0.000000
89	6	-1.855655	-0.095447	0.000000
90	6	-1.385920	1.237656	0.000000
91	6	-3.231811	-0.327721	0.000000
92	6	-2.281321	-2.312483	0.000000
93	6	0.327721	-3.231811	0.000000
94	6	2.312483	-2.281321	0.000000
95	6	3.231811	0.327721	0.000000
96	6	2.281321	2.312483	0.000000
97	6	-0.327721	3.231811	0.000000
98	6	-2.312483	2.281321	0.000000
99	8	-3.510433	-1.681124	0.000000
100	8	1.681124	-3.510433	0.000000
101	8	3.510433	1.681124	0.000000
102	8	-1.681124	3.510433	0.000000
103	6	-2.885277	-6.061720	0.000000
104	6	-1.552094	-6.531483	0.000000
105	6	-0.933115	-7.822022	0.000000
106	6	-1.402683	-9.153432	0.000000
107	6	-2.697780	-9.763634	0.000000
108	6	-4.018868	-9.298132	0.000000
109	6	-4.645358	-8.010836	0.000000
110	6	-4.176554	-6.679156	0.000000
111	6	-6.019677	-8.249724	0.000000
112	6	-5.062191	-10.240284	0.000000
113	6	-2.475545	-11.151720	0.000000
114	6	-0.481697	-10.201099	0.000000
115	6	0.442264	-7.589605	0.000000
116	6	-0.508518	-5.605298	0.000000
117	6	-3.117717	-4.685914	0.000000
118	6	-5.102422	-5.635866	0.000000
119	6	-6.990775	-7.214112	0.000000
120	8	-6.297215	-9.603804	0.000000
121	6	-4.838943	-11.623120	0.000000
122	6	-3.516366	-12.089146	0.000000
123	8	-1.114326	-11.430059	0.000000
124	8	0.720930	-6.235670	0.000000
125	6	-0.706399	-4.201355	0.000000
126	6	-2.083428	-3.716142	0.000000
127	8	-4.470763	-4.406313	0.000000
128	1	-5.672531	-12.318998	0.000000
129	1	-3.303151	-13.153879	0.000000
130	6	-8.010836	4.645358	0.000000
131	6	-6.679156	4.176554	0.000000
132	6	-6.061720	2.885277	0.000000
133	6	-6.531483	1.552094	0.000000
134	6	-7.822022	0.933115	0.000000
135	6	-9.153432	1.402683	0.000000
136	6	-9.763634	2.697780	0.000000
137	6	-9.298132	4.018868	0.000000
138	6	-11.151720	2.475545	0.000000
139	6	-10.201099	0.481697	0.000000
140	6	-7.589605	-0.442264	0.000000
141	6	-5.605298	0.508518	0.000000
142	6	-4.685914	3.117717	0.000000
143	6	-5.635866	5.102422	0.000000
144	6	-8.249724	6.019677	0.000000
145	6	-10.240284	5.062191	0.000000
146	6	-11.623120	4.838943	0.000000
147	6	-12.089146	3.516366	0.000000
148	8	-11.430059	1.114326	0.000000
149	8	-6.235670	-0.720930	0.000000

150	6	-4.201355	0.706399	0.000000
151	6	-3.716142	2.083428	0.000000
152	8	-4.406313	4.470763	0.000000
153	6	-5.835556	6.505493	0.000000
154	6	-7.214112	6.990775	0.000000
155	8	-9.603804	6.297215	0.000000
156	1	-12.318998	5.672531	0.000000
157	1	-13.153879	3.303151	0.000000
158	6	-10.799079	-3.269310	0.000000
159	6	-9.467073	-3.739486	0.000000
160	6	-8.848279	-5.031619	0.000000
161	6	-9.316983	-6.364144	0.000000
162	6	-10.612120	-6.975307	0.000000
163	6	-11.930832	-6.507781	0.000000
164	6	-12.549585	-5.215734	0.000000
165	6	-12.087150	-3.895229	0.000000
166	6	-13.935650	-5.445732	0.000000
167	6	-12.978936	-7.443491	0.000000
168	6	-10.390546	-8.363157	0.000000
169	6	-8.396943	-7.412312	0.000000
170	6	-7.473241	-4.798879	0.000000
171	6	-8.423746	-2.814086	0.000000
172	6	-13.029531	-2.852568	0.000000
173	6	-14.411471	-3.080216	0.000000
174	6	-14.874130	-4.404402	0.000000
175	8	-14.213080	-6.806553	0.000000
176	6	-12.755952	-8.827468	0.000000
177	6	-11.434232	-9.297127	0.000000
178	8	-9.028750	-8.641585	0.000000
179	6	-6.505493	-5.835556	0.000000
180	8	-7.193655	-3.444995	0.000000
181	6	-8.624757	-1.410224	0.000000
182	8	-12.392760	-1.617039	0.000000
183	1	-15.110253	-2.248976	0.000000
184	1	-15.938770	-4.618497	0.000000
185	1	-13.590168	-9.522722	0.000000
186	1	-11.224666	-10.362649	0.000000
187	6	2.697780	9.763634	0.000000
188	6	4.018868	9.298132	0.000000
189	6	4.645358	8.010836	0.000000
190	6	4.176554	6.679156	0.000000
191	6	2.885277	6.061720	0.000000
192	6	1.552094	6.531483	0.000000
193	6	0.933115	7.822022	0.000000
194	6	1.402683	9.153432	0.000000
195	6	-0.442264	7.589605	0.000000
196	6	0.508518	5.605298	0.000000
197	6	3.117717	4.685914	0.000000
198	6	5.102422	5.635866	0.000000
199	6	6.019677	8.249724	0.000000
200	6	5.062191	10.240284	0.000000
201	6	2.475545	11.151720	0.000000
202	6	0.481697	10.201099	0.000000
203	6	-1.410224	8.624757	0.000000
204	8	-0.720930	6.235670	0.000000
205	6	0.706399	4.201355	0.000000
206	6	2.083428	3.716142	0.000000
207	8	4.470763	4.406313	0.000000
208	8	6.297215	9.603804	0.000000
209	6	4.838943	11.623120	0.000000
210	6	3.516366	12.089146	0.000000
211	8	1.114326	11.430059	0.000000
212	6	-5.215734	12.549585	0.000000
213	6	-3.895229	12.087150	0.000000
214	6	-3.269310	10.799079	0.000000
215	6	-3.739486	9.467073	0.000000
216	6	-5.031619	8.848279	0.000000
217	6	-6.364144	9.316983	0.000000
218	6	-6.975307	10.612120	0.000000
219	6	-6.507781	11.930832	0.000000
220	6	-8.363157	10.390546	0.000000
221	6	-7.412312	8.396943	0.000000
222	6	-4.798879	7.473241	0.000000
223	6	-2.814086	8.423746	0.000000
224	6	-1.895413	11.038951	0.000000
225	6	-2.852568	13.029531	0.000000
226	6	-5.445732	13.935650	0.000000
227	6	-7.443491	12.978936	0.000000
228	6	-8.827468	12.755952	0.000000

229	6	-9.297127	11.434232	0.000000
230	8	-8.641585	9.028750	0.000000
231	8	-3.444995	7.193655	0.000000
232	6	-0.924107	10.003018	0.000000
233	8	-1.617039	12.392760	0.000000
234	6	-3.080216	14.411471	0.000000
235	6	-4.404402	14.874130	0.000000
236	8	-6.806553	14.213080	0.000000
237	1	-9.522722	13.590168	0.000000
238	1	-10.362649	11.224666	0.000000
239	6	-11.038951	-1.895413	0.000000
240	6	-10.003018	-0.924107	0.000000
241	1	9.522722	-13.590168	0.000000
242	1	12.318998	-5.672531	0.000000
243	1	13.153879	-3.303151	0.000000
244	1	10.362649	-11.224666	0.000000
245	1	15.110253	2.248976	0.000000
246	1	15.938770	4.618497	0.000000
247	1	13.590168	9.522722	0.000000
248	1	11.224666	10.362649	0.000000
249	1	5.672531	12.318998	0.000000
250	1	3.303151	13.153879	0.000000
251	1	-2.248976	15.110253	0.000000
252	1	-4.618497	15.938770	0.000000

Table S6. The optimized Cartesian coordinates of the compound **3** calculated at the B3LYP/6–21G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	11.604488	6.550636	0.000000
2	6	10.331516	5.832054	0.000000
3	6	-3.685459	11.567329	0.000000
4	6	-4.379333	12.797086	0.000000
5	6	-3.986314	14.173761	0.000000
6	6	-2.766135	14.862077	0.000000
7	6	-1.384554	14.486675	0.000000
8	6	-0.690222	13.257433	0.000000
9	6	-1.075064	11.878820	0.000000
10	6	-2.306218	11.184148	0.000000
11	6	0.114055	11.148483	0.000000
12	6	0.704715	13.268120	0.000000
13	6	-0.660025	15.678895	0.000000
14	6	-2.788901	16.267694	0.000000
15	6	-5.177615	14.920107	0.000000
16	6	-5.774460	12.793386	0.000000
17	6	-4.415448	10.378737	0.000000
18	6	-2.295563	9.788670	0.000000
19	8	1.214702	11.983305	0.000000
20	8	-1.496885	16.778607	0.000000
21	6	-3.977037	17.009614	0.000000
22	6	-5.198282	16.320706	0.000000
23	8	-6.283100	14.078276	0.000000
24	8	-3.579296	9.278024	0.000000
25	1	-3.952274	18.095221	0.000000
26	1	-6.140263	16.860944	0.000000
27	6	3.624405	15.691150	0.000000
28	6	2.929483	16.920722	0.000000
29	6	3.321346	18.298135	0.000000
30	6	4.541022	18.983641	0.000000
31	6	5.921015	18.599492	0.000000
32	6	6.611058	17.382376	0.000000
33	6	6.234845	16.000607	0.000000
34	6	5.004555	15.306957	0.000000
35	6	7.427451	15.277301	0.000000
36	6	8.016195	17.406085	0.000000
37	6	6.659776	19.794625	0.000000
38	6	4.526048	20.388592	0.000000
39	6	2.130566	19.044471	0.000000
40	6	1.534682	16.917675	0.000000
41	6	2.894850	14.502589	0.000000
42	6	5.015043	13.912390	0.000000
43	6	7.477263	13.858213	0.000000
44	8	8.527556	16.113420	0.000000
45	6	8.754109	18.596492	0.000000
46	6	8.061477	19.816072	0.000000
47	8	5.817592	20.898735	0.000000
48	6	3.337042	21.131216	0.000000
49	6	2.113875	20.444938	0.000000
50	8	1.024834	18.201957	0.000000
51	6	0.758789	15.728438	0.000000
52	6	1.477596	14.455907	0.000000
53	8	3.730522	13.401281	0.000000
54	1	9.839876	18.575709	0.000000
55	1	8.600809	20.758662	0.000000
56	1	3.362322	22.216903	0.000000
57	1	1.173540	20.988162	0.000000
58	6	0.442805	4.258123	0.000000
59	6	-0.251937	5.488822	0.000000
60	6	0.131645	6.867022	0.000000
61	6	1.362370	7.561549	0.000000
62	6	2.740651	7.177876	0.000000
63	6	3.435492	5.947328	0.000000
64	6	3.051783	4.569163	0.000000
65	6	1.821065	3.874456	0.000000
66	6	4.240871	3.838613	0.000000
67	6	4.831147	5.958276	0.000000
68	6	3.471382	8.366865	0.000000
69	6	1.351097	8.957090	0.000000
70	6	-1.057609	7.597532	0.000000

71	6	-1.647469	5.477754	0.000000
72	6	-0.287747	3.069107	0.000000
73	6	1.832172	2.478984	0.000000
74	6	3.019132	1.704275	0.000000
75	6	4.290651	2.422037	0.000000
76	8	5.340871	4.674159	0.000000
77	8	2.635323	9.466960	0.000000
78	6	0.163810	9.731646	0.000000
79	6	-1.107827	9.014074	0.000000
80	8	-2.157523	6.761491	0.000000
81	6	-2.422037	4.290651	0.000000
82	6	-1.704275	3.019132	0.000000
83	8	0.548102	1.968964	0.000000
84	6	7.753373	8.383854	0.000000
85	6	7.058240	9.614748	0.000000
86	6	7.441084	10.993917	0.000000
87	6	8.670698	11.687589	0.000000
88	6	10.047530	11.295130	0.000000
89	6	10.736552	10.075349	0.000000
90	6	10.361710	8.693614	0.000000
91	6	9.132222	7.999264	0.000000
92	6	11.554259	7.969581	0.000000
93	6	12.142141	10.098797	0.000000
94	6	10.793307	12.486807	0.000000
95	6	8.666403	13.082692	0.000000
96	6	6.252308	11.723833	0.000000
97	6	5.662791	9.603878	0.000000
98	6	9.143066	6.604446	0.000000
99	8	12.653644	8.806844	0.000000
100	6	12.883527	11.287263	0.000000
101	6	12.193900	12.508101	0.000000
102	8	9.951117	13.591821	0.000000
103	6	6.204326	13.140125	0.000000
104	8	5.151810	10.887331	0.000000
105	6	4.888110	8.416540	0.000000
106	8	7.858441	6.094095	0.000000
107	1	13.969160	11.263073	0.000000
108	1	12.733634	13.450356	0.000000
109	6	-18.298135	3.321346	0.000000
110	6	-18.983641	4.541022	0.000000
111	6	-18.599492	5.921015	0.000000
112	6	-17.382376	6.611058	0.000000
113	6	-16.000607	6.234845	0.000000
114	6	-15.306957	5.004555	0.000000
115	6	-15.691150	3.624405	0.000000
116	6	-16.920722	2.929483	0.000000
117	6	-14.502589	2.894850	0.000000
118	6	-13.912390	5.015043	0.000000
119	6	-15.277301	7.427451	0.000000
120	6	-17.406085	8.016195	0.000000
121	6	-19.794625	6.659776	0.000000
122	6	-20.388592	4.526048	0.000000
123	6	-19.044471	2.130566	0.000000
124	6	-16.917675	1.534682	0.000000
125	8	-13.401281	3.730522	0.000000
126	8	-16.113420	8.527556	0.000000
127	6	-18.596492	8.754109	0.000000
128	6	-19.816072	8.061477	0.000000
129	8	-20.898735	5.817592	0.000000
130	6	-21.131216	3.337042	0.000000
131	6	-20.444938	2.113875	0.000000
132	8	-18.201957	1.024834	0.000000
133	1	-18.575709	9.839876	0.000000
134	1	-20.758662	8.600809	0.000000
135	1	-22.216903	3.362322	0.000000
136	1	-20.988162	1.173540	0.000000
137	6	-10.993917	7.441084	0.000000
138	6	-11.687589	8.670698	0.000000
139	6	-11.295130	10.047530	0.000000
140	6	-10.075349	10.736552	0.000000
141	6	-8.693614	10.361710	0.000000
142	6	-7.999264	9.132222	0.000000
143	6	-8.383854	7.753373	0.000000
144	6	-9.614748	7.058240	0.000000
145	6	-7.194600	7.023205	0.000000
146	6	-6.604446	9.143066	0.000000
147	6	-7.969581	11.554259	0.000000
148	6	-10.098797	12.142141	0.000000
149	6	-12.486807	10.793307	0.000000

150	6	-13.082692	8.666403	0.000000
151	6	-11.723833	6.252308	0.000000
152	6	-9.603878	5.662791	0.000000
153	6	-7.145122	5.606071	0.000000
154	8	-6.094095	7.858441	0.000000
155	6	-5.832054	10.331516	0.000000
156	6	-6.550636	11.604488	0.000000
157	8	-8.806844	12.653644	0.000000
158	6	-11.287263	12.883527	0.000000
159	6	-12.508101	12.193900	0.000000
160	8	-13.591821	9.951117	0.000000
161	6	-13.858213	7.477263	0.000000
162	6	-13.140125	6.204326	0.000000
163	8	-10.887331	5.151810	0.000000
164	1	-11.263073	13.969160	0.000000
165	1	-13.450356	12.733634	0.000000
166	6	-14.173761	-3.986314	0.000000
167	6	-14.862077	-2.766135	0.000000
168	6	-14.486675	-1.384554	0.000000
169	6	-13.257433	-0.690222	0.000000
170	6	-11.878820	-1.075064	0.000000
171	6	-11.184148	-2.306218	0.000000
172	6	-11.567329	-3.685459	0.000000
173	6	-12.797086	-4.379333	0.000000
174	6	-10.378737	-4.415448	0.000000
175	6	-9.788670	-2.295563	0.000000
176	6	-11.148483	0.114055	0.000000
177	6	-13.268120	0.704715	0.000000
178	6	-15.678895	-0.660025	0.000000
179	6	-16.267694	-2.788901	0.000000
180	6	-14.920107	-5.177615	0.000000
181	6	-12.793386	-5.774460	0.000000
182	8	-9.278024	-3.579296	0.000000
183	8	-11.983305	1.214702	0.000000
184	6	-14.455907	1.477596	0.000000
185	6	-15.728438	0.758789	0.000000
186	8	-16.778607	-1.496885	0.000000
187	6	-17.009614	-3.977037	0.000000
188	6	-16.320706	-5.198282	0.000000
189	8	-14.078276	-6.283100	0.000000
190	1	-18.095221	-3.952274	0.000000
191	1	-16.860944	-6.140263	0.000000
192	6	-6.867022	0.131645	0.000000
193	6	-7.561549	1.362370	0.000000
194	6	-7.177876	2.740651	0.000000
195	6	-5.947328	3.435492	0.000000
196	6	-4.569163	3.051783	0.000000
197	6	-3.874456	1.821065	0.000000
198	6	-4.258123	0.442805	0.000000
199	6	-5.488822	-0.251937	0.000000
200	6	-3.069107	-0.287747	0.000000
201	6	-2.478984	1.832172	0.000000
202	6	-3.838613	4.240871	0.000000
203	6	-5.958276	4.831147	0.000000
204	6	-8.366865	3.471382	0.000000
205	6	-8.957090	1.351097	0.000000
206	6	-7.597532	-1.057609	0.000000
207	6	-5.477754	-1.647469	0.000000
208	6	-4.290651	-2.422037	0.000000
209	6	-3.019132	-1.704275	0.000000
210	8	-1.968964	0.548102	0.000000
211	8	-4.674159	5.340871	0.000000
212	6	-8.416540	4.888110	0.000000
213	8	-9.466960	2.635323	0.000000
214	6	-9.731646	0.163810	0.000000
215	6	-9.014074	-1.107827	0.000000
216	8	-6.761491	-2.157523	0.000000
217	6	7.023205	7.194600	0.000000
218	6	5.606071	7.145122	0.000000
219	6	4.569163	-3.051783	0.000000
220	6	3.874456	-1.821065	0.000000
221	6	4.258123	-0.442805	0.000000
222	6	5.488822	0.251937	0.000000
223	6	6.867022	-0.131645	0.000000
224	6	7.561549	-1.362370	0.000000
225	6	7.177876	-2.740651	0.000000
226	6	5.947328	-3.435492	0.000000
227	6	8.366865	-3.471382	0.000000
228	6	8.957090	-1.351097	0.000000

229	6	7.597532	1.057609	0.000000
230	6	5.477754	1.647469	0.000000
231	6	3.069107	0.287747	0.000000
232	6	2.478984	-1.832172	0.000000
233	6	3.838613	-4.240871	0.000000
234	6	5.958276	-4.831147	0.000000
235	8	9.466960	-2.635323	0.000000
236	8	6.761491	2.157523	0.000000
237	8	1.968964	-0.548102	0.000000
238	8	4.674159	-5.340871	0.000000
239	6	11.878820	1.075064	0.000000
240	6	11.184148	2.306218	0.000000
241	6	11.567329	3.685459	0.000000
242	6	12.797086	4.379333	0.000000
243	6	14.173761	3.986314	0.000000
244	6	14.862077	2.766135	0.000000
245	6	14.486675	1.384554	0.000000
246	6	13.257433	0.690222	0.000000
247	6	15.678895	0.660025	0.000000
248	6	16.267694	2.788901	0.000000
249	6	14.920107	5.177615	0.000000
250	6	12.793386	5.774460	0.000000
251	6	10.378737	4.415448	0.000000
252	6	9.788670	2.295563	0.000000
253	6	11.148483	-0.114055	0.000000
254	6	13.268120	-0.704715	0.000000
255	6	15.728438	-0.758789	0.000000
256	8	16.778607	1.496885	0.000000
257	6	17.009614	3.977037	0.000000
258	6	16.320706	5.198282	0.000000
259	8	14.078276	6.283100	0.000000
260	8	9.278024	3.579296	0.000000
261	6	9.014074	1.107827	0.000000
262	6	9.731646	-0.163810	0.000000
263	8	11.983305	-1.214702	0.000000
264	1	18.095221	3.952274	0.000000
265	1	16.860944	6.140263	0.000000
266	6	8.693614	-10.361710	0.000000
267	6	7.999264	-9.132222	0.000000
268	6	8.383854	-7.753373	0.000000
269	6	9.614748	-7.058240	0.000000
270	6	10.993917	-7.441084	0.000000
271	6	11.687589	-8.670698	0.000000
272	6	11.295130	-10.047530	0.000000
273	6	10.075349	-10.736552	0.000000
274	6	12.486807	-10.793307	0.000000
275	6	13.082692	-8.666403	0.000000
276	6	11.723833	-6.252308	0.000000
277	6	9.603878	-5.662791	0.000000
278	6	7.194600	-7.023205	0.000000
279	6	6.604446	-9.143066	0.000000
280	6	7.969581	-11.554259	0.000000
281	6	10.098797	-12.142141	0.000000
282	6	11.287263	-12.883527	0.000000
283	6	12.508101	-12.193900	0.000000
284	8	13.591821	-9.951117	0.000000
285	8	10.887331	-5.151810	0.000000
286	6	8.416540	-4.888110	0.000000
287	6	7.145122	-5.606071	0.000000
288	8	6.094095	-7.858441	0.000000
289	6	5.832054	-10.331516	0.000000
290	6	6.550636	-11.604488	0.000000
291	8	8.806844	-12.653644	0.000000
292	1	11.263073	-13.969160	0.000000
293	1	13.450356	-12.733634	0.000000
294	6	16.000607	-6.234845	0.000000
295	6	15.306957	-5.004555	0.000000
296	6	15.691150	-3.624405	0.000000
297	6	16.920722	-2.929483	0.000000
298	6	18.298135	-3.321346	0.000000
299	6	18.983641	-4.541022	0.000000
300	6	18.599492	-5.921015	0.000000
301	6	17.382376	-6.611058	0.000000
302	6	19.794625	-6.659776	0.000000
303	6	20.388592	-4.526048	0.000000
304	6	19.044471	-2.130566	0.000000
305	6	16.917675	-1.534682	0.000000
306	6	14.502589	-2.894850	0.000000
307	6	13.912390	-5.015043	0.000000

308	6	17.406085	-8.016195	0.000000
309	6	18.596492	-8.754109	0.000000
310	6	19.816072	-8.061477	0.000000
311	8	20.898735	-5.817592	0.000000
312	6	21.131216	-3.337042	0.000000
313	6	20.444938	-2.113875	0.000000
314	8	18.201957	-1.024834	0.000000
315	6	14.455907	-1.477596	0.000000
316	8	13.401281	-3.730522	0.000000
317	6	13.140125	-6.204326	0.000000
318	8	16.113420	-8.527556	0.000000
319	1	18.575709	-9.839876	0.000000
320	1	20.758662	-8.600809	0.000000
321	1	22.216903	-3.362322	0.000000
322	1	20.988162	-1.173540	0.000000
323	6	-10.047530	-11.295130	0.000000
324	6	-10.736552	-10.075349	0.000000
325	6	-10.361710	-8.693614	0.000000
326	6	-9.132222	-7.999264	0.000000
327	6	-7.753373	-8.383854	0.000000
328	6	-7.058240	-9.614748	0.000000
329	6	-7.441084	-10.993917	0.000000
330	6	-8.670698	-11.687589	0.000000
331	6	-6.252308	-11.723833	0.000000
332	6	-5.662791	-9.603878	0.000000
333	6	-7.023205	-7.194600	0.000000
334	6	-9.143066	-6.604446	0.000000
335	6	-11.554259	-7.969581	0.000000
336	6	-12.142141	-10.098797	0.000000
337	6	-10.793307	-12.486807	0.000000
338	6	-8.666403	-13.082692	0.000000
339	8	-5.151810	-10.887331	0.000000
340	8	-7.858441	-6.094095	0.000000
341	6	-10.331516	-5.832054	0.000000
342	6	-11.604488	-6.550636	0.000000
343	8	-12.653644	-8.806844	0.000000
344	6	-12.883527	-11.287263	0.000000
345	6	-12.193900	-12.508101	0.000000
346	8	-9.951117	-13.591821	0.000000
347	1	-13.969160	-11.263073	0.000000
348	1	-12.733634	-13.450356	0.000000
349	6	-2.740651	-7.177876	0.000000
350	6	-3.435492	-5.947328	0.000000
351	6	-3.051783	-4.569163	0.000000
352	6	-1.821065	-3.874456	0.000000
353	6	-0.442805	-4.258123	0.000000
354	6	0.251937	-5.488822	0.000000
355	6	-0.131645	-6.867022	0.000000
356	6	-1.362370	-7.561549	0.000000
357	6	1.057609	-7.597532	0.000000
358	6	1.647469	-5.477754	0.000000
359	6	0.287747	-3.069107	0.000000
360	6	-1.832172	-2.478984	0.000000
361	6	-4.240871	-3.838613	0.000000
362	6	-4.831147	-5.958276	0.000000
363	6	-3.471382	-8.366865	0.000000
364	6	-1.351097	-8.957090	0.000000
365	6	1.107827	-9.014074	0.000000
366	8	2.157523	-6.761491	0.000000
367	6	2.422037	-4.290651	0.000000
368	6	1.704275	-3.019132	0.000000
369	8	-0.548102	-1.968964	0.000000
370	8	-5.340871	-4.674159	0.000000
371	6	-5.606071	-7.145122	0.000000
372	6	-4.888110	-8.416540	0.000000
373	8	-2.635323	-9.466960	0.000000
374	6	-5.921015	-18.599492	0.000000
375	6	-6.611058	-17.382376	0.000000
376	6	-6.234845	-16.000607	0.000000
377	6	-5.004555	-15.306957	0.000000
378	6	-3.624405	-15.691150	0.000000
379	6	-2.929483	-16.920722	0.000000
380	6	-3.321346	-18.298135	0.000000
381	6	-4.541022	-18.983641	0.000000
382	6	-2.130566	-19.044471	0.000000
383	6	-1.534682	-16.917675	0.000000
384	6	-2.894850	-14.502589	0.000000
385	6	-5.015043	-13.912390	0.000000
386	6	-7.427451	-15.277301	0.000000

387	6	-8.016195	-17.406085	0.000000
388	6	-6.659776	-19.794625	0.000000
389	6	-4.526048	-20.388592	0.000000
390	6	-3.337042	-21.131216	0.000000
391	6	-2.113875	-20.444938	0.000000
392	8	-1.024834	-18.201957	0.000000
393	8	-3.730522	-13.401281	0.000000
394	6	-6.204326	-13.140125	0.000000
395	6	-7.477263	-13.858213	0.000000
396	8	-8.527556	-16.113420	0.000000
397	6	-8.754109	-18.596492	0.000000
398	6	-8.061477	-19.816072	0.000000
399	8	-5.817592	-20.898735	0.000000
400	1	-3.362322	-22.216903	0.000000
401	1	-1.173540	-20.988162	0.000000
402	1	-9.839876	-18.575709	0.000000
403	1	-8.600809	-20.758662	0.000000
404	6	1.384554	-14.486675	0.000000
405	6	0.690222	-13.257433	0.000000
406	6	1.075064	-11.878820	0.000000
407	6	2.306218	-11.184148	0.000000
408	6	3.685459	-11.567329	0.000000
409	6	4.379333	-12.797086	0.000000
410	6	3.986314	-14.173761	0.000000
411	6	2.766135	-14.862077	0.000000
412	6	5.177615	-14.920107	0.000000
413	6	5.774460	-12.793386	0.000000
414	6	4.415448	-10.378737	0.000000
415	6	2.295563	-9.788670	0.000000
416	6	-0.114055	-11.148483	0.000000
417	6	-0.704715	-13.268120	0.000000
418	6	0.660025	-15.678895	0.000000
419	6	2.788901	-16.267694	0.000000
420	6	3.977037	-17.009614	0.000000
421	6	5.198282	-16.320706	0.000000
422	8	6.283100	-14.078276	0.000000
423	8	3.579296	-9.278024	0.000000
424	6	-0.163810	-9.731646	0.000000
425	8	-1.214702	-11.983305	0.000000
426	6	-1.477596	-14.455907	0.000000
427	6	-0.758789	-15.728438	0.000000
428	8	1.496885	-16.778607	0.000000
429	1	3.952274	-18.095221	0.000000
430	1	6.140263	-16.860944	0.000000
431	6	15.277301	-7.427451	0.000000
432	6	13.858213	-7.477263	0.000000

Table S7. The optimized Cartesian coordinates of the compound **4** calculated at the B3LYP/6-21G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	3.491077	2.476349
2	6	0.000000	4.903207	2.476662
3	6	0.000000	5.909199	3.495245
4	6	0.000000	5.908949	4.895833
5	6	0.000000	4.902682	5.914126
6	6	0.000000	3.490741	5.914352
7	6	0.000000	2.478968	4.901927
8	6	0.000000	2.479036	3.488578
9	6	0.000000	1.258476	5.578350
10	6	0.000000	2.814561	7.134231
11	6	0.000000	5.584812	7.130869
12	6	0.000000	7.144126	5.566975
13	6	0.000000	7.144579	2.824479
14	6	0.000000	5.585718	1.260152
15	6	0.000000	2.815140	1.256536
16	6	0.000000	1.258642	2.811903
17	8	0.000000	1.444812	6.947393
18	8	0.000000	6.954053	6.942982
19	6	0.000000	8.374199	4.897009
20	6	0.000000	8.374463	3.494779

21	8	0.000000	6.954789	1.448337
22	8	0.000000	1.445344	1.442724
23	1	0.000000	9.307443	5.452158
24	1	0.000000	9.307900	2.939956
25	6	0.000000	3.489841	10.867346
26	6	0.000000	4.902181	10.866893
27	6	0.000000	5.908972	11.885258
28	6	0.000000	5.906254	13.284210
29	6	0.000000	4.893211	14.296952
30	6	0.000000	3.494269	14.299242
31	6	0.000000	2.476152	13.292192
32	6	0.000000	2.476763	11.880035
33	6	0.000000	1.259962	13.974622
34	6	0.000000	2.823724	15.534269
35	6	0.000000	5.570569	15.527800
36	6	0.000000	7.136895	13.961883
37	6	0.000000	7.144197	11.214982
38	6	0.000000	5.585061	9.650971
39	6	0.000000	2.813627	9.647904
40	6	0.000000	1.257259	11.203544
41	6	0.000000	0.000000	13.320084
42	8	0.000000	1.446990	15.344018
43	6	0.000000	3.497408	16.762143
44	6	0.000000	4.900076	16.758818
45	8	0.000000	6.946191	15.337449
46	6	0.000000	8.368114	13.291716
47	6	0.000000	8.371893	11.889066
48	8	0.000000	6.954323	9.838424
49	6	0.000000	4.930850	8.390716
50	6	0.000000	3.469555	8.390925
51	8	0.000000	1.443797	9.833546
52	1	0.000000	2.945363	17.697334
53	1	0.000000	5.455579	17.691961
54	1	0.000000	9.301094	13.847503
55	1	0.000000	9.307275	11.337342
56	6	0.000000	-4.903207	2.476662
57	6	0.000000	-3.491077	2.476349
58	6	0.000000	-2.479036	3.488578
59	6	0.000000	-2.478968	4.901927
60	6	0.000000	-3.490741	5.914352
61	6	0.000000	-4.902682	5.914126
62	6	0.000000	-5.908949	4.895833
63	6	0.000000	-5.909199	3.495245
64	6	0.000000	-7.144126	5.566975
65	6	0.000000	-5.584812	7.130869
66	6	0.000000	-2.814561	7.134231
67	6	0.000000	-1.258476	5.578350
68	6	0.000000	-1.258642	2.811903
69	6	0.000000	-2.815140	1.256536
70	6	0.000000	-5.585718	1.260152
71	6	0.000000	-7.144579	2.824479
72	6	0.000000	-8.374463	3.494779
73	6	0.000000	-8.374199	4.897009
74	8	0.000000	-6.954053	6.942982
75	8	0.000000	-1.444812	6.947393
76	6	0.000000	0.000000	4.925009
77	6	0.000000	0.000000	3.465025
78	8	0.000000	-1.445344	1.442724
79	6	0.000000	-3.470564	0.000000
80	6	0.000000	-4.931984	0.000000
81	8	0.000000	-6.954789	1.448337
82	1	0.000000	-9.307900	2.939956
83	1	0.000000	-9.307443	5.452158
84	6	0.000000	-4.902181	10.866893
85	6	0.000000	-3.489841	10.867346
86	6	0.000000	-2.476763	11.880035
87	6	0.000000	-2.476152	13.292192
88	6	0.000000	-3.494269	14.299242
89	6	0.000000	-4.893211	14.296952
90	6	0.000000	-5.906254	13.284210
91	6	0.000000	-5.908972	11.885258
92	6	0.000000	-7.136895	13.961883
93	6	0.000000	-5.570569	15.527800
94	6	0.000000	-2.823724	15.534269
95	6	0.000000	-1.259962	13.974622
96	6	0.000000	-1.257259	11.203544
97	6	0.000000	-2.813627	9.647904
98	6	0.000000	-7.144197	11.214982
99	6	0.000000	-8.371893	11.889066

100	6	0.000000	-8.368114	13.291716
101	8	0.000000	-6.946191	15.337449
102	6	0.000000	-4.900076	16.758818
103	6	0.000000	-3.497408	16.762143
104	8	0.000000	-1.446990	15.344018
105	6	0.000000	0.000000	11.858900
106	8	0.000000	-1.443797	9.833546
107	6	0.000000	-3.469555	8.390925
108	8	0.000000	-6.954323	9.838424
109	1	0.000000	-9.307275	11.337342
110	1	0.000000	-9.301094	13.847503
111	1	0.000000	-5.455579	17.691961
112	1	0.000000	-2.945363	17.697334
113	6	0.000000	3.494269	-14.299242
114	6	0.000000	4.893211	-14.296952
115	6	0.000000	5.906254	-13.284210
116	6	0.000000	5.908972	-11.885258
117	6	0.000000	4.902181	-10.866893
118	6	0.000000	3.489841	-10.867346
119	6	0.000000	2.476763	-11.880035
120	6	0.000000	2.476152	-13.292192
121	6	0.000000	1.257259	-11.203544
122	6	0.000000	2.813627	-9.647904
123	6	0.000000	5.585061	-9.650971
124	6	0.000000	7.144197	-11.214982
125	6	0.000000	7.136895	-13.961883
126	6	0.000000	5.570569	-15.527800
127	6	0.000000	2.823724	-15.534269
128	6	0.000000	1.259962	-13.974622
129	8	0.000000	1.443797	-9.833546
130	8	0.000000	6.954323	-9.838424
131	6	0.000000	8.371893	-11.889066
132	6	0.000000	8.368114	-13.291716
133	8	0.000000	6.946191	-15.337449
134	6	0.000000	4.900076	-16.758818
135	6	0.000000	3.497408	-16.762143
136	8	0.000000	1.446990	-15.344018
137	1	0.000000	9.307275	-11.337342
138	1	0.000000	9.301094	-13.847503
139	1	0.000000	5.455579	-17.691961
140	1	0.000000	2.945363	-17.697334
141	6	0.000000	3.490741	-5.914352
142	6	0.000000	4.902682	-5.914126
143	6	0.000000	5.908949	-4.895833
144	6	0.000000	5.909199	-3.495245
145	6	0.000000	4.903207	-2.476662
146	6	0.000000	3.491077	-2.476349
147	6	0.000000	2.479036	-3.488578
148	6	0.000000	2.478968	-4.901927
149	6	0.000000	1.258642	-2.811903
150	6	0.000000	2.815140	-1.256536
151	6	0.000000	5.585718	-1.260152
152	6	0.000000	7.144579	-2.824479
153	6	0.000000	7.144126	-5.566975
154	6	0.000000	5.584812	-7.130869
155	6	0.000000	2.814561	-7.134231
156	6	0.000000	1.258476	-5.578350
157	6	0.000000	0.000000	-3.465025
158	8	0.000000	1.445344	-1.442724
159	6	0.000000	3.470564	0.000000
160	6	0.000000	4.931984	0.000000
161	8	0.000000	6.954789	-1.448337
162	6	0.000000	8.374463	-3.494779
163	6	0.000000	8.374199	-4.897009
164	8	0.000000	6.954053	-6.942982
165	6	0.000000	4.930850	-8.390716
166	6	0.000000	3.469555	-8.390925
167	8	0.000000	1.444812	-6.947393
168	1	0.000000	9.307900	-2.939956
169	1	0.000000	9.307443	-5.452158
170	6	0.000000	-4.893211	-14.296952
171	6	0.000000	-3.494269	-14.299242
172	6	0.000000	-2.476152	-13.292192
173	6	0.000000	-2.476763	-11.880035
174	6	0.000000	-3.489841	-10.867346
175	6	0.000000	-4.902181	-10.866893
176	6	0.000000	-5.908972	-11.885258
177	6	0.000000	-5.906254	-13.284210
178	6	0.000000	-7.144197	-11.214982

179	6	0.000000	-5.585061	-9.650971
180	6	0.000000	-2.813627	-9.647904
181	6	0.000000	-1.257259	-11.203544
182	6	0.000000	-1.259962	-13.974622
183	6	0.000000	-2.823724	-15.534269
184	6	0.000000	-5.570569	-15.527800
185	6	0.000000	-7.136895	-13.961883
186	6	0.000000	-8.368114	-13.291716
187	6	0.000000	-8.371893	-11.889066
188	8	0.000000	-6.954323	-9.838424
189	8	0.000000	-1.443797	-9.833546
190	6	0.000000	0.000000	-11.858900
191	6	0.000000	0.000000	-13.320084
192	8	0.000000	-1.446990	-15.344018
193	6	0.000000	-3.497408	-16.762143
194	6	0.000000	-4.900076	-16.758818
195	8	0.000000	-6.946191	-15.337449
196	1	0.000000	-9.301094	-13.847503
197	1	0.000000	-9.307275	-11.337342
198	1	0.000000	-2.945363	-17.697334
199	1	0.000000	-5.455579	-17.691961
200	6	0.000000	-4.902682	-5.914126
201	6	0.000000	-3.490741	-5.914352
202	6	0.000000	-2.478968	-4.901927
203	6	0.000000	-2.479036	-3.488578
204	6	0.000000	-3.491077	-2.476349
205	6	0.000000	-4.903207	-2.476662
206	6	0.000000	-5.909199	-3.495245
207	6	0.000000	-5.908949	-4.895833
208	6	0.000000	-7.144579	-2.824479
209	6	0.000000	-5.585718	-1.260152
210	6	0.000000	-2.815140	-1.256536
211	6	0.000000	-1.258642	-2.811903
212	6	0.000000	-1.258476	-5.578350
213	6	0.000000	-2.814561	-7.134231
214	6	0.000000	-5.584812	-7.130869
215	6	0.000000	-7.144126	-5.566975
216	6	0.000000	-8.374199	-4.897009
217	6	0.000000	-8.374463	-3.494779
218	8	0.000000	-6.954789	-1.448337
219	8	0.000000	-1.445344	-1.442724
220	6	0.000000	0.000000	-4.925009
221	8	0.000000	-1.444812	-6.947393
222	6	0.000000	-3.469555	-8.390925
223	6	0.000000	-4.930850	-8.390716
224	8	0.000000	-6.954053	-6.942982
225	1	0.000000	-9.307443	-5.452158
226	1	0.000000	-9.307900	-2.939956
227	6	0.000000	-5.585061	9.650971
228	6	0.000000	-4.930850	8.390716

Table S8. The optimized Cartesian coordinates of the compound **5** calculated at the B3LYP/6–21G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	10.656674	-0.965946	3.491030
2	6	10.634954	-0.963533	4.904698
3	6	10.587340	0.053257	5.914781
4	6	10.487424	1.452083	5.914781
5	6	10.390036	2.465318	4.904698
6	6	10.411192	2.470794	3.491030
7	6	10.550376	1.464255	2.479208
8	6	10.651383	0.050156	2.479208
9	6	10.391176	2.125394	1.259496
10	6	10.123751	3.659838	2.814135
11	6	10.075850	3.645346	5.579734
12	6	10.264486	2.102200	7.142341
13	6	10.459067	-0.621947	7.142341
14	6	10.491678	-2.176237	5.579734
15	6	10.541152	-2.183774	2.814135
16	6	10.587768	-0.626898	1.259496
17	8	10.141710	3.470841	1.445013
18	8	10.031704	3.455197	6.945770
19	6	10.202952	1.430570	8.368991
20	6	10.302699	0.034119	8.368991
21	8	10.420954	-1.994293	6.945770
22	8	10.532066	-1.994143	1.445013
23	1	10.036761	1.978297	9.291538
24	1	10.216044	-0.531669	9.291538
25	6	8.218433	6.852379	3.491030
26	6	8.201369	6.838727	4.904698
27	6	7.448721	7.524038	5.914781
28	6	6.388951	8.442506	5.914781
29	6	5.603622	9.090108	4.904698
30	6	5.614710	9.108940	3.491030
31	6	6.424857	8.495627	2.479208
32	6	7.496199	7.567131	2.479208
33	6	5.844791	8.850551	1.259496
34	6	4.570676	9.746470	2.814135
35	6	4.547053	9.702351	5.579734
36	6	5.771607	8.744567	7.142341
37	6	7.835460	6.955895	7.142341
38	6	8.957569	5.879904	5.579734
39	6	8.997881	5.909559	2.814135
40	6	7.929966	7.043399	1.259496
41	6	6.344559	8.433120	0.000000
42	8	4.717017	9.625527	1.445013
43	8	4.650293	9.536679	6.945770
44	6	6.203011	8.226142	8.368991
45	6	7.260982	7.309234	8.368991
46	8	8.778905	5.958549	6.945770
47	6	9.642446	4.825550	4.921974
48	6	9.663631	4.836152	3.464592
49	8	8.857367	6.037223	1.445013
50	1	5.698194	8.495929	9.291538
51	1	7.599780	6.847887	9.291538
52	6	10.634954	-0.963533	-4.904698
53	6	10.656674	-0.965946	-3.491030
54	6	10.651383	0.050156	-2.479208
55	6	10.550376	1.464255	-2.479208
56	6	10.411192	2.470794	-3.491030
57	6	10.390036	2.465318	-4.904698
58	6	10.487424	1.452083	-5.914781
59	6	10.587340	0.053257	-5.914781
60	6	10.264486	2.102200	-7.142341
61	6	10.075850	3.645346	-5.579734
62	6	10.123751	3.659838	-2.814135
63	6	10.391176	2.125394	-1.259496
64	6	10.587768	-0.626898	-1.259496
65	6	10.541152	-2.183774	-2.814135
66	6	10.491678	-2.176237	-5.579734
67	6	10.459067	-0.621947	-7.142341
68	6	10.302699	0.034119	-8.368991
69	6	10.202952	1.430570	-8.368991
70	8	10.031704	3.455197	-6.945770

71	8	10.141710	3.470841	-1.445013
72	6	10.449398	1.476836	0.000000
73	6	10.553218	0.023351	0.000000
74	8	10.532066	-1.994143	-1.445013
75	6	10.252895	-3.413543	-3.464592
76	6	10.230418	-3.406060	-4.921974
77	8	10.420954	-1.994293	-6.945770
78	1	10.216044	-0.531669	-9.291538
79	1	10.036761	1.978297	-9.291538
80	6	8.201369	6.838727	-4.904698
81	6	8.218433	6.852379	-3.491030
82	6	7.496199	7.567131	-2.479208
83	6	6.424857	8.495627	-2.479208
84	6	5.614710	9.108940	-3.491030
85	6	5.603622	9.090108	-4.904698
86	6	6.388951	8.442506	-5.914781
87	6	7.448721	7.524038	-5.914781
88	6	5.771607	8.744567	-7.142341
89	6	4.547053	9.702351	-5.579734
90	6	4.570676	9.746470	-2.814135
91	6	5.844791	8.850551	-1.259496
92	6	7.929966	7.043399	-1.259496
93	6	8.997881	5.909559	-2.814135
94	6	7.835460	6.955895	-7.142341
95	6	7.260982	7.309234	-8.368991
96	6	6.203011	8.226142	-8.368991
97	8	4.650293	9.536679	-6.945770
98	8	4.717017	9.625527	-1.445013
99	6	7.445740	7.478764	0.000000
100	8	8.857367	6.037223	-1.445013
101	6	9.663631	4.836152	-3.464592
102	8	8.778905	5.958549	-6.945770
103	1	7.599780	6.847887	-9.291538
104	1	5.698194	8.495929	-9.291538
105	6	-0.965946	-10.656674	3.491030
106	6	-0.963533	-10.634954	4.904698
107	6	0.053257	-10.587340	5.914781
108	6	1.452083	-10.487424	5.914781
109	6	2.465318	-10.390036	4.904698
110	6	2.470794	-10.411192	3.491030
111	6	1.464255	-10.550376	2.479208
112	6	0.050156	-10.651383	2.479208
113	6	2.125394	-10.391176	1.259496
114	6	3.659838	-10.123751	2.814135
115	6	3.645346	-10.075850	5.579734
116	6	2.102200	-10.264486	7.142341
117	6	-0.621947	-10.459067	7.142341
118	6	-2.176237	-10.491678	5.579734
119	6	-2.183774	-10.541152	2.814135
120	6	-0.626898	-10.587768	1.259496
121	8	3.470841	-10.141710	1.445013
122	8	3.455197	-10.031704	6.945770
123	6	1.430570	-10.202952	8.368991
124	6	0.034119	-10.302699	8.368991
125	8	-1.994293	-10.420954	6.945770
126	8	-1.994143	-10.532066	1.445013
127	1	1.978297	-10.036761	9.291538
128	1	-0.531669	-10.216044	9.291538
129	6	6.852379	-8.218433	3.491030
130	6	6.838727	-8.201369	4.904698
131	6	7.524038	-7.448721	5.914781
132	6	8.442506	-6.388951	5.914781
133	6	9.090108	-5.603622	4.904698
134	6	9.108940	-5.614710	3.491030
135	6	8.495627	-6.424857	2.479208
136	6	7.567131	-7.496199	2.479208
137	6	8.850551	-5.844791	1.259496
138	6	9.746470	-4.570676	2.814135
139	6	9.702351	-4.547053	5.579734
140	6	8.744567	-5.771607	7.142341
141	6	6.955895	-7.835460	7.142341
142	6	5.879904	-8.957569	5.579734
143	6	5.909559	-8.997881	2.814135
144	6	7.043399	-7.929966	1.259496
145	6	8.433120	-6.344559	0.000000
146	8	9.625527	-4.717017	1.445013
147	6	10.252895	-3.413543	3.464592
148	6	10.230418	-3.406060	4.921974
149	8	9.536679	-4.650293	6.945770

150	6	8.226142	-6.203011	8.368991
151	6	7.309234	-7.260982	8.368991
152	8	5.958549	-8.778905	6.945770
153	6	4.825550	-9.642446	4.921974
154	6	4.836152	-9.663631	3.464592
155	8	6.037223	-8.857367	1.445013
156	1	8.495929	-5.698194	9.291538
157	1	6.847887	-7.599780	9.291538
158	6	-0.963533	-10.634954	-4.904698
159	6	-0.965946	-10.656674	-3.491030
160	6	0.050156	-10.651383	-2.479208
161	6	1.464255	-10.550376	-2.479208
162	6	2.470794	-10.411192	-3.491030
163	6	2.465318	-10.390036	-4.904698
164	6	1.452083	-10.487424	-5.914781
165	6	0.053257	-10.587340	-5.914781
166	6	2.102200	-10.264486	-7.142341
167	6	3.645346	-10.075850	-5.579734
168	6	3.659838	-10.123751	-2.814135
169	6	2.125394	-10.391176	-1.259496
170	6	-0.626898	-10.587768	-1.259496
171	6	-2.183774	-10.541152	-2.814135
172	6	-2.176237	-10.491678	-5.579734
173	6	-0.621947	-10.459067	-7.142341
174	6	0.034119	-10.302699	-8.368991
175	6	1.430570	-10.202952	-8.368991
176	8	3.455197	-10.031704	-6.945770
177	8	3.470841	-10.141710	-1.445013
178	6	1.476836	-10.449398	0.000000
179	6	0.023351	-10.553218	0.000000
180	8	-1.994143	-10.532066	-1.445013
181	8	-1.994293	-10.420954	-6.945770
182	1	-0.531669	-10.216044	-9.291538
183	1	1.978297	-10.036761	-9.291538
184	6	6.838727	-8.201369	-4.904698
185	6	6.852379	-8.218433	-3.491030
186	6	7.567131	-7.496199	-2.479208
187	6	8.495627	-6.424857	-2.479208
188	6	9.108940	-5.614710	-3.491030
189	6	9.090108	-5.603622	-4.904698
190	6	8.442506	-6.388951	-5.914781
191	6	7.524038	-7.448721	-5.914781
192	6	8.744567	-5.771607	-7.142341
193	6	9.702351	-4.547053	-5.579734
194	6	9.746470	-4.570676	-2.814135
195	6	8.850551	-5.844791	-1.259496
196	6	7.043399	-7.929966	-1.259496
197	6	5.909559	-8.997881	-2.814135
198	6	5.879904	-8.957569	-5.579734
199	6	6.955895	-7.835460	-7.142341
200	6	7.309234	-7.260982	-8.368991
201	6	8.226142	-6.203011	-8.368991
202	8	9.536679	-4.650293	-6.945770
203	8	9.625527	-4.717017	-1.445013
204	6	7.478764	-7.445740	0.000000
205	8	6.037223	-8.857367	-1.445013
206	6	4.836152	-9.663631	-3.464592
207	6	4.825550	-9.642446	-4.921974
208	8	5.958549	-8.778905	-6.945770
209	1	6.847887	-7.599780	-9.291538
210	1	8.495929	-5.698194	-9.291538
211	6	8.957569	5.879904	-5.579734
212	6	9.642446	4.825550	-4.921974
213	6	-9.108940	5.614710	-3.491030
214	6	-9.090108	5.603622	-4.904698
215	6	-8.442506	6.388951	-5.914781
216	6	-7.524038	7.448721	-5.914781
217	6	-6.838727	8.201369	-4.904698
218	6	-6.852379	8.218433	-3.491030
219	6	-7.567131	7.496199	-2.479208
220	6	-8.495627	6.424857	-2.479208
221	6	-7.043399	7.929966	-1.259496
222	6	-5.909559	8.997881	-2.814135
223	6	-5.879904	8.957569	-5.579734
224	6	-6.955895	7.835460	-7.142341
225	6	-8.744567	5.771607	-7.142341
226	6	-9.702351	4.547053	-5.579734
227	6	-9.746470	4.570676	-2.814135
228	6	-8.850551	5.844791	-1.259496

229	8	-6.037223	8.857367	-1.445013
230	8	-5.958549	8.778905	-6.945770
231	6	-7.309234	7.260982	-8.368991
232	6	-8.226142	6.203011	-8.368991
233	8	-9.536679	4.650293	-6.945770
234	8	-9.625527	4.717017	-1.445013
235	1	-6.847887	7.599780	-9.291538
236	1	-8.495929	5.698194	-9.291538
237	6	-2.470794	10.411192	-3.491030
238	6	-2.465318	10.390036	-4.904698
239	6	-1.452083	10.487424	-5.914781
240	6	-0.053257	10.587340	-5.914781
241	6	0.963533	10.634954	-4.904698
242	6	0.965946	10.656674	-3.491030
243	6	-0.050156	10.651383	-2.479208
244	6	-1.464255	10.550376	-2.479208
245	6	0.626898	10.587768	-1.259496
246	6	2.183774	10.541152	-2.814135
247	6	2.176237	10.491678	-5.579734
248	6	0.621947	10.459067	-7.142341
249	6	-2.102200	10.264486	-7.142341
250	6	-3.645346	10.075850	-5.579734
251	6	-3.659838	10.123751	-2.814135
252	6	-2.125394	10.391176	-1.259496
253	6	-0.023351	10.553218	0.000000
254	8	1.994143	10.532066	-1.445013
255	6	3.413543	10.252895	-3.464592
256	6	3.406060	10.230418	-4.921974
257	8	1.994293	10.420954	-6.945770
258	6	-0.034119	10.302699	-8.368991
259	6	-1.430570	10.202952	-8.368991
260	8	-3.455197	10.031704	-6.945770
261	6	-4.825550	9.642446	-4.921974
262	6	-4.836152	9.663631	-3.464592
263	8	-3.470841	10.141710	-1.445013
264	1	0.531669	10.216044	-9.291538
265	1	-1.978297	10.036761	-9.291538
266	6	-9.090108	5.603622	4.904698
267	6	-9.108940	5.614710	3.491030
268	6	-8.495627	6.424857	2.479208
269	6	-7.567131	7.496199	2.479208
270	6	-6.852379	8.218433	3.491030
271	6	-6.838727	8.201369	4.904698
272	6	-7.524038	7.448721	5.914781
273	6	-8.442506	6.388951	5.914781
274	6	-6.955895	7.835460	7.142341
275	6	-5.879904	8.957569	5.579734
276	6	-5.909559	8.997881	2.814135
277	6	-7.043399	7.929966	1.259496
278	6	-8.850551	5.844791	1.259496
279	6	-9.746470	4.570676	2.814135
280	6	-9.702351	4.547053	5.579734
281	6	-8.744567	5.771607	7.142341
282	6	-8.226142	6.203011	8.368991
283	6	-7.309234	7.260982	8.368991
284	8	-5.958549	8.778905	6.945770
285	8	-6.037223	8.857367	1.445013
286	6	-7.478764	7.445740	0.000000
287	6	-8.433120	6.344559	0.000000
288	8	-9.625527	4.717017	1.445013
289	6	-10.252895	3.413543	3.464592
290	6	-10.230418	3.406060	4.921974
291	8	-9.536679	4.650293	6.945770
292	1	-8.495929	5.698194	9.291538
293	1	-6.847887	7.599780	9.291538
294	6	-2.465318	10.390036	4.904698
295	6	-2.470794	10.411192	3.491030
296	6	-1.464255	10.550376	2.479208
297	6	-0.050156	10.651383	2.479208
298	6	0.965946	10.656674	3.491030
299	6	0.963533	10.634954	4.904698
300	6	-0.053257	10.587340	5.914781
301	6	-1.452083	10.487424	5.914781
302	6	0.621947	10.459067	7.142341
303	6	2.176237	10.491678	5.579734
304	6	2.183774	10.541152	2.814135
305	6	0.626898	10.587768	1.259496
306	6	-2.125394	10.391176	1.259496
307	6	-3.659838	10.123751	2.814135

308	6	-2.102200	10.264486	7.142341
309	6	-1.430570	10.202952	8.368991
310	6	-0.034119	10.302699	8.368991
311	8	1.994293	10.420954	6.945770
312	6	3.406060	10.230418	4.921974
313	6	3.413543	10.252895	3.464592
314	8	1.994143	10.532066	1.445013
315	6	-1.476836	10.449398	0.000000
316	8	-3.470841	10.141710	1.445013
317	6	-4.836152	9.663631	3.464592
318	8	-3.455197	10.031704	6.945770
319	1	-1.978297	10.036761	9.291538
320	1	0.531669	10.216044	9.291538
321	6	-5.614710	-9.108940	-3.491030
322	6	-5.603622	-9.090108	-4.904698
323	6	-6.388951	-8.442506	-5.914781
324	6	-7.448721	-7.524038	-5.914781
325	6	-8.201369	-6.838727	-4.904698
326	6	-8.218433	-6.852379	-3.491030
327	6	-7.496199	-7.567131	-2.479208
328	6	-6.424857	-8.495627	-2.479208
329	6	-7.929966	-7.043399	-1.259496
330	6	-8.997881	-5.909559	-2.814135
331	6	-8.957569	-5.879904	-5.579734
332	6	-7.835460	-6.955895	-7.142341
333	6	-5.771607	-8.744567	-7.142341
334	6	-4.547053	-9.702351	-5.579734
335	6	-4.570676	-9.746470	-2.814135
336	6	-5.844791	-8.850551	-1.259496
337	8	-8.857367	-6.037223	-1.445013
338	8	-8.778905	-5.958549	-6.945770
339	6	-7.260982	-7.309234	-8.368991
340	6	-6.203011	-8.226142	-8.368991
341	8	-4.650293	-9.536679	-6.945770
342	6	-3.406060	-10.230418	-4.921974
343	6	-3.413543	-10.252895	-3.464592
344	8	-4.717017	-9.625527	-1.445013
345	1	-7.599780	-6.847887	-9.291538
346	1	-5.698194	-8.495929	-9.291538
347	6	-10.411192	-2.470794	-3.491030
348	6	-10.390036	-2.465318	-4.904698
349	6	-10.487424	-1.452083	-5.914781
350	6	-10.587340	-0.053257	-5.914781
351	6	-10.634954	0.963533	-4.904698
352	6	-10.656674	0.965946	-3.491030
353	6	-10.651383	-0.050156	-2.479208
354	6	-10.550376	-1.464255	-2.479208
355	6	-10.587768	0.626898	-1.259496
356	6	-10.541152	2.183774	-2.814135
357	6	-10.491678	2.176237	-5.579734
358	6	-10.459067	0.621947	-7.142341
359	6	-10.264486	-2.102200	-7.142341
360	6	-10.075850	-3.645346	-5.579734
361	6	-10.123751	-3.659838	-2.814135
362	6	-10.391176	-2.125394	-1.259496
363	6	-10.553218	-0.023351	0.000000
364	8	-10.532066	1.994143	-1.445013
365	6	-10.252895	3.413543	-3.464592
366	6	-10.230418	3.406060	-4.921974
367	8	-10.420954	1.994293	-6.945770
368	6	-10.302699	-0.034119	-8.368991
369	6	-10.202952	-1.430570	-8.368991
370	8	-10.031704	-3.455197	-6.945770
371	6	-9.642446	-4.825550	-4.921974
372	6	-9.663631	-4.836152	-3.464592
373	8	-10.141710	-3.470841	-1.445013
374	1	-10.216044	0.531669	-9.291538
375	1	-10.036761	-1.978297	-9.291538
376	6	-5.603622	-9.090108	4.904698
377	6	-5.614710	-9.108940	3.491030
378	6	-6.424857	-8.495627	2.479208
379	6	-7.496199	-7.567131	2.479208
380	6	-8.218433	-6.852379	3.491030
381	6	-8.201369	-6.838727	4.904698
382	6	-7.448721	-7.524038	5.914781
383	6	-6.388951	-8.442506	5.914781
384	6	-7.835460	-6.955895	7.142341
385	6	-8.957569	-5.879904	5.579734
386	6	-8.997881	-5.909559	2.814135

387	6	-7.929966	-7.043399	1.259496
388	6	-5.844791	-8.850551	1.259496
389	6	-4.570676	-9.746470	2.814135
390	6	-4.547053	-9.702351	5.579734
391	6	-5.771607	-8.744567	7.142341
392	6	-6.203011	-8.226142	8.368991
393	6	-7.260982	-7.309234	8.368991
394	8	-8.778905	-5.958549	6.945770
395	8	-8.857367	-6.037223	1.445013
396	6	-7.445740	-7.478764	0.000000
397	6	-6.344559	-8.433120	0.000000
398	8	-4.717017	-9.625527	1.445013
399	6	-3.413543	-10.252895	3.464592
400	6	-3.406060	-10.230418	4.921974
401	8	-4.650293	-9.536679	6.945770
402	1	-5.698194	-8.495929	9.291538
403	1	-7.599780	-6.847887	9.291538
404	6	-10.390036	-2.465318	4.904698
405	6	-10.411192	-2.470794	3.491030
406	6	-10.550376	-1.464255	2.479208
407	6	-10.651383	-0.050156	2.479208
408	6	-10.656674	0.965946	3.491030
409	6	-10.634954	0.963533	4.904698
410	6	-10.587340	-0.053257	5.914781
411	6	-10.487424	-1.452083	5.914781
412	6	-10.459067	0.621947	7.142341
413	6	-10.491678	2.176237	5.579734
414	6	-10.541152	2.183774	2.814135
415	6	-10.587768	0.626898	1.259496
416	6	-10.391176	-2.125394	1.259496
417	6	-10.123751	-3.659838	2.814135
418	6	-10.075850	-3.645346	5.579734
419	6	-10.264486	-2.102200	7.142341
420	6	-10.202952	-1.430570	8.368991
421	6	-10.302699	-0.034119	8.368991
422	8	-10.420954	1.994293	6.945770
423	8	-10.532066	1.994143	1.445013
424	6	-10.449398	-1.476836	0.000000
425	8	-10.141710	-3.470841	1.445013
426	6	-9.663631	-4.836152	3.464592
427	6	-9.642446	-4.825550	4.921974
428	8	-10.031704	-3.455197	6.945770
429	1	-10.036761	-1.978297	9.291538
430	1	-10.216044	0.531669	9.291538
431	6	-3.645346	10.075850	5.579734
432	6	-4.825550	9.642446	4.921974

Table S9. The optimized Cartesian coordinates of the 1D ribbons (n=2) calculated at the B3LYP/6–21G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	1	0.000000	2.943420	5.110970
2	1	0.000000	5.453130	5.106563
3	1	0.000000	9.300066	1.254142
4	6	0.000000	8.365114	0.701478
5	6	0.000000	8.365114	-0.701478
6	1	0.000000	9.300066	-1.254142
7	6	0.000000	7.136094	-1.375724
8	6	0.000000	5.905565	-0.698734
9	6	0.000000	5.905565	0.698734
10	6	0.000000	7.136094	1.375724
11	8	0.000000	6.945354	2.752101
12	6	0.000000	5.569448	2.941857
13	6	0.000000	4.898010	4.173132
14	6	0.000000	3.495821	4.175937
15	6	0.000000	2.821806	2.947520
16	6	0.000000	3.492671	1.712953
17	6	0.000000	4.891824	1.711528
18	6	0.000000	4.891824	-1.711528
19	6	0.000000	3.492671	-1.712953
20	6	0.000000	2.473410	-0.705499
21	6	0.000000	2.473410	0.705499
22	8	0.000000	1.444771	2.757731

23	6	0.000000	1.258577	1.387993
24	6	0.000000	0.000000	0.730893
25	6	0.000000	1.258577	-1.387993
26	6	0.000000	2.821806	-2.947520
27	8	0.000000	1.444771	-2.757731
28	6	0.000000	5.569448	-2.941857
29	6	0.000000	4.898010	-4.173132
30	6	0.000000	3.495821	-4.175937
31	1	0.000000	2.943420	-5.110970
32	1	0.000000	5.453130	-5.106563
33	8	0.000000	6.945354	-2.752101
34	1	0.000000	-5.453130	5.106563
35	1	0.000000	-2.943420	5.110970
36	6	0.000000	0.000000	-0.730893
37	6	0.000000	-1.258577	-1.387993
38	6	0.000000	-2.473410	-0.705499
39	6	0.000000	-2.473410	0.705499
40	6	0.000000	-1.258577	1.387993
41	8	0.000000	-1.444771	2.757731
42	6	0.000000	-2.821806	2.947520
43	6	0.000000	-3.495821	4.175937
44	6	0.000000	-4.898010	4.173132
45	6	0.000000	-5.569448	2.941857
46	6	0.000000	-4.891824	1.711528
47	6	0.000000	-3.492671	1.712953
48	6	0.000000	-3.492671	-1.712953
49	6	0.000000	-4.891824	-1.711528
50	6	0.000000	-5.905565	-0.698734
51	6	0.000000	-5.905565	0.698734
52	8	0.000000	-6.945354	2.752101
53	6	0.000000	-7.136094	1.375724
54	6	0.000000	-8.365114	0.701478
55	1	0.000000	-9.300066	1.254142
56	6	0.000000	-8.365114	-0.701478
57	6	0.000000	-7.136094	-1.375724
58	1	0.000000	-9.300066	-1.254142
59	6	0.000000	-5.569448	-2.941857
60	8	0.000000	-6.945354	-2.752101
61	6	0.000000	-2.821806	-2.947520
62	6	0.000000	-3.495821	-4.175937
63	6	0.000000	-4.898010	-4.173132
64	1	0.000000	-5.453130	-5.106563
65	1	0.000000	-2.943420	-5.110970
66	8	0.000000	-1.444771	-2.757731

Table S10. The optimized Cartesian coordinates of the 1D ribbons (n=3) calculated at the B3LYP/6-21G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	0.000000	2.752144	11.139336
2	6	0.000000	-2.947797	7.015744
3	6	0.000000	-1.387997	5.452151
4	6	0.000000	1.387997	5.452151
5	6	0.000000	2.947797	7.015744
6	6	0.000000	2.941949	9.763420
7	6	0.000000	1.375737	11.330053
8	6	0.000000	-1.713124	7.686512
9	6	0.000000	-1.711621	9.085658
10	6	0.000000	-0.698734	10.099478
11	6	0.000000	0.698734	10.099478
12	6	0.000000	1.711621	9.085658
13	6	0.000000	1.713124	7.686512
14	6	0.000000	0.705607	6.667156
15	6	0.000000	-0.705607	6.667156
16	6	0.000000	-2.941949	9.763420
17	6	0.000000	-1.375737	11.330053
18	6	0.000000	-4.173239	9.092171
19	6	0.000000	-4.176128	7.689806
20	6	0.000000	4.173239	9.092171
21	6	0.000000	4.176128	7.689806
22	6	0.000000	0.701547	12.559066
23	6	0.000000	-0.701547	12.559066
24	8	0.000000	-2.758237	5.638797

25	8	0.000000	-2.752144	11.139336
26	8	0.000000	2.758237	5.638797
27	1	0.000000	-5.106631	9.647288
28	1	0.000000	-5.111244	7.137605
29	1	0.000000	1.254046	13.494080
30	1	0.000000	-1.254046	13.494080
31	1	0.000000	5.106631	9.647288
32	1	0.000000	5.111244	7.137605
33	8	0.000000	2.757346	2.747651
34	6	0.000000	-2.946807	-1.371397
35	6	0.000000	-1.387232	-2.935257
36	6	0.000000	1.387232	-2.935257
37	6	0.000000	2.946807	-1.371397
38	6	0.000000	2.946807	1.371397
39	6	0.000000	1.387232	2.935257
40	6	0.000000	-1.711759	-0.700237
41	6	0.000000	-1.711759	0.700237
42	6	0.000000	-0.705272	1.719318
43	6	0.000000	0.705272	1.719318
44	6	0.000000	1.711759	0.700237
45	6	0.000000	1.711759	-0.700237
46	6	0.000000	0.705272	-1.719318
47	6	0.000000	-0.705272	-1.719318
48	6	0.000000	-2.946807	1.371397
49	6	0.000000	-1.387232	2.935257
50	6	0.000000	-4.177103	0.701021
51	6	0.000000	-4.177103	-0.701021
52	6	0.000000	4.177103	0.701021
53	6	0.000000	4.177103	-0.701021
54	6	0.000000	0.731208	4.193357
55	6	0.000000	-0.731208	4.193357
56	8	0.000000	-2.757346	-2.747651
57	8	0.000000	-2.757346	2.747651
58	8	0.000000	2.757346	-2.747651
59	1	0.000000	-5.110468	1.256053
60	1	0.000000	-5.110468	-1.256053
61	1	0.000000	5.110468	1.256053
62	1	0.000000	5.110468	-1.256053
63	8	0.000000	2.758237	-5.638797
64	6	0.000000	-2.941949	-9.763420
65	6	0.000000	-1.375737	-11.330053
66	6	0.000000	1.375737	-11.330053
67	6	0.000000	2.941949	-9.763420
68	6	0.000000	2.947797	-7.015744
69	6	0.000000	1.387997	-5.452151
70	6	0.000000	-1.711621	-9.085658
71	6	0.000000	-1.713124	-7.686512
72	6	0.000000	-0.705607	-6.667156
73	6	0.000000	0.705607	-6.667156
74	6	0.000000	1.713124	-7.686512
75	6	0.000000	1.711621	-9.085658
76	6	0.000000	0.698734	-10.099478
77	6	0.000000	-0.698734	-10.099478
78	6	0.000000	-2.947797	-7.015744
79	6	0.000000	-1.387997	-5.452151
80	6	0.000000	-4.176128	-7.689806
81	6	0.000000	-4.173239	-9.092171
82	6	0.000000	4.176128	-7.689806
83	6	0.000000	4.173239	-9.092171
84	6	0.000000	0.731208	-4.193357
85	6	0.000000	-0.731208	-4.193357
86	6	0.000000	0.701547	-12.559066
87	6	0.000000	-0.701547	-12.559066
88	8	0.000000	-2.752144	-11.139336
89	8	0.000000	-2.758237	-5.638797
90	8	0.000000	2.752144	-11.139336
91	1	0.000000	-5.111244	-7.137605
92	1	0.000000	-5.106631	-9.647288
93	1	0.000000	5.111244	-7.137605
94	1	0.000000	5.106631	-9.647288
95	1	0.000000	1.254046	-13.494080
96	1	0.000000	-1.254046	-13.494080

Table S11. The optimized Cartesian coordinates of the 1D ribbons (n=4) calculated at the B3LYP/6–21G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	13.285875	4.173345
2	6	0.000000	11.209592	2.947809
3	6	0.000000	11.883525	4.176242
4	6	0.000000	13.956997	2.941968
5	8	0.000000	-15.333026	2.752136
6	6	0.000000	-11.209592	-2.947809
7	6	0.000000	-9.645802	-1.387941
8	6	0.000000	-9.645802	1.387941
9	6	0.000000	-11.209592	2.947809
10	6	0.000000	-13.956997	2.941968
11	6	0.000000	-15.523789	1.375616
12	6	0.000000	-11.880228	-1.713069
13	6	0.000000	-13.279374	-1.711570
14	6	0.000000	-14.293161	-0.698733
15	6	0.000000	-14.293161	0.698733
16	6	0.000000	-13.279374	1.711570
17	6	0.000000	-11.880228	1.713069
18	6	0.000000	-10.860880	0.705587
19	6	0.000000	-10.860880	-0.705587
20	6	0.000000	-13.956997	-2.941968
21	6	0.000000	-15.523789	-1.375616
22	6	0.000000	-13.285875	-4.173345
23	6	0.000000	-11.883525	-4.176242
24	6	0.000000	-13.285875	4.173345
25	6	0.000000	-11.883525	4.176242
26	6	0.000000	-16.752884	0.701544
27	6	0.000000	-16.752884	-0.701544
28	8	0.000000	-9.832542	-2.758220
29	8	0.000000	-15.333026	-2.752136
30	8	0.000000	-9.832542	2.758220
31	1	0.000000	-13.841104	-5.106685
32	1	0.000000	-11.331215	-5.111306
33	1	0.000000	-17.687860	1.254131
34	1	0.000000	-17.687860	-1.254131
35	1	0.000000	-13.841104	5.106685
36	1	0.000000	-11.331215	5.111306
37	8	0.000000	-6.941216	2.757418
38	6	0.000000	-2.822196	-2.946911
39	6	0.000000	-1.258324	-1.387423
40	6	0.000000	-1.258324	1.387423
41	6	0.000000	-2.822196	2.946911
42	6	0.000000	-5.564951	2.946800
43	6	0.000000	-7.128878	1.387268
44	6	0.000000	-3.493230	-1.711796
45	6	0.000000	-4.893825	-1.711742
46	6	0.000000	-5.912886	-0.705310
47	6	0.000000	-5.912886	0.705310
48	6	0.000000	-4.893825	1.711742
49	6	0.000000	-3.493230	1.711796
50	6	0.000000	-2.474097	0.705430
51	6	0.000000	-2.474097	-0.705430
52	6	0.000000	-5.564951	-2.946800
53	6	0.000000	-7.128878	-1.387268
54	6	0.000000	-4.894589	-4.177180
55	6	0.000000	-3.492585	-4.177245
56	6	0.000000	-4.894589	4.177180
57	6	0.000000	-3.492585	4.177245
58	6	0.000000	-8.387004	0.731285
59	6	0.000000	-8.387004	-0.731285
60	8	0.000000	-1.445853	-2.757512
61	8	0.000000	-6.941216	-2.757418
62	8	0.000000	-1.445853	2.757512
63	1	0.000000	-5.449727	-5.110475
64	1	0.000000	-2.937550	-5.110594
65	1	0.000000	-5.449727	5.110475
66	1	0.000000	-2.937550	5.110594
67	8	0.000000	1.445853	2.757512
68	6	0.000000	5.564951	-2.946800
69	6	0.000000	7.128878	-1.387268
70	6	0.000000	7.128878	1.387268
71	6	0.000000	5.564951	2.946800
72	6	0.000000	2.822196	2.946911

73	6	0.000000	1.258324	1.387423
74	6	0.000000	4.893825	-1.711742
75	6	0.000000	3.493230	-1.711796
76	6	0.000000	2.474097	-0.705430
77	6	0.000000	2.474097	0.705430
78	6	0.000000	3.493230	1.711796
79	6	0.000000	4.893825	1.711742
80	6	0.000000	5.912886	0.705310
81	6	0.000000	5.912886	-0.705310
82	6	0.000000	2.822196	-2.946911
83	6	0.000000	1.258324	-1.387423
84	6	0.000000	3.492585	-4.177245
85	6	0.000000	4.894589	-4.177180
86	6	0.000000	3.492585	4.177245
87	6	0.000000	4.894589	4.177180
88	6	0.000000	0.000000	0.731396
89	6	0.000000	0.000000	-0.731396
90	6	0.000000	8.387004	-0.731285
91	8	0.000000	6.941216	-2.757418
92	8	0.000000	1.445853	-2.757512
93	8	0.000000	6.941216	2.757418
94	1	0.000000	2.937550	-5.110594
95	1	0.000000	5.449727	-5.110475
96	1	0.000000	2.937550	5.110594
97	1	0.000000	5.449727	5.110475
98	6	0.000000	8.387004	0.731285
99	6	0.000000	9.645802	-1.387941
100	6	0.000000	9.645802	1.387941
101	6	0.000000	10.860880	0.705587
102	6	0.000000	10.860880	-0.705587
103	6	0.000000	11.880228	1.713069
104	6	0.000000	13.279374	1.711570
105	6	0.000000	14.293161	0.698733
106	6	0.000000	14.293161	-0.698733
107	6	0.000000	13.279374	-1.711570
108	6	0.000000	11.880228	-1.713069
109	6	0.000000	15.523789	1.375616
110	6	0.000000	16.752884	0.701544
111	6	0.000000	16.752884	-0.701544
112	6	0.000000	15.523789	-1.375616
113	6	0.000000	11.209592	-2.947809
114	6	0.000000	11.883525	-4.176242
115	6	0.000000	13.285875	-4.173345
116	6	0.000000	13.956997	-2.941968
117	8	0.000000	9.832542	-2.758220
118	8	0.000000	15.333026	-2.752136
119	8	0.000000	15.333026	2.752136
120	8	0.000000	9.832542	2.758220
121	1	0.000000	13.841104	5.106685
122	1	0.000000	11.331215	5.111306
123	1	0.000000	17.687860	1.254131
124	1	0.000000	17.687860	-1.254131
125	1	0.000000	11.331215	-5.111306
126	1	0.000000	13.841104	-5.106685

Table S12. The optimized Cartesian coordinates of the 1D ribbons (n=9) calculated at the B3LYP/6-21G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	4.177058	7.685522
2	6	0.000000	2.946713	9.757744
3	6	0.000000	4.177054	9.087462
4	6	0.000000	2.946711	7.015236
5	8	0.000000	2.752039	36.298291
6	6	0.000000	-2.947622	32.174981
7	6	0.000000	-1.387957	30.611274
8	6	0.000000	1.387957	30.611274
9	6	0.000000	2.947622	32.174981
10	6	0.000000	2.941845	34.922371
11	6	0.000000	1.375656	36.489046
12	6	0.000000	-1.712937	32.845510

13	6	0.000000	-1.711492	34.244710
14	6	0.000000	-0.698760	35.258483
15	6	0.000000	0.698760	35.258483
16	6	0.000000	1.711492	34.244710
17	6	0.000000	1.712937	32.845510
18	6	0.000000	0.705487	31.826315
19	6	0.000000	-0.705487	31.826315
20	6	0.000000	-2.941845	34.922371
21	6	0.000000	-1.375656	36.489046
22	6	0.000000	-4.173204	34.251101
23	6	0.000000	-4.176034	32.848805
24	6	0.000000	4.173204	34.251101
25	6	0.000000	4.176034	32.848805
26	6	0.000000	0.701466	37.718098
27	6	0.000000	-0.701466	37.718098
28	8	0.000000	-2.757754	30.797776
29	8	0.000000	-2.752039	36.298291
30	8	0.000000	2.757754	30.797776
31	1	0.000000	-5.106535	34.806427
32	1	0.000000	-5.111046	32.296397
33	1	0.000000	1.254119	38.653034
34	1	0.000000	-1.254119	38.653034
35	1	0.000000	5.106535	34.806427
36	1	0.000000	5.111046	32.296397
37	8	0.000000	2.757012	27.907352
38	6	0.000000	-2.946720	23.788366
39	6	0.000000	-1.387471	22.224481
40	6	0.000000	1.387471	22.224481
41	6	0.000000	2.946720	23.788366
42	6	0.000000	2.946578	26.530932
43	6	0.000000	1.387291	28.094844
44	6	0.000000	-1.711628	24.459251
45	6	0.000000	-1.711564	25.859899
46	6	0.000000	-0.705212	26.878881
47	6	0.000000	0.705212	26.878881
48	6	0.000000	1.711564	25.859899
49	6	0.000000	1.711628	24.459251
50	6	0.000000	0.705333	23.440210
51	6	0.000000	-0.705333	23.440210
52	6	0.000000	-2.946578	26.530932
53	6	0.000000	-1.387291	28.094844
54	6	0.000000	-4.176944	25.860646
55	6	0.000000	-4.177042	24.458691
56	6	0.000000	4.176944	25.860646
57	6	0.000000	4.177042	24.458691
58	6	0.000000	0.731186	29.352763
59	6	0.000000	-0.731186	29.352763
60	8	0.000000	-2.757158	22.411843
61	8	0.000000	-2.757012	27.907352
62	8	0.000000	2.757158	22.411843
63	1	0.000000	-5.110131	26.415985
64	1	0.000000	-5.110314	23.903484
65	1	0.000000	5.110131	26.415985
66	1	0.000000	5.110314	23.903484
67	8	0.000000	2.757125	19.520712
68	6	0.000000	-2.946715	15.401779
69	6	0.000000	-1.387456	13.837936
70	6	0.000000	1.387456	13.837936
71	6	0.000000	2.946715	15.401779
72	6	0.000000	2.946710	18.144301
73	6	0.000000	1.387439	19.708135
74	6	0.000000	-1.711632	16.072714
75	6	0.000000	-1.711619	17.473373
76	6	0.000000	-0.705337	18.492390
77	6	0.000000	0.705337	18.492390
78	6	0.000000	1.711619	17.473373
79	6	0.000000	1.711632	16.072714
80	6	0.000000	0.705334	15.053693
81	6	0.000000	-0.705334	15.053693
82	6	0.000000	-2.946710	18.144301
83	6	0.000000	-1.387439	19.708135
84	6	0.000000	-4.177068	17.474021
85	6	0.000000	-4.177083	16.072037
86	6	0.000000	4.177068	17.474021
87	6	0.000000	4.177083	16.072037
88	6	0.000000	0.731320	20.966340
89	6	0.000000	-0.731320	20.966340
90	6	0.000000	-0.731323	12.579768
91	8	0.000000	-2.757122	14.025334

92	8	0.000000	-2.757125	19.520712
93	8	0.000000	2.757122	14.025334
94	1	0.000000	-5.110330	18.029278
95	1	0.000000	-5.110350	15.516793
96	1	0.000000	5.110330	18.029278
97	1	0.000000	5.110350	15.516793
98	6	0.000000	0.731323	12.579768
99	6	0.000000	-1.387458	11.321591
100	6	0.000000	1.387458	11.321591
101	6	0.000000	0.705338	10.105858
102	6	0.000000	-0.705338	10.105858
103	6	0.000000	1.711617	9.086844
104	6	0.000000	1.711628	7.686185
105	6	0.000000	0.705346	6.667163
106	6	0.000000	-0.705346	6.667163
107	6	0.000000	-1.711628	7.686185
108	6	0.000000	-1.711617	9.086844
109	6	0.000000	1.387464	5.451425
110	6	0.000000	-0.731303	4.193264
111	6	0.000000	-1.387464	5.451425
112	6	0.000000	-2.946713	9.757744
113	6	0.000000	-4.177054	9.087462
114	6	0.000000	-4.177058	7.685522
115	6	0.000000	-2.946711	7.015236
116	8	0.000000	-2.757140	11.134199
117	8	0.000000	-2.757140	5.638821
118	8	0.000000	2.757140	5.638821
119	8	0.000000	2.757140	11.134199
120	1	0.000000	5.110301	7.130273
121	1	0.000000	5.110295	9.642720
122	1	0.000000	-5.110295	9.642720
123	1	0.000000	-5.110301	7.130273
124	8	0.000000	2.757128	2.747687
125	6	0.000000	-2.946719	-1.371284
126	6	0.000000	-1.387464	-2.935097
127	6	0.000000	1.387464	-2.935097
128	6	0.000000	2.946719	-1.371284
129	6	0.000000	2.946719	1.371284
130	6	0.000000	1.387464	2.935097
131	6	0.000000	-1.711633	-0.700334
132	6	0.000000	-1.711633	0.700334
133	6	0.000000	-0.705344	1.719360
134	6	0.000000	0.705344	1.719360
135	6	0.000000	1.711633	0.700334
136	6	0.000000	1.711633	-0.700334
137	6	0.000000	0.705344	-1.719360
138	6	0.000000	-0.705344	-1.719360
139	6	0.000000	-2.946719	1.371284
140	6	0.000000	-1.387464	2.935097
141	6	0.000000	-4.177064	0.700982
142	6	0.000000	-4.177064	-0.700982
143	6	0.000000	4.177064	0.700982
144	6	0.000000	4.177064	-0.700982
145	6	0.000000	0.731303	4.193264
146	8	0.000000	-2.757128	-2.747687
147	8	0.000000	-2.757128	2.747687
148	8	0.000000	2.757128	-2.747687
149	1	0.000000	-5.110316	1.256227
150	1	0.000000	-5.110316	-1.256227
151	1	0.000000	5.110316	1.256227
152	1	0.000000	5.110316	-1.256227
153	8	0.000000	2.757140	-5.638821
154	6	0.000000	-2.946713	-9.757744
155	6	0.000000	-1.387458	-11.321591
156	6	0.000000	1.387458	-11.321591
157	6	0.000000	2.946713	-9.757744
158	6	0.000000	2.946711	-7.015236
159	6	0.000000	1.387464	-5.451425
160	6	0.000000	-1.711617	-9.086844
161	6	0.000000	-1.711628	-7.686185
162	6	0.000000	-0.705346	-6.667163
163	6	0.000000	0.705346	-6.667163
164	6	0.000000	1.711628	-7.686185
165	6	0.000000	1.711617	-9.086844
166	6	0.000000	0.705338	-10.105858
167	6	0.000000	-0.705338	-10.105858
168	6	0.000000	-2.946711	-7.015236
169	6	0.000000	-1.387464	-5.451425
170	6	0.000000	-4.177058	-7.685522

171	6	0.000000	-4.177054	-9.087462
172	6	0.000000	4.177058	-7.685522
173	6	0.000000	4.177054	-9.087462
174	6	0.000000	0.731303	-4.193264
175	6	0.000000	-0.731303	-4.193264
176	8	0.000000	-2.757140	-11.134199
177	8	0.000000	-2.757140	-5.638821
178	8	0.000000	2.757140	-11.134199
179	1	0.000000	-5.110301	-7.130273
180	1	0.000000	-5.110295	-9.642720
181	1	0.000000	5.110301	-7.130273
182	1	0.000000	5.110295	-9.642720
183	8	0.000000	2.757122	-14.025334
184	6	0.000000	-2.946710	-18.144301
185	6	0.000000	-1.387439	-19.708135
186	6	0.000000	1.387439	-19.708135
187	6	0.000000	2.946710	-18.144301
188	6	0.000000	2.946715	-15.401779
189	6	0.000000	1.387456	-13.837936
190	6	0.000000	-1.711619	-17.473373
191	6	0.000000	-1.711632	-16.072714
192	6	0.000000	-0.705334	-15.053693
193	6	0.000000	0.705334	-15.053693
194	6	0.000000	1.711632	-16.072714
195	6	0.000000	1.711619	-17.473373
196	6	0.000000	0.705337	-18.492390
197	6	0.000000	-0.705337	-18.492390
198	6	0.000000	-2.946715	-15.401779
199	6	0.000000	-1.387456	-13.837936
200	6	0.000000	-4.177083	-16.072037
201	6	0.000000	-4.177068	-17.474021
202	6	0.000000	4.177083	-16.072037
203	6	0.000000	4.177068	-17.474021
204	6	0.000000	0.731323	-12.579768
205	6	0.000000	-0.731323	-12.579768
206	6	0.000000	-0.731320	-20.966340
207	8	0.000000	-2.757125	-19.520712
208	8	0.000000	-2.757122	-14.025334
209	8	0.000000	2.757125	-19.520712
210	1	0.000000	-5.110350	-15.516793
211	1	0.000000	-5.110330	-18.029278
212	1	0.000000	5.110350	-15.516793
213	1	0.000000	5.110330	-18.029278
214	6	0.000000	0.731320	-20.966340
215	6	0.000000	4.176944	-25.860646
216	6	0.000000	2.946720	-23.788366
217	6	0.000000	4.177042	-24.458691
218	6	0.000000	2.946578	-26.530932
219	6	0.000000	-1.387471	-22.224481
220	6	0.000000	1.387471	-22.224481
221	6	0.000000	0.705333	-23.440210
222	6	0.000000	-0.705333	-23.440210
223	6	0.000000	1.711628	-24.459251
224	6	0.000000	1.711564	-25.859899
225	6	0.000000	0.705212	-26.878881
226	6	0.000000	-0.705212	-26.878881
227	6	0.000000	-1.711564	-25.859899
228	6	0.000000	-1.711628	-24.459251
229	6	0.000000	1.387291	-28.094844
230	6	0.000000	0.731186	-29.352763
231	6	0.000000	-0.731186	-29.352763
232	6	0.000000	-1.387291	-28.094844
233	6	0.000000	-2.946720	-23.788366
234	6	0.000000	-4.177042	-24.458691
235	6	0.000000	-4.176944	-25.860646
236	6	0.000000	-2.946578	-26.530932
237	8	0.000000	-2.757158	-22.411843
238	8	0.000000	-2.757012	-27.907352
239	8	0.000000	2.757012	-27.907352
240	8	0.000000	2.757158	-22.411843
241	1	0.000000	5.110131	-26.415985
242	1	0.000000	5.110314	-23.903484
243	1	0.000000	-5.110314	-23.903484
244	1	0.000000	-5.110131	-26.415985
245	6	0.000000	4.173204	-34.251101
246	6	0.000000	2.947622	-32.174981
247	6	0.000000	4.176034	-32.848805
248	6	0.000000	2.941845	-34.922371
249	6	0.000000	-1.387957	-30.611274

250	6	0.000000	1.387957	-30.611274
251	6	0.000000	0.705487	-31.826315
252	6	0.000000	-0.705487	-31.826315
253	6	0.000000	1.712937	-32.845510
254	6	0.000000	1.711492	-34.244710
255	6	0.000000	0.698760	-35.258483
256	6	0.000000	-0.698760	-35.258483
257	6	0.000000	-1.711492	-34.244710
258	6	0.000000	-1.712937	-32.845510
259	6	0.000000	1.375656	-36.489046
260	6	0.000000	0.701466	-37.718098
261	6	0.000000	-0.701466	-37.718098
262	6	0.000000	-1.375656	-36.489046
263	6	0.000000	-2.947622	-32.174981
264	6	0.000000	-4.176034	-32.848805
265	6	0.000000	-4.173204	-34.251101
266	6	0.000000	-2.941845	-34.922371
267	8	0.000000	-2.757754	-30.797776
268	8	0.000000	-2.752039	-36.298291
269	8	0.000000	2.752039	-36.298291
270	8	0.000000	2.757754	-30.797776
271	1	0.000000	5.106535	-34.806427
272	1	0.000000	5.111046	-32.296397
273	1	0.000000	1.254119	-38.653034
274	1	0.000000	-1.254119	-38.653034
275	1	0.000000	-5.111046	-32.296397
276	1	0.000000	-5.106535	-34.806427

Table S13. The optimized Cartesian coordinates of the 1D ribbons (n=16) calculated at the B3LYP/6–21G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	-37.038658	4.177036
2	6	0.000000	-39.110899	2.946681
3	6	0.000000	-38.440614	4.177013
4	6	0.000000	-36.368344	2.946693
5	8	0.000000	-65.651764	2.752082
6	6	0.000000	-61.528397	-2.947665
7	6	0.000000	-59.964739	-1.388139
8	6	0.000000	-59.964739	1.388139
9	6	0.000000	-61.528397	2.947665
10	6	0.000000	-64.275910	2.941869
11	6	0.000000	-65.842517	1.375731
12	6	0.000000	-62.199015	-1.713002
13	6	0.000000	-63.598225	-1.711535
14	6	0.000000	-64.611986	-0.698756
15	6	0.000000	-64.611986	0.698756
16	6	0.000000	-63.598225	1.711535
17	6	0.000000	-62.199015	1.713002
18	6	0.000000	-61.179778	0.705533
19	6	0.000000	-61.179778	-0.705533
20	6	0.000000	-64.275910	-2.941869
21	6	0.000000	-65.842517	-1.375731
22	6	0.000000	-63.604631	-4.173187
23	6	0.000000	-62.202359	-4.176049
24	6	0.000000	-63.604631	4.173187
25	6	0.000000	-62.202359	4.176049
26	6	0.000000	-67.071569	0.701491
27	6	0.000000	-67.071569	-0.701491
28	8	0.000000	-60.151244	-2.758022
29	8	0.000000	-65.651764	-2.752082
30	8	0.000000	-60.151244	2.758022
31	1	0.000000	-64.159877	-5.106527
32	1	0.000000	-61.649963	-5.111073
33	1	0.000000	-68.006558	1.254083
34	1	0.000000	-68.006558	-1.254083
35	1	0.000000	-64.159877	5.106527
36	1	0.000000	-61.649963	5.111073
37	8	0.000000	-57.260514	2.757111
38	6	0.000000	-53.141576	-2.946698
39	6	0.000000	-51.577741	-1.387541
40	6	0.000000	-51.577741	1.387541
41	6	0.000000	-53.141576	2.946698

42	6	0.000000	-55.884189	2.946580
43	6	0.000000	-57.448044	1.387368
44	6	0.000000	-53.812523	-1.711627
45	6	0.000000	-55.213140	-1.711563
46	6	0.000000	-56.232106	-0.705210
47	6	0.000000	-56.232106	0.705210
48	6	0.000000	-55.213140	1.711563
49	6	0.000000	-53.812523	1.711627
50	6	0.000000	-52.793476	0.705325
51	6	0.000000	-52.793476	-0.705325
52	6	0.000000	-55.884189	-2.946580
53	6	0.000000	-57.448044	-1.387368
54	6	0.000000	-55.213871	-4.176922
55	6	0.000000	-53.811912	-4.177007
56	6	0.000000	-55.213871	4.176922
57	6	0.000000	-53.811912	4.177007
58	6	0.000000	-58.706083	0.731264
59	6	0.000000	-58.706083	-0.731264
60	8	0.000000	-51.765123	-2.757197
61	8	0.000000	-57.260514	-2.757111
62	8	0.000000	-51.765123	2.757197
63	1	0.000000	-55.769115	-5.110159
64	1	0.000000	-53.256776	-5.110306
65	1	0.000000	-55.769115	5.110159
66	1	0.000000	-53.256776	5.110306
67	8	0.000000	-48.873956	2.757317
68	6	0.000000	-44.754891	-2.946785
69	6	0.000000	-43.191137	-1.387643
70	6	0.000000	-43.191137	1.387643
71	6	0.000000	-44.754891	2.946785
72	6	0.000000	-47.497569	2.946780
73	6	0.000000	-49.061309	1.387625
74	6	0.000000	-45.425889	-1.711718
75	6	0.000000	-46.826577	-1.711704
76	6	0.000000	-47.845591	-0.705382
77	6	0.000000	-47.845591	0.705382
78	6	0.000000	-46.826577	1.711704
79	6	0.000000	-45.425889	1.711718
80	6	0.000000	-44.406873	0.705376
81	6	0.000000	-44.406873	-0.705376
82	6	0.000000	-47.497569	-2.946780
83	6	0.000000	-49.061309	-1.387625
84	6	0.000000	-46.827197	-4.177076
85	6	0.000000	-45.425242	-4.177092
86	6	0.000000	-46.827197	4.177076
87	6	0.000000	-45.425242	4.177092
88	6	0.000000	-50.319530	0.731387
89	6	0.000000	-50.319530	-0.731387
90	6	0.000000	-41.932966	-0.731390
91	8	0.000000	-43.378464	-2.757320
92	8	0.000000	-48.873956	-2.757317
93	8	0.000000	-43.378464	2.757320
94	1	0.000000	-47.382376	-5.110347
95	1	0.000000	-44.870074	-5.110368
96	1	0.000000	-47.382376	5.110347
97	1	0.000000	-44.870074	5.110368
98	6	0.000000	-41.932966	0.731390
99	6	0.000000	-40.674708	-1.387505
100	6	0.000000	-40.674708	1.387505
101	6	0.000000	-39.458972	0.705325
102	6	0.000000	-39.458972	-0.705325
103	6	0.000000	-38.439947	1.711606
104	6	0.000000	-37.039330	1.711613
105	6	0.000000	-36.020313	0.705330
106	6	0.000000	-36.020313	-0.705330
107	6	0.000000	-37.039330	-1.711613
108	6	0.000000	-38.439947	-1.711606
109	6	0.000000	-34.804578	1.387501
110	6	0.000000	-33.546352	-0.731394
111	6	0.000000	-34.804578	-1.387501
112	6	0.000000	-39.110899	-2.946681
113	6	0.000000	-38.440614	-4.177013
114	6	0.000000	-37.038658	-4.177036
115	6	0.000000	-36.368344	-2.946693
116	8	0.000000	-40.487299	-2.757160
117	8	0.000000	-34.992017	-2.757194
118	8	0.000000	-34.992017	2.757194
119	8	0.000000	-40.487299	2.757160
120	1	0.000000	-36.483475	5.110310

121	1	0.000000	-38.995819	5.110274
122	1	0.000000	-38.995819	-5.110274
123	1	0.000000	-36.483475	-5.110310
124	8	0.000000	-32.100736	2.757301
125	6	0.000000	-27.981732	-2.946764
126	6	0.000000	-26.417981	-1.387620
127	6	0.000000	-26.417981	1.387620
128	6	0.000000	-27.981732	2.946764
129	6	0.000000	-30.724418	2.946772
130	6	0.000000	-32.288132	1.387592
131	6	0.000000	-28.652731	-1.711700
132	6	0.000000	-30.053402	-1.711695
133	6	0.000000	-31.072411	-0.705377
134	6	0.000000	-31.072411	0.705377
135	6	0.000000	-30.053402	1.711695
136	6	0.000000	-28.652731	1.711700
137	6	0.000000	-27.633722	0.705369
138	6	0.000000	-27.633722	-0.705369
139	6	0.000000	-30.724418	-2.946772
140	6	0.000000	-32.288132	-1.387592
141	6	0.000000	-30.054028	-4.177084
142	6	0.000000	-28.652081	-4.177075
143	6	0.000000	-30.054028	4.177084
144	6	0.000000	-28.652081	4.177075
145	6	0.000000	-33.546352	0.731394
146	8	0.000000	-26.605313	-2.757278
147	8	0.000000	-32.100736	-2.757301
148	8	0.000000	-26.605313	2.757278
149	1	0.000000	-30.609198	-5.110364
150	1	0.000000	-28.096901	-5.110347
151	1	0.000000	-30.609198	5.110364
152	1	0.000000	-28.096901	5.110347
153	8	0.000000	-23.714163	2.757217
154	6	0.000000	-19.595189	-2.946720
155	6	0.000000	-18.031403	-1.387553
156	6	0.000000	-18.031403	1.387553
157	6	0.000000	-19.595189	2.946720
158	6	0.000000	-22.337765	2.946718
159	6	0.000000	-23.901546	1.387550
160	6	0.000000	-20.266155	-1.711642
161	6	0.000000	-21.666803	-1.711639
162	6	0.000000	-22.685813	-0.705340
163	6	0.000000	-22.685813	0.705340
164	6	0.000000	-21.666803	1.711639
165	6	0.000000	-20.266155	1.711642
166	6	0.000000	-19.247142	0.705342
167	6	0.000000	-19.247142	-0.705342
168	6	0.000000	-22.337765	-2.946718
169	6	0.000000	-23.901546	-1.387550
170	6	0.000000	-21.667452	-4.177043
171	6	0.000000	-20.265500	-4.177047
172	6	0.000000	-21.667452	4.177043
173	6	0.000000	-20.265500	4.177047
174	6	0.000000	-25.159775	0.731382
175	6	0.000000	-25.159775	-0.731382
176	8	0.000000	-18.218785	-2.757220
177	8	0.000000	-23.714163	-2.757217
178	8	0.000000	-18.218785	2.757220
179	1	0.000000	-22.222634	-5.110314
180	1	0.000000	-19.710318	-5.110318
181	1	0.000000	-22.222634	5.110314
182	1	0.000000	-19.710318	5.110318
183	8	0.000000	-15.327599	2.757264
184	6	0.000000	-11.208575	-2.946751
185	6	0.000000	-9.644809	-1.387590
186	6	0.000000	-9.644809	1.387590
187	6	0.000000	-11.208575	2.946751
188	6	0.000000	-13.951195	2.946751
189	6	0.000000	-15.514960	1.387592
190	6	0.000000	-11.879552	-1.711674
191	6	0.000000	-13.280218	-1.711674
192	6	0.000000	-14.299226	-0.705360
193	6	0.000000	-14.299226	0.705360
194	6	0.000000	-13.280218	1.711674
195	6	0.000000	-11.879552	1.711674
196	6	0.000000	-10.860544	0.705359
197	6	0.000000	-10.860544	-0.705359
198	6	0.000000	-13.951195	-2.946751
199	6	0.000000	-15.514960	-1.387592

200	6	0.000000	-13.280860	-4.177067
201	6	0.000000	-11.878909	-4.177068
202	6	0.000000	-13.280860	4.177067
203	6	0.000000	-11.878909	4.177068
204	6	0.000000	-16.773177	0.731382
205	6	0.000000	-16.773177	-0.731382
206	6	0.000000	-8.386595	-0.731382
207	8	0.000000	-9.832170	-2.757261
208	8	0.000000	-15.327599	-2.757264
209	8	0.000000	-9.832170	2.757261
210	1	0.000000	-13.836036	-5.110339
211	1	0.000000	-11.323732	-5.110341
212	1	0.000000	-13.836036	5.110339
213	1	0.000000	-11.323732	5.110341
214	6	0.000000	-8.386595	0.731382
215	6	0.000000	-3.492325	4.177057
216	6	0.000000	-5.564597	2.946736
217	6	0.000000	-4.894277	4.177057
218	6	0.000000	-2.822007	2.946735
219	6	0.000000	-7.128374	-1.387570
220	6	0.000000	-7.128374	1.387570
221	6	0.000000	-5.912641	0.705349
222	6	0.000000	-5.912641	-0.705349
223	6	0.000000	-4.893631	1.711656
224	6	0.000000	-3.492973	1.711655
225	6	0.000000	-2.473966	0.705349
226	6	0.000000	-2.473966	-0.705349
227	6	0.000000	-3.492973	-1.711655
228	6	0.000000	-4.893631	-1.711656
229	6	0.000000	-1.258224	1.387575
230	6	0.000000	-1.258224	-1.387575
231	6	0.000000	-5.564597	-2.946736
232	6	0.000000	-4.894277	-4.177057
233	6	0.000000	-3.492325	-4.177057
234	6	0.000000	-2.822007	-2.946735
235	8	0.000000	-6.941001	-2.757239
236	8	0.000000	-1.445594	-2.757237
237	8	0.000000	-1.445594	2.757237
238	8	0.000000	-6.941001	2.757239
239	1	0.000000	-2.937145	5.110328
240	1	0.000000	-5.449457	5.110330
241	1	0.000000	-5.449457	-5.110330
242	1	0.000000	-2.937145	-5.110328
243	6	0.000000	30.054028	4.177084
244	6	0.000000	27.981732	2.946764
245	6	0.000000	28.652081	4.177075
246	6	0.000000	30.724418	2.946772
247	8	0.000000	1.445594	2.757237
248	6	0.000000	5.564597	-2.946736
249	6	0.000000	7.128374	-1.387570
250	6	0.000000	7.128374	1.387570
251	6	0.000000	5.564597	2.946736
252	6	0.000000	2.822007	2.946735
253	6	0.000000	1.258224	1.387575
254	6	0.000000	4.893631	-1.711656
255	6	0.000000	3.492973	-1.711655
256	6	0.000000	2.473966	-0.705349
257	6	0.000000	2.473966	0.705349
258	6	0.000000	3.492973	1.711655
259	6	0.000000	4.893631	1.711656
260	6	0.000000	5.912641	0.705349
261	6	0.000000	5.912641	-0.705349
262	6	0.000000	2.822007	-2.946735
263	6	0.000000	1.258224	-1.387575
264	6	0.000000	3.492325	-4.177057
265	6	0.000000	4.894277	-4.177057
266	6	0.000000	3.492325	4.177057
267	6	0.000000	4.894277	4.177057
268	6	0.000000	0.000000	0.731398
269	6	0.000000	0.000000	-0.731398
270	8	0.000000	6.941001	-2.757239
271	8	0.000000	1.445594	-2.757237
272	8	0.000000	6.941001	2.757239
273	1	0.000000	2.937145	-5.110328
274	1	0.000000	5.449457	-5.110330
275	1	0.000000	2.937145	5.110328
276	1	0.000000	5.449457	5.110330
277	8	0.000000	9.832170	2.757261
278	6	0.000000	13.951195	-2.946751

279	6	0.000000	15.514960	-1.387592
280	6	0.000000	15.514960	1.387592
281	6	0.000000	13.951195	2.946751
282	6	0.000000	11.208575	2.946751
283	6	0.000000	9.644809	1.387590
284	6	0.000000	13.280218	-1.711674
285	6	0.000000	11.879552	-1.711674
286	6	0.000000	10.860544	-0.705359
287	6	0.000000	10.860544	0.705359
288	6	0.000000	11.879552	1.711674
289	6	0.000000	13.280218	1.711674
290	6	0.000000	14.299226	0.705360
291	6	0.000000	14.299226	-0.705360
292	6	0.000000	11.208575	-2.946751
293	6	0.000000	9.644809	-1.387590
294	6	0.000000	11.878909	-4.177068
295	6	0.000000	13.280860	-4.177067
296	6	0.000000	11.878909	4.177068
297	6	0.000000	13.280860	4.177067
298	6	0.000000	8.386595	0.731382
299	6	0.000000	8.386595	-0.731382
300	8	0.000000	15.327599	-2.757264
301	8	0.000000	9.832170	-2.757261
302	8	0.000000	15.327599	2.757264
303	1	0.000000	11.323732	-5.110341
304	1	0.000000	13.836036	-5.110339
305	1	0.000000	11.323732	5.110341
306	1	0.000000	13.836036	5.110339
307	8	0.000000	18.218785	2.757220
308	6	0.000000	22.337765	-2.946718
309	6	0.000000	23.901546	-1.387550
310	6	0.000000	23.901546	1.387550
311	6	0.000000	22.337765	2.946718
312	6	0.000000	19.595189	2.946720
313	6	0.000000	18.031403	1.387553
314	6	0.000000	21.666803	-1.711639
315	6	0.000000	20.266155	-1.711642
316	6	0.000000	19.247142	-0.705342
317	6	0.000000	19.247142	0.705342
318	6	0.000000	20.266155	1.711642
319	6	0.000000	21.666803	1.711639
320	6	0.000000	22.685813	0.705340
321	6	0.000000	22.685813	-0.705340
322	6	0.000000	19.595189	-2.946720
323	6	0.000000	18.031403	-1.387553
324	6	0.000000	20.265500	-4.177047
325	6	0.000000	21.667452	-4.177043
326	6	0.000000	20.265500	4.177047
327	6	0.000000	21.667452	4.177043
328	6	0.000000	16.773177	0.731382
329	6	0.000000	16.773177	-0.731382
330	6	0.000000	25.159775	-0.731382
331	8	0.000000	23.714163	-2.757217
332	8	0.000000	18.218785	-2.757220
333	8	0.000000	23.714163	2.757217
334	1	0.000000	19.710318	-5.110318
335	1	0.000000	22.222634	-5.110314
336	1	0.000000	19.710318	5.110318
337	1	0.000000	22.222634	5.110314
338	6	0.000000	25.159775	0.731382
339	6	0.000000	26.417981	-1.387620
340	6	0.000000	26.417981	1.387620
341	6	0.000000	27.633722	0.705369
342	6	0.000000	27.633722	-0.705369
343	6	0.000000	28.652731	1.711700
344	6	0.000000	30.053402	1.711695
345	6	0.000000	31.072411	0.705377
346	6	0.000000	31.072411	-0.705377
347	6	0.000000	30.053402	-1.711695
348	6	0.000000	28.652731	-1.711700
349	6	0.000000	32.288132	1.387592
350	6	0.000000	33.546352	-0.731394
351	6	0.000000	32.288132	-1.387592
352	6	0.000000	27.981732	-2.946764
353	6	0.000000	28.652081	-4.177075
354	6	0.000000	30.054028	-4.177084
355	6	0.000000	30.724418	-2.946772
356	8	0.000000	26.605313	-2.757278
357	8	0.000000	32.100736	-2.757301

358	8	0.000000	32.100736	2.757301
359	8	0.000000	26.605313	2.757278
360	1	0.000000	30.609198	5.110364
361	1	0.000000	28.096901	5.110347
362	1	0.000000	28.096901	-5.110347
363	1	0.000000	30.609198	-5.110364
364	8	0.000000	34.992017	2.757194
365	6	0.000000	39.110899	-2.946681
366	6	0.000000	40.674708	-1.387505
367	6	0.000000	40.674708	1.387505
368	6	0.000000	39.110899	2.946681
369	6	0.000000	36.368344	2.946693
370	6	0.000000	34.804578	1.387501
371	6	0.000000	38.439947	-1.711606
372	6	0.000000	37.039330	-1.711613
373	6	0.000000	36.020313	-0.705330
374	6	0.000000	36.020313	0.705330
375	6	0.000000	37.039330	1.711613
376	6	0.000000	38.439947	1.711606
377	6	0.000000	39.458972	0.705325
378	6	0.000000	39.458972	-0.705325
379	6	0.000000	36.368344	-2.946693
380	6	0.000000	34.804578	-1.387501
381	6	0.000000	37.038658	-4.177036
382	6	0.000000	38.440614	-4.177013
383	6	0.000000	37.038658	4.177036
384	6	0.000000	38.440614	4.177013
385	6	0.000000	33.546352	0.731394
386	8	0.000000	40.487299	-2.757160
387	8	0.000000	34.992017	-2.757194
388	8	0.000000	40.487299	2.757160
389	1	0.000000	36.483475	-5.110310
390	1	0.000000	38.995819	-5.110274
391	1	0.000000	36.483475	5.110310
392	1	0.000000	38.995819	5.110274
393	8	0.000000	43.378464	2.757320
394	6	0.000000	47.497569	-2.946780
395	6	0.000000	49.061309	-1.387625
396	6	0.000000	49.061309	1.387625
397	6	0.000000	47.497569	2.946780
398	6	0.000000	44.754891	2.946785
399	6	0.000000	43.191137	1.387643
400	6	0.000000	46.826577	-1.711704
401	6	0.000000	45.425889	-1.711718
402	6	0.000000	44.406873	-0.705376
403	6	0.000000	44.406873	0.705376
404	6	0.000000	45.425889	1.711718
405	6	0.000000	46.826577	1.711704
406	6	0.000000	47.845591	0.705382
407	6	0.000000	47.845591	-0.705382
408	6	0.000000	44.754891	-2.946785
409	6	0.000000	43.191137	-1.387643
410	6	0.000000	45.425242	-4.177092
411	6	0.000000	46.827197	-4.177076
412	6	0.000000	45.425242	4.177092
413	6	0.000000	46.827197	4.177076
414	6	0.000000	41.932966	0.731390
415	6	0.000000	41.932966	-0.731390
416	8	0.000000	48.873956	-2.757317
417	8	0.000000	43.378464	-2.757320
418	8	0.000000	48.873956	2.757317
419	1	0.000000	44.870074	-5.110368
420	1	0.000000	47.382376	-5.110347
421	1	0.000000	44.870074	5.110368
422	1	0.000000	47.382376	5.110347
423	8	0.000000	51.765123	2.757197
424	6	0.000000	55.884189	-2.946580
425	6	0.000000	57.448044	-1.387368
426	6	0.000000	57.448044	1.387368
427	6	0.000000	55.884189	2.946580
428	6	0.000000	53.141576	2.946698
429	6	0.000000	51.577741	1.387541
430	6	0.000000	55.213140	-1.711563
431	6	0.000000	53.812523	-1.711627
432	6	0.000000	52.793476	-0.705325
433	6	0.000000	52.793476	0.705325
434	6	0.000000	53.812523	1.711627
435	6	0.000000	55.213140	1.711563
436	6	0.000000	56.232106	0.705210

437	6	0.000000	56.232106	-0.705210
438	6	0.000000	53.141576	-2.946698
439	6	0.000000	51.577741	-1.387541
440	6	0.000000	53.811912	-4.177007
441	6	0.000000	55.213871	-4.176922
442	6	0.000000	53.811912	4.177007
443	6	0.000000	55.213871	4.176922
444	6	0.000000	50.319530	0.731387
445	6	0.000000	50.319530	-0.731387
446	6	0.000000	58.706083	-0.731264
447	8	0.000000	57.260514	-2.757111
448	8	0.000000	51.765123	-2.757197
449	8	0.000000	57.260514	2.757111
450	1	0.000000	53.256776	-5.110306
451	1	0.000000	55.769115	-5.110159
452	1	0.000000	53.256776	5.110306
453	1	0.000000	55.769115	5.110159
454	6	0.000000	58.706083	0.731264
455	6	0.000000	63.604631	4.173187
456	6	0.000000	61.528397	2.947665
457	6	0.000000	62.202359	4.176049
458	6	0.000000	64.275910	2.941869
459	6	0.000000	59.964739	-1.388139
460	6	0.000000	59.964739	1.388139
461	6	0.000000	61.179778	0.705533
462	6	0.000000	61.179778	-0.705533
463	6	0.000000	62.199015	1.713002
464	6	0.000000	63.598225	1.711535
465	6	0.000000	64.611986	0.698756
466	6	0.000000	64.611986	-0.698756
467	6	0.000000	63.598225	-1.711535
468	6	0.000000	62.199015	-1.713002
469	6	0.000000	65.842517	1.375731
470	6	0.000000	67.071569	0.701491
471	6	0.000000	67.071569	-0.701491
472	6	0.000000	65.842517	-1.375731
473	6	0.000000	61.528397	-2.947665
474	6	0.000000	62.202359	-4.176049
475	6	0.000000	63.604631	-4.173187
476	6	0.000000	64.275910	-2.941869
477	8	0.000000	60.151244	-2.758022
478	8	0.000000	65.651764	-2.752082
479	8	0.000000	65.651764	2.752082
480	8	0.000000	60.151244	2.758022
481	1	0.000000	64.159877	5.106527
482	1	0.000000	61.649963	5.111073
483	1	0.000000	61.649963	-5.111073
484	1	0.000000	64.159877	-5.106527
485	1	0.000000	68.006558	1.254083
486	1	0.000000	68.006558	-1.254083
