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Computational study of the structure, UV-vis absorption spectra and conductivity of biphenylene-based polymers and their boron nitride analogues

Nataliya N. Karaush,*[a] Sergey V. Bondarchuk, [a] Gleb V. Baryshnikov,[a,c] Valentina A. Minaeva,[a] Wen-Hua Sun[b] and Boris F. Minaev[a,b]

[a]*Bohdan Khmelnytsky National University, Cherkasy, 18031, Ukraine; E-mail: karaush22@ukr.net, bfmin@rambler.ru*

[b] *Key Laboratory of Engineering Plastics and Beijing National Laboratory for Molecular Science, Institute of Chemistry, Chinese Academy of Science, 100190 Beijing, China*

[c] *Department of Theoretical Chemistry and Biology, School of Biotechnology, KTH Royal Institute of Technology, SE-106 91 Stockholm, Sweden*

Electronic Supplementary Information

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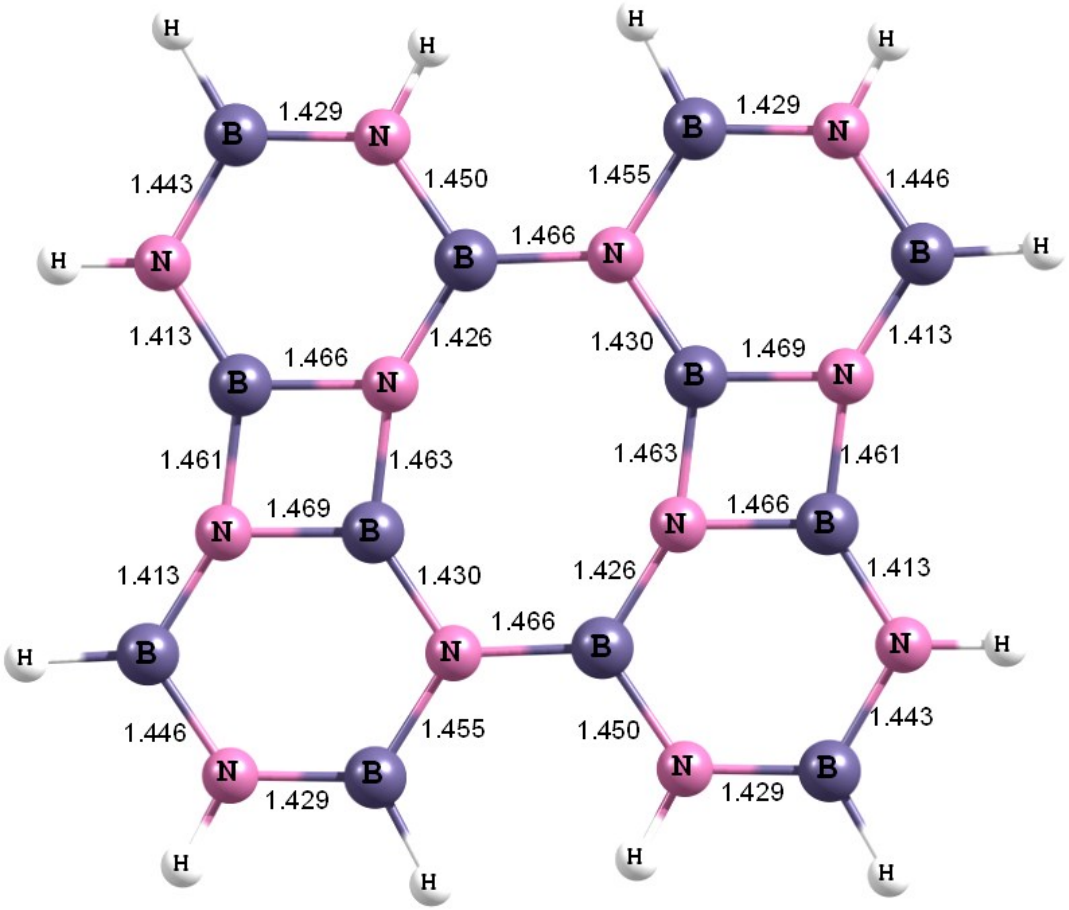

Figure S1. The optimized structure and bond lengths for the S_0 state of the simplest boron nitride ribbon **2** calculated at the B3LYP/6-31G(d) level of theory.

Table S1. Total energy of the ground singlet state of the biphenylene- and boron nitride compounds calculated at the B3LYP/6–31G(d) level of theory

Biphenylene compounds	n×m	E_{tot}, *a.u*	Boron nitride compounds	n×m	E_{tot}, *a.u.*
1	3×1.5	–2068.3054	**1**	3×1.5	–2162.8022
2	3×2	–2755.2797	**2**	3×2	–2881.3638
3	3×3	–4129.2283	**3**	3×3	–4318.4869
4	4×2	–3672.11976	**4**	4×2	–3840.2776
1D armchair ribbons (m=1)	1	–462.0320	1D armchair ribbons (m=1)	1	–482.9572
	2	–921.6809		2	–963.5994
	3	–1381.3305		3	–1444.2423
	4	–1840.9801		4	–1924.8854
	5	–2300.6297		5	–2405.5282
	6	–2760.2793		6	–2886.1712
	7	–3219.9289		7	–3366.8142
	8	–3679.5786		8	–3847.4572
	9	–4139.2282		9	–4328.1002
	10	–4598.8778		10	–4808.7432
1D zigzag ribbons (n=2)	2	–1838.4396	1D zigzag ribbons (n=2)	2	–1922.4502
	3	–2755.1975		3	–2881.3017
	4	–3671.9554		4	–3840.1531
	5	–4588.7133		5	–4799.0044

Table S2. The absorption maxima (λ), assignment and oscillator strength (f) in the electronic absorption spectra of the Bp-based ribbons and sheets calculated by the TD DFT/B3LYP/6-31G(d) method

n×m	State	Assignment	λ_{max}, nm	f	State	Assignment	λ_{max}, nm	f
	I band				II band			
1D armchair Bp-ribbons								
1×1	S_2	$X^1A_g \rightarrow 1^1B_{1u}$	310	0.084	S_4	$X^1A_g \rightarrow 2^1B_{1u}$	231	1.146
2×1	S_3	$X^1A_g \rightarrow 1^1B_{2u}$	407	0.059	S_6	$X^1A_g \rightarrow 3^1B_{2u}$	332	0.087
3×1	S_5	$X^1A_g \rightarrow 3^1B_{2u}$	419	0.089	S_{13}	$X^1A_g \rightarrow 1^1B_{1u}$	331	0.488
4×1	S_7	$X^1A_g \rightarrow 3^1B_{2u}$	436	0.051	S_{16}	$X^1A_g \rightarrow 1^1B_{1u}$	360	0.914
	S_8	$X^1A_g \rightarrow 4^1B_{2u}$	430	0.033				
5×1	S_9	$X^1A_g \rightarrow 5^1B_{2u}$	446	0.030	S_{21}	$X^1A_g \rightarrow 1^1B_{1u}$	380	1.355
6×1	S_{11}	$X^1A_g \rightarrow 5^1B_{2u}$	456	0.021	S_{25}	$X^1A_g \rightarrow 1^1B_{1u}$	394	1.803
	S_{13}	$X^1A_g \rightarrow 6^1B_{2u}$	453	0.016				
7×1	S_{15}	$X^1A_g \rightarrow 8^1B_{2u}$	457	0.068	–	–	–	–
8×1	S_{17}	$X^1A_g \rightarrow 8^1B_{2u}$	460	0.063	–	–	–	–
9×1	S_{19}	$X^1A_g \rightarrow 10^1B_{2u}$	463	0.067	–	–	–	–
10×1	S_{24}	$X^1A_g \rightarrow 12^1B_{2u}$	461	0.034		–	–	–
1D zigzag Bp-ribbons								
2×2	S_5	$X^1Ag \rightarrow 3^1B_{1u}$	583	0.586	S_{17}	$X^1Ag \rightarrow 8^1B_{1u}$	376	0.115
2×3	S_6	$X^1Ag \rightarrow 3^1B_{1u}$	734	1.391	S_{12}	$X^1A_g \rightarrow 4^1B_{2u}$	584	0.021
2×4	S_9	$X^1Ag \rightarrow 3^1B_{1u}$	854	2.370	–	–	–	–
2×5	S_{10}	$X^1Ag \rightarrow 3^1B_{1u}$	957	3.422	–	–	–	–
2D Bp-sheet								
3×1.5	S_6	$X^1Ag \rightarrow 3^1B_{2u}$	552	0.262	S_{24}	$X^1Ag \rightarrow 11^1B_{1u}$	362	0.111
3×2	S_7	$X^1Ag \rightarrow 2^1B_{1u}$	675	0.455	S_{24}	$X^1Ag \rightarrow 10^1B_{1u}$	460	0.251
3×3	S_7	$X^1Ag \rightarrow 1^1B_{1u}$	885	1.029	–	–	–	–
4×2	S_8	$X^1Ag \rightarrow 4^1B_{2u}$	729	0.380	S_{25}	$X^1Ag \rightarrow 12B_{2u}$	538	0.295

Table S3. The wavelength (λ), assignment and oscillator strength (f) in the electronic absorption spectra of the BN-based ribbons and sheets calculated by the TD DFT/B3LYP/6-31G(d) method

n×m	State	Assignment	λ, nm	*f*	State	Assignment	λ, nm	*f*
	I band				II band			
1D armchair BN-ribbons								
1×1	S_2	$X^1A_g \rightarrow 1^1B_u$	214	0.182	–	–	–	–
2×1	S_3	$X^1A_g \rightarrow 1^1B_u$	228	0.051	S_9	$X^1A_g \rightarrow 4^1B_u$	196	0.284
	S_4	$X^1A_g \rightarrow 2^1B_u$	226	0.114	S_{10}	$X^1A_g \rightarrow 5^1B_u$	191	0.149
3×1	S_4	$X^1A_g \rightarrow 2^1B_u$	230	0.057	S_{16}	$X^1A_g \rightarrow 8^1B_u$	201	0.650
	S_6	$X^1A_g \rightarrow 3^1B_u$	228	0.134	S_{18}	$X^1A_g \rightarrow 9^1B_u$	197	0.169
					S_{19}	$X^1A_g \rightarrow 10^1B_u$	195	0.299
4×1	S_6	$X^1A_g \rightarrow 3^1B_u$	229	0.153	S_{22}	$X^1A_g \rightarrow 11^1B_u$	204	1.424
	S_8	$X^1A_g \rightarrow 4^1B_u$	228	0.067	S_{28}	$X^1A_g \rightarrow 14^1B_u$	198	0.271
					S_{30}	$X^1A_g \rightarrow 16^1B_u$	196	0.150
5×1	S_8	$X^1A_g \rightarrow 4^1B_u$	230	0.189	S_{26}	$X^1A_g \rightarrow 18^1B_u$	207	0.564
	S_{10}	$X^1A_g \rightarrow 5^1B_u$	228	0.074	S_{28}	$X^1A_g \rightarrow 19^1B_u$	206	1.376
					S_{29}	$X^1A_g \rightarrow 20^1B_u$	205	0.119
6×1	S_{10}	$X^1A_g \rightarrow 5^1B_u$	230	0.249	S_{32}	$X^1A_g \rightarrow 16^1B_u$	208	1.872
	S_{12}	$X^1A_g \rightarrow 6^1B_u$	228	0.052	S_{34}	$X^1A_g \rightarrow 17^1B_u$	207	0.391
					S_{35}	$X^1A_g \rightarrow 18^1B_u$	206	0.395
7×1	S_{12}	$X^1A_g \rightarrow 6^1B_u$	230	0.297	S_{37}	$X^1A_g \rightarrow 18^1B_u$	210	0.180
	S_{14}	$X^1A_g \rightarrow 7^1B_u$	228	0.049	S_{38}	$X^1A_g \rightarrow 19^1B_u$	209	1.633
					S_{39}	$X^1A_g \rightarrow 20^1B_u$	209	0.680
8×1	S_{14}	$X^1A_g \rightarrow 7^1B_u$	230	0.349	S_{43}	$X^1A_g \rightarrow 21^1B_u$	210	2.127
	S_{16}	$X^1A_g \rightarrow 8^1B_u$	228	0.042	S_{44}	$X^1A_g \rightarrow 22^1B_u$	209	0.335
9×1	S_{16}	$X^1A_g \rightarrow 8^1B_u$	230	0.400	S_{49}	$X^1A_g \rightarrow 25^1B_u$	211	2.347
					S_{51}	$X^1A_g \rightarrow 26^1B_u$	210	1.004
10×1	S_{18}	$X^1A_g \rightarrow 9^1B_{2u}$	230	0.449	S_{55}	$X^1A_g \rightarrow 27^1B_u$	211	0.366
					S_{56}	$X^1A_g \rightarrow 28^1B_u$	211	3.008
					S_{57}	$X^1A_g \rightarrow 29^1B_u$	210	0.468
1D zigzag BN-ribbons								
2×2	S_2	$X^1Ag \rightarrow 1^1B_u$	254	0.658	S_6	$X^1Ag \rightarrow 3^1B_u$	235	0.119
					S_{12}	$X^1Ag \rightarrow 6^1B_u$	220	0.192
					S_{24}	$X^1Ag \rightarrow 12^1B_u$	202	0.581
2×3	S_2	$X^1Ag \rightarrow 1^1B_u$	264	1.357	S_{14}	$X^1A_g \rightarrow 7^1B_u$	231	0.451
					S_{26}	$X^1A_g \rightarrow 13^1B_u$	217	0.734
2×4	S_2	$X^1Ag \rightarrow 1^1B_u$	268	2.140	S_7	$X^1A_g \rightarrow 4^1B_u$	245	0.036
					S_{14}	$X^1A_g \rightarrow 7^1B_u$	237	0.314
					S_{29}	$X^1A_g \rightarrow 15^1B_u$	225	0.579
2×5	S_1	$X^1Ag \rightarrow 1^1B_{1u}$	270	3.015	S_7	$X^1A_g \rightarrow 4^1B_u$	252	0.159
					S_{29}	$X^1A_g \rightarrow 15^1B_u$	231	0.516
2D BN-sheet								
3×1.5	S_1	$X^1A_1 \rightarrow 1^1B_2$	257	0.003				
	S_2	$X^1A_1 \rightarrow 2^1B_2$	254	0.071				
	S_3	$X^1A_1 \rightarrow 3^1B_2$	244	0.318				
	S_6	$X^1A_1 \rightarrow 3^1A_1$	238	0.006				
3×2	S_1	$X^1Ag \rightarrow 1^1B_u$	262	0.022	S_9	$X^1Ag \rightarrow 5^1B_u$	235	0.190
	S_3	$X^1Ag \rightarrow 2^1B_u$	256	0.707	S_{12}	$X^1Ag \rightarrow 6^1B_u$	232	0.055
3×3	S_1	$X^1Ag \rightarrow 1^1B_u$	268	0.342	S_{14}	$X^1Ag \rightarrow 7^1B_u$	239	0.153

	S_3	$X^1Ag \rightarrow 2^1B_u$	264	1.152	S_{17}	$X^1Ag \rightarrow 8^1B_u$	237	0.198
	S_5	$X^1Ag \rightarrow 3^1B_u$	255	0.040	S_{18}	$X^1Ag \rightarrow 9^1B_u$	236	0.258
					S_{19}	$X^1Ag \rightarrow 10^1B_u$	235	0.122
					S_{21}	$X^1Ag \rightarrow 11^1B_u$	234	0.162
4×2	S_2	$X^1Ag \rightarrow 1^1B_u$	262	0.019	S_9	$X^1Ag \rightarrow 6^1B_u$	238	0.095
	S_4	$X^1Ag \rightarrow 2^1B_u$	256	0.844	S_{11}	$X^1Ag \rightarrow 7^1B_u$	237	0.061
					S_{14}	$X^1Ag \rightarrow 8^1B_u$	236	0.207

Table S4. The optimized Cartesian coordinates of the biphenylene sheet **1** (n×m = 3×1.5) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	2.957375
2	6	0.000000	0.000000	1.495698
3	6	0.000000	1.154511	0.705612
4	6	0.000000	1.154511	-0.705612
5	6	0.000000	1.154901	3.745164
6	6	0.000000	0.000000	5.941085
7	6	0.000000	1.156990	5.160876
8	6	0.000000	0.000000	-1.495698
9	6	0.000000	3.811360	1.480454
10	6	0.000000	2.664160	0.710063
11	6	0.000000	3.811360	-1.480454
12	6	0.000000	5.007522	-0.691809
13	6	0.000000	5.007522	0.691809
14	6	0.000000	3.812775	2.960402
15	6	0.000000	5.019094	3.736327
16	6	0.000000	2.663094	3.729414
17	6	0.000000	5.025271	5.121491
18	6	0.000000	2.668131	5.152183
19	6	0.000000	3.825264	5.885851
20	6	0.000000	2.664160	-0.710063
21	1	0.000000	0.000000	7.026291
22	1	0.000000	5.971464	-1.189360
23	1	0.000000	5.971464	1.189360
24	1	0.000000	5.976627	3.226692
25	1	0.000000	5.980206	5.640075
26	1	0.000000	3.851758	6.971204
27	6	0.000000	-3.811360	1.480454
28	6	0.000000	-5.007522	0.691809
29	6	0.000000	-3.811360	-1.480454
30	6	0.000000	-2.664160	-0.710063
31	6	0.000000	-2.664160	0.710063
32	6	0.000000	-3.812775	2.960402
33	6	0.000000	-1.154511	0.705612
34	6	0.000000	-2.663094	3.729414
35	6	0.000000	-1.154901	3.745164
36	6	0.000000	-1.154511	-0.705612
37	6	0.000000	-5.019094	3.736327
38	6	0.000000	-1.156990	5.160876
39	6	0.000000	-2.668131	5.152183
40	6	0.000000	-5.025271	5.121491
41	6	0.000000	-3.825264	5.885851
42	6	0.000000	-5.007522	-0.691809
43	1	0.000000	-3.851758	6.971204
44	6	0.000000	0.000000	-5.941085
45	6	0.000000	1.156990	-5.160876
46	6	0.000000	0.000000	-2.957375
47	6	0.000000	1.154901	-3.745164
48	6	0.000000	3.825264	-5.885851
49	6	0.000000	5.025271	-5.121491
50	6	0.000000	2.668131	-5.152183
51	6	0.000000	5.019094	-3.736327
52	6	0.000000	2.663094	-3.729414

53	6	0.000000	3.812775	-2.960402
54	1	0.000000	5.980206	-5.640075
55	1	0.000000	5.976627	-3.226692
56	6	0.000000	-3.825264	-5.885851
57	6	0.000000	-2.668131	-5.152183
58	6	0.000000	-1.156990	-5.160876
59	6	0.000000	-1.154901	-3.745164
60	6	0.000000	-2.663094	-3.729414
61	6	0.000000	-5.019094	-3.736327
62	6	0.000000	-3.812775	-2.960402
63	6	0.000000	-5.025271	-5.121491
64	1	0.000000	-5.971464	1.189360
65	1	0.000000	-5.976627	3.226692
66	1	0.000000	-5.980206	5.640075
67	1	0.000000	-5.971464	-1.189360
68	1	0.000000	0.000000	-7.026291
69	1	0.000000	3.851758	-6.971204
70	1	0.000000	-3.851758	-6.971204
71	1	0.000000	-5.976627	-3.226692
72	1	0.000000	-5.980206	-5.640075

Table S5. The optimized Cartesian coordinates of the biphenylene sheet **2** (n×m = 3×2) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	5.957199	1.915693
2	6	0.000000	5.166444	3.070185
3	6	0.000000	2.967438	1.899671
4	6	0.000000	3.753891	3.062266
5	6	0.000000	5.885307	5.738192
6	6	0.000000	5.116965	6.937549
7	6	0.000000	5.154814	4.580525
8	6	0.000000	3.733227	6.927344
9	6	0.000000	3.731190	4.570483
10	6	0.000000	2.959479	5.717235
11	1	0.000000	5.633582	7.893497
12	1	0.000000	3.220239	7.882977
13	6	0.000000	-2.967438	1.899671
14	6	0.000000	-1.503027	1.900389
15	6	0.000000	-0.704844	3.057561
16	6	0.000000	0.704844	3.057561
17	6	0.000000	-3.753891	3.062266
18	6	0.000000	-5.957199	1.915693
19	6	0.000000	-5.166444	3.070185
20	6	0.000000	1.503027	1.900389
21	6	0.000000	-1.480344	5.713409
22	6	0.000000	-0.710520	4.567082
23	6	0.000000	1.480344	5.713409
24	6	0.000000	0.690863	6.911438
25	6	0.000000	-0.690863	6.911438
26	6	0.000000	-2.959479	5.717235
27	6	0.000000	-3.733227	6.927344
28	6	0.000000	-3.731190	4.570483
29	6	0.000000	-5.116965	6.937549
30	6	0.000000	-5.154814	4.580525
31	6	0.000000	-5.885307	5.738192
32	6	0.000000	0.710520	4.567082
33	1	0.000000	-7.042266	1.924716
34	1	0.000000	1.189364	7.874786
35	1	0.000000	-1.189364	7.874786
36	1	0.000000	-3.220239	7.882977
37	1	0.000000	-5.633582	7.893497
38	1	0.000000	-6.970494	5.767862
39	6	0.000000	5.957199	-1.915693
40	6	0.000000	5.186106	-0.757111
41	6	0.000000	5.186106	0.757111
42	6	0.000000	3.766779	0.752590
43	6	0.000000	3.766779	-0.752590
44	6	0.000000	3.753891	-3.062266

45	6	0.000000	2.967438	-1.899671
46	6	0.000000	-1.503027	-1.900389
47	6	0.000000	-0.704844	-3.057561
48	6	0.000000	1.503027	-1.900389
49	6	0.000000	0.708011	-0.752792
50	6	0.000000	-0.708011	-0.752792
51	6	0.000000	-2.967438	-1.899671
52	6	0.000000	-0.708011	0.752792
53	6	0.000000	-3.766779	-0.752590
54	6	0.000000	-3.766779	0.752590
55	6	0.000000	0.708011	0.752792
56	6	0.000000	-3.753891	-3.062266
57	6	0.000000	-5.186106	0.757111
58	6	0.000000	-5.186106	-0.757111
59	6	0.000000	-5.166444	-3.070185
60	6	0.000000	-5.957199	-1.915693
61	6	0.000000	0.704844	-3.057561
62	1	0.000000	-7.042266	-1.924716
63	6	0.000000	5.166444	-3.070185
64	6	0.000000	5.885307	-5.738192
65	6	0.000000	5.154814	-4.580525
66	6	0.000000	5.116965	-6.937549
67	6	0.000000	3.731190	-4.570483
68	6	0.000000	3.733227	-6.927344
69	6	0.000000	2.959479	-5.717235
70	1	0.000000	3.220239	-7.882977
71	1	0.000000	5.633582	-7.893497
72	6	0.000000	-1.480344	-5.713409
73	6	0.000000	-0.690863	-6.911438
74	6	0.000000	1.480344	-5.713409
75	6	0.000000	0.710520	-4.567082
76	6	0.000000	-0.710520	-4.567082
77	6	0.000000	-2.959479	-5.717235
78	6	0.000000	-3.731190	-4.570483
79	6	0.000000	-3.733227	-6.927344
80	6	0.000000	-5.154814	-4.580525
81	6	0.000000	-5.116965	-6.937549
82	6	0.000000	-5.885307	-5.738192
83	1	0.000000	-5.633582	-7.893497
84	1	0.000000	-1.189364	-7.874786
85	1	0.000000	-3.220239	-7.882977
86	6	0.000000	0.690863	-6.911438
87	1	0.000000	1.189364	-7.874786
88	1	0.000000	-6.970494	-5.767862
89	1	0.000000	7.042266	1.924716
90	1	0.000000	6.970494	5.767862
91	1	0.000000	7.042266	-1.924716
92	1	0.000000	6.970494	-5.767862

Table S6. The optimized Cartesian coordinates of the biphenylene sheet **3** (n×m = 3×3) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.479762	9.525605
2	6	0.000000	0.710557	8.378337
3	6	0.000000	-1.479762	9.525605
4	6	0.000000	-0.690569	10.723596
5	6	0.000000	0.690569	10.723596
6	6	0.000000	2.957376	9.531704
7	6	0.000000	3.730663	10.742369
8	6	0.000000	3.729332	8.385367
9	6	0.000000	5.114310	10.753410
10	6	0.000000	5.152696	8.396674
11	6	0.000000	5.883093	9.554356
12	6	0.000000	-0.710557	8.378337
13	1	0.000000	6.968336	9.583567
14	6	0.000000	1.503025	5.709392
15	6	0.000000	0.708472	4.562391
16	6	0.000000	-1.503025	5.709392

17	6	0.000000	-0.704206	6.867990
18	6	0.000000	0.704206	6.867990
19	6	0.000000	2.965805	5.712139
20	6	0.000000	3.752302	6.877093
21	6	0.000000	3.766763	4.568046
22	6	0.000000	5.164138	6.886849
23	6	0.000000	5.186738	4.576484
24	6	0.000000	5.957137	5.733202
25	6	0.000000	-0.708472	4.562391
26	1	0.000000	7.042112	5.743133
27	6	0.000000	-5.883093	9.554356
28	6	0.000000	-5.114310	10.753410
29	6	0.000000	-3.730663	10.742369
30	6	0.000000	-3.729332	8.385367
31	6	0.000000	-2.957376	9.531704
32	6	0.000000	-5.152696	8.396674
33	6	0.000000	-5.957137	5.733202
34	6	0.000000	-5.164138	6.886849
35	6	0.000000	-5.186738	4.576484
36	6	0.000000	-3.752302	6.877093
37	6	0.000000	-3.766763	4.568046
38	6	0.000000	-2.965805	5.712139
39	6	0.000000	2.975842	-1.905668
40	6	0.000000	1.509680	-1.903791
41	6	0.000000	0.707732	-0.753968
42	6	0.000000	-0.707732	-0.753968
43	6	0.000000	3.775189	-0.753612
44	6	0.000000	5.973116	-1.909990
45	6	0.000000	5.192247	-0.755678
46	6	0.000000	-1.509680	-1.903791
47	6	0.000000	1.509680	1.903791
48	6	0.000000	0.707732	0.753968
49	6	0.000000	-1.509680	1.903791
50	6	0.000000	-0.706714	3.055356
51	6	0.000000	0.706714	3.055356
52	6	0.000000	2.975842	1.905668
53	6	0.000000	3.773427	3.061843
54	6	0.000000	3.775189	0.753612
55	6	0.000000	5.188925	3.064556
56	6	0.000000	5.192247	0.755678
57	6	0.000000	5.973116	1.909990
58	6	0.000000	-0.707732	0.753968
59	1	0.000000	7.058058	-1.911154
60	1	0.000000	7.058058	1.911154
61	6	0.000000	1.503025	-5.709392
62	6	0.000000	0.704206	-6.867990
63	6	0.000000	-1.503025	-5.709392
64	6	0.000000	-0.708472	-4.562391
65	6	0.000000	0.708472	-4.562391
66	6	0.000000	2.965805	-5.712139
67	6	0.000000	0.706714	-3.055356
68	6	0.000000	3.766763	-4.568046
69	6	0.000000	3.773427	-3.061843
70	6	0.000000	-0.706714	-3.055356
71	6	0.000000	3.752302	-6.877093
72	6	0.000000	5.188925	-3.064556
73	6	0.000000	5.186738	-4.576484
74	6	0.000000	5.164138	-6.886849
75	6	0.000000	5.957137	-5.733202
76	6	0.000000	-0.704206	-6.867990
77	1	0.000000	7.042112	-5.743133
78	6	0.000000	1.479762	-9.525605
79	6	0.000000	0.690569	-10.723596
80	6	0.000000	-1.479762	-9.525605
81	6	0.000000	-0.710557	-8.378337
82	6	0.000000	0.710557	-8.378337
83	6	0.000000	2.957376	-9.531704
84	6	0.000000	3.729332	-8.385367
85	6	0.000000	3.730663	-10.742369
86	6	0.000000	5.152696	-8.396674
87	6	0.000000	5.114310	-10.753410
88	6	0.000000	5.883093	-9.554356
89	1	0.000000	5.630040	-11.709912
90	1	0.000000	1.189172	-11.686850
91	1	0.000000	3.217453	-11.697836
92	6	0.000000	-0.690569	-10.723596
93	1	0.000000	-1.189172	-11.686850
94	1	0.000000	6.968336	-9.583567
95	6	0.000000	-5.973116	-1.909990

96	6	0.000000	-5.192247	-0.755678
97	6	0.000000	-2.975842	-1.905668
98	6	0.000000	-3.775189	-0.753612
99	6	0.000000	-5.973116	1.909990
100	6	0.000000	-5.188925	3.064556
101	6	0.000000	-5.192247	0.755678
102	6	0.000000	-3.773427	3.061843
103	6	0.000000	-3.775189	0.753612
104	6	0.000000	-2.975842	1.905668
105	6	0.000000	-5.957137	-5.733202
106	6	0.000000	-5.186738	-4.576484
107	6	0.000000	-5.188925	-3.064556
108	6	0.000000	-3.773427	-3.061843
109	6	0.000000	-3.766763	-4.568046
110	6	0.000000	-3.752302	-6.877093
111	6	0.000000	-2.965805	-5.712139
112	6	0.000000	-5.164138	-6.886849
113	6	0.000000	-5.883093	-9.554356
114	6	0.000000	-5.152696	-8.396674
115	6	0.000000	-5.114310	-10.753410
116	6	0.000000	-3.729332	-8.385367
117	6	0.000000	-3.730663	-10.742369
118	6	0.000000	-2.957376	-9.531704
119	1	0.000000	-3.217453	-11.697836
120	1	0.000000	-5.630040	-11.709912
121	1	0.000000	-1.189172	11.686850
122	1	0.000000	1.189172	11.686850
123	1	0.000000	3.217453	11.697836
124	1	0.000000	5.630040	11.709912
125	1	0.000000	-5.630040	11.709912
126	1	0.000000	-3.217453	11.697836
127	1	0.000000	-6.968336	9.583567
128	1	0.000000	-7.042112	5.743133
129	1	0.000000	-7.058058	-1.911154
130	1	0.000000	-7.058058	1.911154
131	1	0.000000	-7.042112	-5.743133
132	1	0.000000	-6.968336	-9.583567

Table S7. The optimized Cartesian coordinates of the biphenylene sheet **4** (n×m = 4×2) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.900275	5.196607
2	6	0.000000	1.902041	3.733206
3	6	0.000000	3.059378	2.935322
4	6	0.000000	3.057685	1.526060
5	6	0.000000	3.063305	5.980921
6	6	0.000000	1.918022	8.184391
7	6	0.000000	3.072564	7.393443
8	6	0.000000	1.901222	0.730434
9	6	0.000000	5.717361	3.703309
10	6	0.000000	4.569715	2.935436
11	6	0.000000	5.710565	0.739412
12	6	0.000000	6.909793	1.527093
13	6	0.000000	6.912800	2.909941
14	6	0.000000	5.719959	5.182896
15	6	0.000000	6.929567	5.955827
16	6	0.000000	4.572483	5.955616
17	6	0.000000	6.940690	7.340129
18	6	0.000000	4.583635	7.378970
19	6	0.000000	5.742475	8.108709
20	6	0.000000	4.566319	1.514574
21	1	0.000000	1.927778	9.269482
22	1	0.000000	7.872182	1.026399
23	1	0.000000	7.877782	3.405344
24	1	0.000000	7.885034	5.442472
25	1	0.000000	7.897268	7.855566
26	1	0.000000	5.772092	9.193942
27	6	0.000000	-1.902041	3.733206
28	6	0.000000	-3.059378	2.935322

29	6	0.000000	-1.901222	0.730434
30	6	0.000000	-0.752809	1.524425
31	6	0.000000	-0.753431	2.939542
32	6	0.000000	-1.900275	5.196607
33	6	0.000000	0.753431	2.939542
34	6	0.000000	-0.752861	5.995724
35	6	0.000000	0.752861	5.995724
36	6	0.000000	0.752809	1.524425
37	6	0.000000	-3.063305	5.980921
38	6	0.000000	0.757890	7.414696
39	6	0.000000	-0.757890	7.414696
40	6	0.000000	-3.072564	7.393443
41	6	0.000000	-1.918022	8.184391
42	6	0.000000	-3.057685	1.526060
43	1	0.000000	-1.927778	9.269482
44	6	0.000000	-5.717361	3.703309
45	6	0.000000	-6.912800	2.909941
46	6	0.000000	-5.710565	0.739412
47	6	0.000000	-4.566319	1.514574
48	6	0.000000	-4.569715	2.935436
49	6	0.000000	-5.719959	5.182896
50	6	0.000000	-4.572483	5.955616
51	6	0.000000	-6.929567	5.955827
52	6	0.000000	-4.583635	7.378970
53	6	0.000000	-6.940690	7.340129
54	6	0.000000	-5.742475	8.108709
55	1	0.000000	-7.897268	7.855566
56	1	0.000000	-7.877782	3.405344
57	1	0.000000	-7.885034	5.442472
58	6	0.000000	-6.909793	1.527093
59	1	0.000000	-7.872182	1.026399
60	1	0.000000	-5.772092	9.193942
61	6	0.000000	1.902041	-3.733206
62	6	0.000000	3.059378	-2.935322
63	6	0.000000	1.901222	-0.730434
64	6	0.000000	3.057685	-1.526060
65	6	0.000000	5.717361	-3.703309
66	6	0.000000	6.912800	-2.909941
67	6	0.000000	4.569715	-2.935436
68	6	0.000000	6.909793	-1.527093
69	6	0.000000	4.566319	-1.514574
70	6	0.000000	5.710565	-0.739412
71	1	0.000000	7.877782	-3.405344
72	1	0.000000	7.872182	-1.026399
73	6	0.000000	-1.902041	-3.733206
74	6	0.000000	-0.753431	-2.939542
75	6	0.000000	0.753431	-2.939542
76	6	0.000000	0.752809	-1.524425
77	6	0.000000	-0.752809	-1.524425
78	6	0.000000	-3.057685	-1.526060
79	6	0.000000	-1.901222	-0.730434
80	6	0.000000	-3.059378	-2.935322
81	6	0.000000	-5.717361	-3.703309
82	6	0.000000	-4.569715	-2.935436
83	6	0.000000	-6.912800	-2.909941
84	6	0.000000	-4.566319	-1.514574
85	6	0.000000	-6.909793	-1.527093
86	6	0.000000	-5.710565	-0.739412
87	1	0.000000	-7.872182	-1.026399
88	1	0.000000	-7.877782	-3.405344
89	6	0.000000	1.918022	-8.184391
90	6	0.000000	3.072564	-7.393443
91	6	0.000000	1.900275	-5.196607
92	6	0.000000	3.063305	-5.980921
93	6	0.000000	5.742475	-8.108709
94	6	0.000000	6.940690	-7.340129
95	6	0.000000	4.583635	-7.378970
96	6	0.000000	6.929567	-5.955827
97	6	0.000000	4.572483	-5.955616
98	1	0.000000	7.897268	-7.855566
99	1	0.000000	7.885034	-5.442472
100	6	0.000000	-1.918022	-8.184391
101	6	0.000000	-0.757890	-7.414696
102	6	0.000000	0.757890	-7.414696
103	6	0.000000	0.752861	-5.995724
104	6	0.000000	-0.752861	-5.995724
105	6	0.000000	-3.063305	-5.980921
106	6	0.000000	-1.900275	-5.196607
107	6	0.000000	-3.072564	-7.393443

108	6	0.000000	-5.742475	-8.108709
109	6	0.000000	-4.583635	-7.378970
110	6	0.000000	-6.940690	-7.340129
111	6	0.000000	-4.572483	-5.955616
112	6	0.000000	-6.929567	-5.955827
113	6	0.000000	-5.719959	-5.182896
114	1	0.000000	-7.885034	-5.442472
115	1	0.000000	-7.897268	-7.855566
116	1	0.000000	1.927778	-9.269482
117	1	0.000000	5.772092	-9.193942
118	1	0.000000	-1.927778	-9.269482
119	1	0.000000	-5.772092	-9.193942
120	6	0.000000	5.719959	-5.182896

Table S8. The optimized Cartesian coordinates of the biphenylene molecule calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.695067	3.121754
2	6	0.000000	1.445119	1.915410
3	6	0.000000	0.711943	0.754433
4	6	0.000000	-0.711943	0.754433
5	6	0.000000	-0.695067	3.121754
6	6	0.000000	-1.445119	1.915410
7	1	0.000000	-2.531190	1.936247
8	6	0.000000	1.445119	-1.915410
9	6	0.000000	0.711943	-0.754433
10	6	0.000000	-1.445119	-1.915410
11	6	0.000000	-0.695067	-3.121754
12	6	0.000000	0.695067	-3.121754
13	6	0.000000	-0.711943	-0.754433
14	1	0.000000	-2.531190	-1.936247
15	1	0.000000	-1.224532	-4.070869
16	1	0.000000	1.224532	-4.070869
17	1	0.000000	1.224532	4.070869
18	1	0.000000	-1.224532	4.070869
19	1	0.000000	2.531190	1.936247
20	1	0.000000	2.531190	-1.936247

Table S9. The optimized Cartesian coordinates of the armchair biphenylene ribbon (n×m = 2×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	3.114530	1.521541
2	6	0.000000	3.114530	-1.521541
3	6	0.000000	1.918077	-0.740380
4	6	0.000000	1.918077	0.740380
5	6	0.000000	0.757388	1.493604
6	6	0.000000	0.753461	2.913172
7	6	0.000000	3.109860	2.909700
8	6	0.000000	3.109860	-2.909700
9	6	0.000000	0.757388	-1.493604
10	6	0.000000	1.905733	-3.658843
11	6	0.000000	0.753461	-2.913172
12	6	0.000000	1.905733	3.658843
13	1	0.000000	1.919702	4.744474
14	6	0.000000	-1.918077	0.740380
15	6	0.000000	-0.757388	1.493604
16	6	0.000000	-1.905733	3.658843
17	6	0.000000	-3.109860	2.909700
18	6	0.000000	-3.114530	1.521541
19	6	0.000000	-1.918077	-0.740380
20	6	0.000000	-3.114530	-1.521541
21	6	0.000000	-0.757388	-1.493604
22	6	0.000000	-3.109860	-2.909700

23	6	0.000000	-0.753461	-2.913172
24	6	0.000000	-1.905733	-3.658843
25	6	0.000000	-0.753461	2.913172
26	1	0.000000	-1.919702	4.744474
27	1	0.000000	-4.060672	3.435953
28	1	0.000000	-4.076026	1.019034
29	1	0.000000	-4.076026	-1.019034
30	1	0.000000	-4.060672	-3.435953
31	1	0.000000	4.076026	1.019034
32	1	0.000000	4.076026	-1.019034
33	1	0.000000	4.060672	3.435953
34	1	0.000000	4.060672	-3.435953
35	1	0.000000	1.919702	-4.744474
36	1	0.000000	-1.919702	-4.744474

Table S10. The optimized Cartesian coordinates of the armchair biphenylene ribbon (n×m = 3×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	3.110117	5.119614
2	6	0.000000	1.907167	5.871575
3	6	0.000000	3.112461	3.731798
4	6	0.000000	0.753950	5.127908
5	6	0.000000	1.913759	2.952146
6	6	0.000000	0.756117	3.708207
7	6	0.000000	-1.907167	5.871575
8	6	0.000000	-3.110117	5.119614
9	6	0.000000	-0.753950	5.127908
10	6	0.000000	-3.112461	3.731798
11	6	0.000000	-0.756117	3.708207
12	6	0.000000	-1.913759	2.952146
13	1	0.000000	-4.061547	5.644316
14	1	0.000000	-4.072909	3.227864
15	6	0.000000	3.105557	-0.692488
16	6	0.000000	3.112461	-3.731798
17	6	0.000000	1.913759	-2.952146
18	6	0.000000	1.911511	-1.472797
19	6	0.000000	0.757509	-0.708021
20	6	0.000000	0.757509	0.708021
21	6	0.000000	3.105557	0.692488
22	6	0.000000	3.110117	-5.119614
23	6	0.000000	0.756117	-3.708207
24	6	0.000000	1.907167	-5.871575
25	6	0.000000	0.753950	-5.127908
26	6	0.000000	1.911511	1.472797
27	6	0.000000	-1.911511	-1.472797
28	6	0.000000	-0.757509	-0.708021
29	6	0.000000	-1.911511	1.472797
30	6	0.000000	-3.105557	0.692488
31	6	0.000000	-3.105557	-0.692488
32	6	0.000000	-1.913759	-2.952146
33	6	0.000000	-3.112461	-3.731798
34	6	0.000000	-0.756117	-3.708207
35	6	0.000000	-3.110117	-5.119614
36	6	0.000000	-0.753950	-5.127908
37	6	0.000000	-1.907167	-5.871575
38	6	0.000000	-0.757509	0.708021
39	1	0.000000	1.923650	-6.957113
40	1	0.000000	-4.067870	1.192745
41	1	0.000000	-4.067870	-1.192745
42	1	0.000000	-4.072909	-3.227864
43	1	0.000000	-4.061547	-5.644316
44	1	0.000000	-1.923650	-6.957113
45	1	0.000000	4.061547	5.644316
46	1	0.000000	1.923650	6.957113
47	1	0.000000	4.072909	3.227864
48	1	0.000000	-1.923650	6.957113
49	1	0.000000	4.067870	-1.192745
50	1	0.000000	4.072909	-3.227864
51	1	0.000000	4.067870	1.192745
52	1	0.000000	4.061547	-5.644316

Table S11. The optimized Cartesian coordinates of the armchair biphenylene ribbon (n×m = 4×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	3.112400	5.943044
2	6	0.000000	3.104497	2.903204
3	6	0.000000	1.911268	3.685028
4	6	0.000000	1.913660	5.163746
5	6	0.000000	0.756435	5.919678
6	6	0.000000	0.753686	7.338612
7	6	0.000000	3.110133	7.331117
8	6	0.000000	3.103568	1.517811
9	6	0.000000	0.757536	2.921014
10	6	0.000000	1.907920	0.738630
11	6	0.000000	0.756433	1.506321
12	6	0.000000	1.907076	8.082985
13	1	0.000000	1.924021	9.168494
14	6	0.000000	-1.913660	5.163746
15	6	0.000000	-0.756435	5.919678
16	6	0.000000	-1.907076	8.082985
17	6	0.000000	-3.110133	7.331117
18	6	0.000000	-3.112400	5.943044
19	6	0.000000	-1.911268	3.685028
20	6	0.000000	-3.104497	2.903204
21	6	0.000000	-0.757536	2.921014
22	6	0.000000	-3.103568	1.517811
23	6	0.000000	-0.756433	1.506321
24	6	0.000000	-1.907920	0.738630
25	6	0.000000	-0.753686	7.338612
26	1	0.000000	-1.924021	9.168494
27	1	0.000000	-4.061428	7.856156
28	1	0.000000	-4.073256	5.440036
29	1	0.000000	-4.067907	3.401229
30	1	0.000000	-4.066068	1.017625
31	6	0.000000	3.104497	-2.903204
32	6	0.000000	3.112400	-5.943044
33	6	0.000000	1.913660	-5.163746
34	6	0.000000	1.911268	-3.685028
35	6	0.000000	0.757536	-2.921014
36	6	0.000000	0.756433	-1.506321
37	6	0.000000	3.103568	-1.517811
38	6	0.000000	3.110133	-7.331117
39	6	0.000000	0.756435	-5.919678
40	6	0.000000	1.907076	-8.082985
41	6	0.000000	0.753686	-7.338612
42	6	0.000000	1.907920	-0.738630
43	6	0.000000	-1.911268	-3.685028
44	6	0.000000	-0.757536	-2.921014
45	6	0.000000	-1.907920	-0.738630
46	6	0.000000	-3.103568	-1.517811
47	6	0.000000	-3.104497	-2.903204
48	6	0.000000	-1.913660	-5.163746
49	6	0.000000	-3.112400	-5.943044
50	6	0.000000	-0.756435	-5.919678
51	6	0.000000	-3.110133	-7.331117
52	6	0.000000	-0.753686	-7.338612
53	6	0.000000	-1.907076	-8.082985
54	6	0.000000	-0.756433	-1.506321
55	1	0.000000	1.924021	-9.168494
56	1	0.000000	-4.066068	-1.017625
57	1	0.000000	-4.067907	-3.401229
58	1	0.000000	-4.073256	-5.440036
59	1	0.000000	-4.061428	-7.856156
60	1	0.000000	-1.924021	-9.168494
61	1	0.000000	4.073256	5.440036
62	1	0.000000	4.067907	3.401229
63	1	0.000000	4.061428	7.856156
64	1	0.000000	4.066068	1.017625
65	1	0.000000	4.067907	-3.401229
66	1	0.000000	4.073256	-5.440036
67	1	0.000000	4.066068	-1.017625
68	1	0.000000	4.061428	-7.856156

Table S12. The optimized Cartesian coordinates of the armchair biphenylene ribbon (n×m = 5×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	3.113023	8.153092
2	6	0.000000	1.912659	5.895375
3	6	0.000000	1.914925	7.373948
4	6	0.000000	0.756512	8.129491
5	6	0.000000	0.753630	9.548970
6	6	0.000000	3.110343	9.541011
7	6	0.000000	3.104462	3.728846
8	6	0.000000	0.757607	5.131804
9	6	0.000000	1.909503	2.949903
10	6	0.000000	0.756633	3.716404
11	6	0.000000	1.907589	10.292654
12	1	0.000000	1.923725	11.378296
13	6	0.000000	-1.914925	7.373948
14	6	0.000000	-0.756512	8.129491
15	6	0.000000	-1.907589	10.292654
16	6	0.000000	-3.110343	9.541011
17	6	0.000000	-3.113023	8.153092
18	6	0.000000	-1.912659	5.895375
19	6	0.000000	-3.105481	5.113878
20	6	0.000000	-0.757607	5.131804
21	6	0.000000	-3.104462	3.728846
22	6	0.000000	-0.756633	3.716404
23	6	0.000000	-1.909503	2.949903
24	6	0.000000	-0.753630	9.548970
25	1	0.000000	-1.923725	11.378296
26	1	0.000000	-4.061920	10.065692
27	1	0.000000	-4.073777	7.649611
28	1	0.000000	-4.068508	5.612911
29	1	0.000000	-4.066563	3.228032
30	6	0.000000	3.103756	-0.692504
31	6	0.000000	1.909560	-1.473244
32	6	0.000000	0.756560	-0.707609
33	6	0.000000	0.756560	0.707609
34	6	0.000000	3.103756	0.692504
35	6	0.000000	1.909560	1.473244
36	6	0.000000	-1.909560	-1.473244
37	6	0.000000	-0.756560	-0.707609
38	6	0.000000	-1.909560	1.473244
39	6	0.000000	-3.103756	0.692504
40	6	0.000000	-3.103756	-0.692504
41	6	0.000000	-0.756560	0.707609
42	1	0.000000	-4.066445	1.192167
43	1	0.000000	-4.066445	-1.192167
44	1	0.000000	4.073777	7.649611
45	1	0.000000	4.061920	10.065692
46	1	0.000000	4.066563	3.228032
47	1	0.000000	4.066445	-1.192167
48	1	0.000000	4.066445	1.192167
49	6	0.000000	3.104462	-3.728846
50	6	0.000000	1.909503	-2.949903
51	6	0.000000	3.105481	-5.113878
52	6	0.000000	0.756633	-3.716404
53	6	0.000000	1.912659	-5.895375
54	6	0.000000	0.757607	-5.131804
55	6	0.000000	-1.909503	-2.949903
56	6	0.000000	-3.104462	-3.728846
57	6	0.000000	-0.756633	-3.716404
58	6	0.000000	-3.105481	-5.113878
59	6	0.000000	-0.757607	-5.131804
60	6	0.000000	-1.912659	-5.895375
61	1	0.000000	-4.066563	-3.228032
62	1	0.000000	-4.068508	-5.612911
63	1	0.000000	4.066563	-3.228032
64	1	0.000000	4.068508	-5.612911
65	6	0.000000	3.113023	-8.153092
66	6	0.000000	1.914925	-7.373948
67	6	0.000000	3.110343	-9.541011
68	6	0.000000	0.756512	-8.129491
69	6	0.000000	1.907589	-10.292654
70	6	0.000000	0.753630	-9.548970

71	6	0.000000	-1.914925	-7.373948
72	6	0.000000	-3.113023	-8.153092
73	6	0.000000	-0.756512	-8.129491
74	6	0.000000	-3.110343	-9.541011
75	6	0.000000	-0.753630	-9.548970
76	6	0.000000	-1.907589	-10.292654
77	1	0.000000	1.923725	-11.378296
78	1	0.000000	-4.073777	-7.649611
79	1	0.000000	-4.061920	-10.065692
80	1	0.000000	-1.923725	-11.378296
81	1	0.000000	4.073777	-7.649611
82	1	0.000000	4.061920	-10.065692
83	6	0.000000	3.105481	5.113878
84	1	0.000000	4.068508	5.612911

Table S13. The optimized Cartesian coordinates of the armchair biphenylene ribbon (n×m = 6×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	3.112566	10.363746
2	6	0.000000	1.912341	8.106587
3	6	0.000000	1.914560	9.584802
4	6	0.000000	0.756486	10.340436
5	6	0.000000	0.753612	11.759542
6	6	0.000000	3.110078	11.752031
7	6	0.000000	3.104196	5.939951
8	6	0.000000	0.757665	7.342816
9	6	0.000000	1.909439	5.160910
10	6	0.000000	0.756608	5.927636
11	6	0.000000	1.907498	12.503540
12	1	0.000000	1.923301	13.589204
13	6	0.000000	-1.914560	9.584802
14	6	0.000000	-0.756486	10.340436
15	6	0.000000	-1.907498	12.503540
16	6	0.000000	-3.110078	11.752031
17	6	0.000000	-3.112566	10.363746
18	6	0.000000	-1.912341	8.106587
19	6	0.000000	-3.105018	7.325328
20	6	0.000000	-0.757665	7.342816
21	6	0.000000	-3.104196	5.939951
22	6	0.000000	-0.756608	5.927636
23	6	0.000000	-1.909439	5.160910
24	6	0.000000	-0.753612	11.759542
25	1	0.000000	-1.923301	13.589204
26	1	0.000000	-4.061934	12.276311
27	1	0.000000	-4.073576	9.860598
28	1	0.000000	-4.068279	7.824028
29	1	0.000000	-4.066599	5.439546
30	6	0.000000	3.103789	1.518623
31	6	0.000000	1.909863	0.738046
32	6	0.000000	0.756773	1.503586
33	6	0.000000	0.756584	2.918562
34	6	0.000000	3.103661	2.903966
35	6	0.000000	1.909521	3.684545
36	6	0.000000	-1.909863	0.738046
37	6	0.000000	-0.756773	1.503586
38	6	0.000000	-1.909521	3.684545
39	6	0.000000	-3.103661	2.903966
40	6	0.000000	-3.103789	1.518623
41	6	0.000000	-0.756584	2.918562
42	1	0.000000	-4.066493	3.403492
43	1	0.000000	-4.066711	1.019279
44	1	0.000000	4.073576	9.860598
45	1	0.000000	4.061934	12.276311
46	1	0.000000	4.066599	5.439546
47	1	0.000000	4.066711	1.019279
48	1	0.000000	4.066493	3.403492
49	6	0.000000	3.103789	-1.518623
50	6	0.000000	1.909863	-0.738046

51	6	0.000000	3.103661	-2.903966
52	6	0.000000	0.756773	-1.503586
53	6	0.000000	1.909521	-3.684545
54	6	0.000000	0.756584	-2.918562
55	6	0.000000	-1.909863	-0.738046
56	6	0.000000	-3.103789	-1.518623
57	6	0.000000	-0.756773	-1.503586
58	6	0.000000	-3.103661	-2.903966
59	6	0.000000	-0.756584	-2.918562
60	6	0.000000	-1.909521	-3.684545
61	1	0.000000	-4.066711	-1.019279
62	1	0.000000	-4.066493	-3.403492
63	1	0.000000	4.066711	-1.019279
64	1	0.000000	4.066493	-3.403492
65	6	0.000000	3.104196	-5.939951
66	6	0.000000	1.909439	-5.160910
67	6	0.000000	3.105018	-7.325328
68	6	0.000000	0.756608	-5.927636
69	6	0.000000	1.912341	-8.106587
70	6	0.000000	0.757665	-7.342816
71	6	0.000000	-1.909439	-5.160910
72	6	0.000000	-3.104196	-5.939951
73	6	0.000000	-0.756608	-5.927636
74	6	0.000000	-3.105018	-7.325328
75	6	0.000000	-0.757665	-7.342816
76	6	0.000000	-1.912341	-8.106587
77	1	0.000000	-4.066599	-5.439546
78	1	0.000000	-4.068279	-7.824028
79	1	0.000000	4.066599	-5.439546
80	1	0.000000	4.068279	-7.824028
81	6	0.000000	3.105018	7.325328
82	1	0.000000	4.068279	7.824028
83	6	0.000000	3.110078	-11.752031
84	6	0.000000	1.907498	-12.503540
85	6	0.000000	0.753612	-11.759542
86	6	0.000000	0.756486	-10.340436
87	6	0.000000	3.112566	-10.363746
88	6	0.000000	1.914560	-9.584802
89	6	0.000000	-1.907498	-12.503540
90	6	0.000000	-0.753612	-11.759542
91	6	0.000000	-1.914560	-9.584802
92	6	0.000000	-3.112566	-10.363746
93	6	0.000000	-3.110078	-11.752031
94	6	0.000000	-0.756486	-10.340436
95	1	0.000000	-4.073576	-9.860598
96	1	0.000000	-4.061934	-12.276311
97	1	0.000000	4.061934	-12.276311
98	1	0.000000	4.073576	-9.860598
99	1	0.000000	1.923301	-13.589204
100	1	0.000000	-1.923301	-13.589204

Table S14. The optimized Cartesian coordinates of the armchair biphenylene ribbon (n×m = 7×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	3.113113	12.575101
2	6	0.000000	1.912603	10.317191
3	6	0.000000	1.915058	11.795661
4	6	0.000000	0.756471	12.551251
5	6	0.000000	0.753678	13.970684
6	6	0.000000	3.110123	13.963293
7	6	0.000000	3.103643	8.149817
8	6	0.000000	0.757456	9.553391
9	6	0.000000	1.908436	7.371544
10	6	0.000000	0.756565	8.138347
11	6	0.000000	1.907419	14.714517
12	1	0.000000	1.923058	15.800117
13	6	0.000000	-1.915058	11.795661
14	6	0.000000	-0.756471	12.551251

15	6	0.000000	-1.907419	14.714517
16	6	0.000000	-3.110123	13.963293
17	6	0.000000	-3.113113	12.575101
18	6	0.000000	-1.912603	10.317191
19	6	0.000000	-3.105415	9.535245
20	6	0.000000	-0.757456	9.553391
21	6	0.000000	-3.103643	8.149817
22	6	0.000000	-0.756565	8.138347
23	6	0.000000	-1.908436	7.371544
24	6	0.000000	-0.753678	13.970684
25	1	0.000000	-1.923058	15.800117
26	1	0.000000	-4.061862	14.487695
27	1	0.000000	-4.074122	12.071655
28	1	0.000000	-4.068828	10.034056
29	1	0.000000	-4.065964	7.649258
30	6	0.000000	3.103178	3.729773
31	6	0.000000	1.908738	2.949147
32	6	0.000000	0.756369	3.715031
33	6	0.000000	0.756329	5.129340
34	6	0.000000	3.102780	5.115297
35	6	0.000000	1.908208	5.895514
36	6	0.000000	-1.908738	2.949147
37	6	0.000000	-0.756369	3.715031
38	6	0.000000	-1.908208	5.895514
39	6	0.000000	-3.102780	5.115297
40	6	0.000000	-3.103178	3.729773
41	6	0.000000	-0.756329	5.129340
42	1	0.000000	-4.065756	5.614668
43	1	0.000000	-4.066296	3.230383
44	1	0.000000	4.074122	12.071655
45	1	0.000000	4.061862	14.487695
46	1	0.000000	4.065964	7.649258
47	1	0.000000	4.066296	3.230383
48	1	0.000000	4.065756	5.614668
49	6	0.000000	3.103416	0.692802
50	6	0.000000	1.908803	1.473151
51	6	0.000000	3.103416	-0.692802
52	6	0.000000	0.756422	0.707133
53	6	0.000000	1.908803	-1.473151
54	6	0.000000	0.756422	-0.707133
55	6	0.000000	-1.908803	1.473151
56	6	0.000000	-3.103416	0.692802
57	6	0.000000	-0.756422	0.707133
58	6	0.000000	-3.103416	-0.692802
59	6	0.000000	-0.756422	-0.707133
60	6	0.000000	-1.908803	-1.473151
61	1	0.000000	-4.066425	1.192387
62	1	0.000000	-4.066425	-1.192387
63	1	0.000000	4.066425	1.192387
64	1	0.000000	4.066425	-1.192387
65	6	0.000000	3.103178	-3.729773
66	6	0.000000	1.908738	-2.949147
67	6	0.000000	3.102780	-5.115297
68	6	0.000000	0.756369	-3.715031
69	6	0.000000	1.908208	-5.895514
70	6	0.000000	0.756329	-5.129340
71	6	0.000000	-1.908738	-2.949147
72	6	0.000000	-3.103178	-3.729773
73	6	0.000000	-0.756369	-3.715031
74	6	0.000000	-3.102780	-5.115297
75	6	0.000000	-0.756329	-5.129340
76	6	0.000000	-1.908208	-5.895514
77	1	0.000000	-4.066296	-3.230383
78	1	0.000000	-4.065756	-5.614668
79	1	0.000000	4.066296	-3.230383
80	1	0.000000	4.065756	-5.614668
81	6	0.000000	3.105415	9.535245
82	1	0.000000	4.068828	10.034056
83	6	0.000000	3.105415	-9.535245
84	6	0.000000	1.915058	-11.795661
85	6	0.000000	1.912603	-10.317191
86	6	0.000000	0.757456	-9.553391
87	6	0.000000	0.756565	-8.138347
88	6	0.000000	3.103643	-8.149817
89	6	0.000000	3.110123	-13.963293
90	6	0.000000	0.756471	-12.551251
91	6	0.000000	1.907419	-14.714517
92	6	0.000000	0.753678	-13.970684
93	6	0.000000	1.908436	-7.371544

94	6	0.000000	-1.912603	-10.317191
95	6	0.000000	-0.757456	-9.553391
96	6	0.000000	-1.908436	-7.371544
97	6	0.000000	-3.103643	-8.149817
98	6	0.000000	-3.105415	-9.535245
99	6	0.000000	-1.915058	-11.795661
100	6	0.000000	-3.113113	-12.575101
101	6	0.000000	-0.756471	-12.551251
102	6	0.000000	-3.110123	-13.963293
103	6	0.000000	-0.753678	-13.970684
104	6	0.000000	-1.907419	-14.714517
105	6	0.000000	-0.756565	-8.138347
106	1	0.000000	-4.065964	-7.649258
107	1	0.000000	-4.068828	-10.034056
108	1	0.000000	-4.074122	-12.071655
109	1	0.000000	-4.061862	-14.487695
110	1	0.000000	4.068828	-10.034056
111	1	0.000000	4.065964	-7.649258
112	1	0.000000	4.061862	-14.487695
113	6	0.000000	3.113113	-12.575101
114	1	0.000000	4.074122	-12.071655
115	1	0.000000	1.923058	-15.800117
116	1	0.000000	-1.923058	-15.800117

Table S15. The optimized Cartesian coordinates of the armchair biphenylene ribbon (n×m = 8×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	3.112537	14.785697
2	6	0.000000	1.911854	12.528545
3	6	0.000000	1.914270	14.006778
4	6	0.000000	0.756357	14.762482
5	6	0.000000	0.753585	16.181677
6	6	0.000000	3.110079	16.173915
7	6	0.000000	3.103701	10.361623
8	6	0.000000	0.757402	11.764657
9	6	0.000000	1.908479	9.582954
10	6	0.000000	0.756431	10.349808
11	6	0.000000	1.907417	16.925539
12	1	0.000000	1.923423	18.011200
13	6	0.000000	-1.914270	14.006778
14	6	0.000000	-0.756357	14.762482
15	6	0.000000	-1.907417	16.925539
16	6	0.000000	-3.110079	16.173915
17	6	0.000000	-3.112537	14.785697
18	6	0.000000	-1.911854	12.528545
19	6	0.000000	-3.104847	11.747084
20	6	0.000000	-0.757402	11.764657
21	6	0.000000	-3.103701	10.361623
22	6	0.000000	-0.756431	10.349808
23	6	0.000000	-1.908479	9.582954
24	6	0.000000	-0.753585	16.181677
25	1	0.000000	-1.923423	18.011200
26	1	0.000000	-4.061928	16.698266
27	1	0.000000	-4.073496	14.282304
28	1	0.000000	-4.068195	12.245855
29	1	0.000000	-4.066143	9.861119
30	6	0.000000	3.103468	5.940940
31	6	0.000000	1.909092	5.160288
32	6	0.000000	0.756473	5.926022
33	6	0.000000	0.756376	7.340563
34	6	0.000000	3.103118	7.326415
35	6	0.000000	1.908520	8.106748
36	6	0.000000	-1.909092	5.160288
37	6	0.000000	-0.756473	5.926022
38	6	0.000000	-1.908520	8.106748
39	6	0.000000	-3.103118	7.326415
40	6	0.000000	-3.103468	5.940940
41	6	0.000000	-0.756376	7.340563
42	1	0.000000	-4.066041	7.825963

43	1	0.000000	-4.066540	5.441545
44	1	0.000000	4.073496	14.282304
45	1	0.000000	4.061928	16.698266
46	1	0.000000	4.066143	9.861119
47	1	0.000000	4.066540	5.441545
48	1	0.000000	4.066041	7.825963
49	6	0.000000	3.103610	2.903792
50	6	0.000000	1.909102	3.684228
51	6	0.000000	3.103547	1.518313
52	6	0.000000	0.756498	2.918331
53	6	0.000000	1.909005	0.737999
54	6	0.000000	0.756510	1.503874
55	6	0.000000	-1.909102	3.684228
56	6	0.000000	-3.103610	2.903792
57	6	0.000000	-0.756498	2.918331
58	6	0.000000	-3.103547	1.518313
59	6	0.000000	-0.756510	1.503874
60	6	0.000000	-1.909005	0.737999
61	1	0.000000	-4.066549	3.403426
62	1	0.000000	-4.066489	1.018740
63	1	0.000000	4.066549	3.403426
64	1	0.000000	4.066489	1.018740
65	6	0.000000	3.103547	-1.518313
66	6	0.000000	1.909005	-0.737999
67	6	0.000000	3.103610	-2.903792
68	6	0.000000	0.756510	-1.503874
69	6	0.000000	1.909102	-3.684228
70	6	0.000000	0.756498	-2.918331
71	6	0.000000	-1.909005	-0.737999
72	6	0.000000	-3.103547	-1.518313
73	6	0.000000	-0.756510	-1.503874
74	6	0.000000	-3.103610	-2.903792
75	6	0.000000	-0.756498	-2.918331
76	6	0.000000	-1.909102	-3.684228
77	1	0.000000	-4.066489	-1.018740
78	1	0.000000	-4.066549	-3.403426
79	1	0.000000	4.066489	-1.018740
80	1	0.000000	4.066549	-3.403426
81	6	0.000000	3.104847	11.747084
82	1	0.000000	4.068195	12.245855
83	6	0.000000	3.103118	-7.326415
84	6	0.000000	1.908479	-9.582954
85	6	0.000000	1.908520	-8.106748
86	6	0.000000	0.756376	-7.340563
87	6	0.000000	0.756473	-5.926022
88	6	0.000000	3.103468	-5.940940
89	6	0.000000	3.104847	-11.747084
90	6	0.000000	0.756431	-10.349808
91	6	0.000000	1.911854	-12.528545
92	6	0.000000	0.757402	-11.764657
93	6	0.000000	1.909092	-5.160288
94	6	0.000000	-1.908520	-8.106748
95	6	0.000000	-0.756376	-7.340563
96	6	0.000000	-1.909092	-5.160288
97	6	0.000000	-3.103468	-5.940940
98	6	0.000000	-3.103118	-7.326415
99	6	0.000000	-1.908479	-9.582954
100	6	0.000000	-3.103701	-10.361623
101	6	0.000000	-0.756431	-10.349808
102	6	0.000000	-3.104847	-11.747084
103	6	0.000000	-0.757402	-11.764657
104	6	0.000000	-1.911854	-12.528545
105	6	0.000000	-0.756473	-5.926022
106	1	0.000000	-4.066540	-5.441545
107	1	0.000000	-4.066041	-7.825963
108	1	0.000000	-4.066143	-9.861119
109	1	0.000000	-4.068195	-12.245855
110	6	0.000000	3.110079	-16.173915
111	6	0.000000	1.907417	-16.925539
112	6	0.000000	0.753585	-16.181677
113	6	0.000000	0.756357	-14.762482
114	6	0.000000	3.112537	-14.785697
115	6	0.000000	1.914270	-14.006778
116	6	0.000000	-1.907417	-16.925539
117	6	0.000000	-0.753585	-16.181677
118	6	0.000000	-1.914270	-14.006778
119	6	0.000000	-3.112537	-14.785697
120	6	0.000000	-3.110079	-16.173915
121	6	0.000000	-0.756357	-14.762482

122	1	0.000000	-4.073496	-14.282304
123	1	0.000000	-4.061928	-16.698266
124	1	0.000000	4.066041	-7.825963
125	1	0.000000	4.066540	-5.441545
126	1	0.000000	4.068195	-12.245855
127	1	0.000000	4.061928	-16.698266
128	1	0.000000	4.073496	-14.282304
129	6	0.000000	3.103701	-10.361623
130	1	0.000000	4.066143	-9.861119
131	1	0.000000	1.923423	-18.011200
132	1	0.000000	-1.923423	-18.011200

Table S16. The optimized Cartesian coordinates of the armchair biphenylene ribbon (n×m = 9×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	3.112900	16.996652
2	6	0.000000	1.912389	14.739348
3	6	0.000000	1.914733	16.217659
4	6	0.000000	0.756519	16.973333
5	6	0.000000	0.753664	18.392554
6	6	0.000000	3.110216	18.384847
7	6	0.000000	3.104123	12.572601
8	6	0.000000	0.757598	13.975495
9	6	0.000000	1.909114	11.793746
10	6	0.000000	0.756674	12.560453
11	6	0.000000	1.907510	19.136389
12	1	0.000000	1.923701	20.222021
13	6	0.000000	-1.914733	16.217659
14	6	0.000000	-0.756519	16.973333
15	6	0.000000	-1.907510	19.136389
16	6	0.000000	-3.110216	18.384847
17	6	0.000000	-3.112900	16.996652
18	6	0.000000	-1.912389	14.739348
19	6	0.000000	-3.105242	13.957939
20	6	0.000000	-0.757598	13.975495
21	6	0.000000	-3.104123	12.572601
22	6	0.000000	-0.756674	12.560453
23	6	0.000000	-1.909114	11.793746
24	6	0.000000	-0.753664	18.392554
25	1	0.000000	-1.923701	20.222021
26	1	0.000000	-4.062014	18.909161
27	1	0.000000	-4.073899	16.493312
28	1	0.000000	-4.068613	14.456636
29	1	0.000000	-4.066525	12.072244
30	6	0.000000	3.103823	8.151771
31	6	0.000000	1.909646	7.371135
32	6	0.000000	0.756696	8.136686
33	6	0.000000	0.756610	9.551441
34	6	0.000000	3.103601	9.537048
35	6	0.000000	1.909191	10.317447
36	6	0.000000	-1.909646	7.371135
37	6	0.000000	-0.756696	8.136686
38	6	0.000000	-1.909191	10.317447
39	6	0.000000	-3.103601	9.537048
40	6	0.000000	-3.103823	8.151771
41	6	0.000000	-0.756610	9.551441
42	1	0.000000	-4.066522	10.036390
43	1	0.000000	-4.066721	7.652286
44	1	0.000000	4.073899	16.493312
45	1	0.000000	4.062014	18.909161
46	1	0.000000	4.066525	12.072244
47	1	0.000000	4.066721	7.652286
48	1	0.000000	4.066522	10.036390
49	6	0.000000	3.104032	5.114698
50	6	0.000000	1.909744	5.895077
51	6	0.000000	3.104031	3.729426
52	6	0.000000	0.756756	5.129380
53	6	0.000000	1.909721	2.949073

54	6	0.000000	0.756709	3.714705
55	6	0.000000	-1.909744	5.895077
56	6	0.000000	-3.104032	5.114698
57	6	0.000000	-0.756756	5.129380
58	6	0.000000	-3.104031	3.729426
59	6	0.000000	-0.756709	3.714705
60	6	0.000000	-1.909721	2.949073
61	1	0.000000	-4.066920	5.614176
62	1	0.000000	-4.066815	3.229742
63	1	0.000000	4.066920	5.614176
64	1	0.000000	4.066815	3.229742
65	6	0.000000	3.103976	0.692648
66	6	0.000000	1.909726	1.473025
67	6	0.000000	3.103976	-0.692648
68	6	0.000000	0.756722	0.707327
69	6	0.000000	1.909726	-1.473025
70	6	0.000000	0.756722	-0.707327
71	6	0.000000	-1.909726	1.473025
72	6	0.000000	-3.103976	0.692648
73	6	0.000000	-0.756722	0.707327
74	6	0.000000	-3.103976	-0.692648
75	6	0.000000	-0.756722	-0.707327
76	6	0.000000	-1.909726	-1.473025
77	1	0.000000	-4.066856	1.192147
78	1	0.000000	-4.066856	-1.192147
79	1	0.000000	4.066856	1.192147
80	1	0.000000	4.066856	-1.192147
81	6	0.000000	3.105242	13.957939
82	1	0.000000	4.068613	14.456636
83	6	0.000000	3.104032	-5.114698
84	6	0.000000	1.909646	-7.371135
85	6	0.000000	1.909744	-5.895077
86	6	0.000000	0.756756	-5.129380
87	6	0.000000	0.756709	-3.714705
88	6	0.000000	3.104031	-3.729426
89	6	0.000000	3.103601	-9.537048
90	6	0.000000	0.756696	-8.136686
91	6	0.000000	1.909191	-10.317447
92	6	0.000000	0.756610	-9.551441
93	6	0.000000	1.909721	-2.949073
94	6	0.000000	-1.909744	-5.895077
95	6	0.000000	-0.756756	-5.129380
96	6	0.000000	-1.909721	-2.949073
97	6	0.000000	-3.104031	-3.729426
98	6	0.000000	-3.104032	-5.114698
99	6	0.000000	-1.909646	-7.371135
100	6	0.000000	-3.103823	-8.151771
101	6	0.000000	-0.756696	-8.136686
102	6	0.000000	-3.103601	-9.537048
103	6	0.000000	-0.756610	-9.551441
104	6	0.000000	-1.909191	-10.317447
105	6	0.000000	-0.756709	-3.714705
106	1	0.000000	-4.066815	-3.229742
107	1	0.000000	-4.066920	-5.614176
108	1	0.000000	-4.066721	-7.652286
109	1	0.000000	-4.066522	-10.036390
110	6	0.000000	3.105242	-13.957939
111	6	0.000000	1.912389	-14.739348
112	6	0.000000	0.757598	-13.975495
113	6	0.000000	0.756674	-12.560453
114	6	0.000000	3.104123	-12.572601
115	6	0.000000	1.909114	-11.793746
116	6	0.000000	-1.912389	-14.739348
117	6	0.000000	-0.757598	-13.975495
118	6	0.000000	-1.909114	-11.793746
119	6	0.000000	-3.104123	-12.572601
120	6	0.000000	-3.105242	-13.957939
121	6	0.000000	-0.756674	-12.560453
122	1	0.000000	-4.066525	-12.072244
123	1	0.000000	-4.068613	-14.456636
124	1	0.000000	4.066920	-5.614176
125	1	0.000000	4.066815	-3.229742
126	1	0.000000	4.066522	-10.036390
127	1	0.000000	4.068613	-14.456636
128	1	0.000000	4.066525	-12.072244
129	6	0.000000	3.112900	-16.996652
130	6	0.000000	1.914733	-16.217659
131	6	0.000000	3.110216	-18.384847
132	6	0.000000	0.756519	-16.973333

133	6	0.000000	1.907510	-19.136389
134	6	0.000000	0.753664	-18.392554
135	6	0.000000	-1.914733	-16.217659
136	6	0.000000	-3.112900	-16.996652
137	6	0.000000	-0.756519	-16.973333
138	6	0.000000	-3.110216	-18.384847
139	6	0.000000	-0.753664	-18.392554
140	6	0.000000	-1.907510	-19.136389
141	1	0.000000	-4.073899	-16.493312
142	1	0.000000	-4.062014	-18.909161
143	1	0.000000	4.073899	-16.493312
144	1	0.000000	4.062014	-18.909161
145	6	0.000000	3.103823	-8.151771
146	1	0.000000	4.066721	-7.652286
147	1	0.000000	1.923701	-20.222021
148	1	0.000000	-1.923701	-20.222021

Table S17. The optimized Cartesian coordinates of the armchair biphenylene ribbon (n×m = 10×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	3.112893	19.208560
2	6	0.000000	1.912426	16.950923
3	6	0.000000	1.914758	18.429349
4	6	0.000000	0.756457	19.184904
5	6	0.000000	0.753625	20.604282
6	6	0.000000	3.110159	20.596683
7	6	0.000000	3.104047	14.784037
8	6	0.000000	0.757533	16.187197
9	6	0.000000	1.909021	14.005403
10	6	0.000000	0.756597	14.772043
11	6	0.000000	1.907458	21.348140
12	1	0.000000	1.923315	22.433774
13	6	0.000000	-1.914758	18.429349
14	6	0.000000	-0.756457	19.184904
15	6	0.000000	-1.907458	21.348140
16	6	0.000000	-3.110159	20.596683
17	6	0.000000	-3.112893	19.208560
18	6	0.000000	-1.912426	16.950923
19	6	0.000000	-3.105280	16.169309
20	6	0.000000	-0.757533	16.187197
21	6	0.000000	-3.104047	14.784037
22	6	0.000000	-0.756597	14.772043
23	6	0.000000	-1.909021	14.005403
24	6	0.000000	-0.753625	20.604282
25	1	0.000000	-1.923315	22.433774
26	1	0.000000	-4.061865	21.121166
27	1	0.000000	-4.073825	18.705188
28	1	0.000000	-4.068531	16.668157
29	1	0.000000	-4.066332	14.283433
30	6	0.000000	3.103813	10.363411
31	6	0.000000	1.909665	9.582648
32	6	0.000000	0.756669	10.348186
33	6	0.000000	0.756511	11.763102
34	6	0.000000	3.103443	11.748683
35	6	0.000000	1.909038	12.529101
36	6	0.000000	-1.909665	9.582648
37	6	0.000000	-0.756669	10.348186
38	6	0.000000	-1.909038	12.529101
39	6	0.000000	-3.103443	11.748683
40	6	0.000000	-3.103813	10.363411
41	6	0.000000	-0.756511	11.763102
42	1	0.000000	-4.066200	12.248332
43	1	0.000000	-4.066756	9.863994
44	1	0.000000	4.073825	18.705188
45	1	0.000000	4.061865	21.121166
46	1	0.000000	4.066332	14.283433
47	1	0.000000	4.066756	9.863994
48	1	0.000000	4.066200	12.248332
49	6	0.000000	3.103963	7.325837

50	6	0.000000	1.909652	8.106450
51	6	0.000000	3.103770	5.940585
52	6	0.000000	0.756676	7.340722
53	6	0.000000	1.909424	5.160299
54	6	0.000000	0.756637	5.925919
55	6	0.000000	-1.909652	8.106450
56	6	0.000000	-3.103963	7.325837
57	6	0.000000	-0.756676	7.340722
58	6	0.000000	-3.103770	5.940585
59	6	0.000000	-0.756637	5.925919
60	6	0.000000	-1.909424	5.160299
61	1	0.000000	-4.066787	7.825482
62	1	0.000000	-4.066480	5.440839
63	1	0.000000	4.066787	7.825482
64	1	0.000000	4.066480	5.440839
65	6	0.000000	3.103768	2.904060
66	6	0.000000	1.909491	3.684319
67	6	0.000000	3.104008	1.518772
68	6	0.000000	0.756699	2.918623
69	6	0.000000	1.909760	0.738131
70	6	0.000000	0.756653	1.503835
71	6	0.000000	-1.909491	3.684319
72	6	0.000000	-3.103768	2.904060
73	6	0.000000	-0.756699	2.918623
74	6	0.000000	-3.104008	1.518772
75	6	0.000000	-0.756653	1.503835
76	6	0.000000	-1.909760	0.738131
77	1	0.000000	-4.066522	3.403711
78	1	0.000000	-4.066873	1.019200
79	1	0.000000	4.066522	3.403711
80	1	0.000000	4.066873	1.019200
81	6	0.000000	3.105280	16.169309
82	1	0.000000	4.068531	16.668157
83	6	0.000000	3.103768	-2.904060
84	6	0.000000	1.909424	-5.160299
85	6	0.000000	1.909491	-3.684319
86	6	0.000000	0.756699	-2.918623
87	6	0.000000	0.756653	-1.503835
88	6	0.000000	3.104008	-1.518772
89	6	0.000000	3.103963	-7.325837
90	6	0.000000	0.756637	-5.925919
91	6	0.000000	1.909652	-8.106450
92	6	0.000000	0.756676	-7.340722
93	6	0.000000	1.909760	-0.738131
94	6	0.000000	-1.909491	-3.684319
95	6	0.000000	-0.756699	-2.918623
96	6	0.000000	-1.909760	-0.738131
97	6	0.000000	-3.104008	-1.518772
98	6	0.000000	-3.103768	-2.904060
99	6	0.000000	-1.909424	-5.160299
100	6	0.000000	-3.103770	-5.940585
101	6	0.000000	-0.756637	-5.925919
102	6	0.000000	-3.103963	-7.325837
103	6	0.000000	-0.756676	-7.340722
104	6	0.000000	-1.909652	-8.106450
105	6	0.000000	-0.756653	-1.503835
106	1	0.000000	-4.066873	-1.019200
107	1	0.000000	-4.066522	-3.403711
108	1	0.000000	-4.066480	-5.440839
109	1	0.000000	-4.066787	-7.825482
110	6	0.000000	3.103443	-11.748683
111	6	0.000000	1.909038	-12.529101
112	6	0.000000	0.756511	-11.763102
113	6	0.000000	0.756669	-10.348186
114	6	0.000000	3.103813	-10.363411
115	6	0.000000	1.909665	-9.582648
116	6	0.000000	-1.909038	-12.529101
117	6	0.000000	-0.756511	-11.763102
118	6	0.000000	-1.909665	-9.582648
119	6	0.000000	-3.103813	-10.363411
120	6	0.000000	-3.103443	-11.748683
121	6	0.000000	-0.756669	-10.348186
122	1	0.000000	-4.066756	-9.863994
123	1	0.000000	-4.066200	-12.248332
124	1	0.000000	4.066522	-3.403711
125	1	0.000000	4.066873	-1.019200
126	1	0.000000	4.066787	-7.825482
127	1	0.000000	4.066200	-12.248332
128	1	0.000000	4.066756	-9.863994

129	6	0.000000	3.104047	-14.784037
130	6	0.000000	1.909021	-14.005403
131	6	0.000000	3.105280	-16.169309
132	6	0.000000	0.756597	-14.772043
133	6	0.000000	1.912426	-16.950923
134	6	0.000000	0.757533	-16.187197
135	6	0.000000	-1.909021	-14.005403
136	6	0.000000	-3.104047	-14.784037
137	6	0.000000	-0.756597	-14.772043
138	6	0.000000	-3.105280	-16.169309
139	6	0.000000	-0.757533	-16.187197
140	6	0.000000	-1.912426	-16.950923
141	1	0.000000	-4.066332	-14.283433
142	1	0.000000	-4.068531	-16.668157
143	1	0.000000	4.066332	-14.283433
144	1	0.000000	4.068531	-16.668157
145	6	0.000000	3.112893	-19.208560
146	6	0.000000	1.914758	-18.429349
147	6	0.000000	3.110159	-20.596683
148	6	0.000000	0.756457	-19.184904
149	6	0.000000	1.907458	-21.348140
150	6	0.000000	0.753625	-20.604282
151	6	0.000000	-1.914758	-18.429349
152	6	0.000000	-3.112893	-19.208560
153	6	0.000000	-0.756457	-19.184904
154	6	0.000000	-3.110159	-20.596683
155	6	0.000000	-0.753625	-20.604282
156	6	0.000000	-1.907458	-21.348140
157	1	0.000000	1.923315	-22.433774
158	1	0.000000	-4.073825	-18.705188
159	1	0.000000	-4.061865	-21.121166
160	1	0.000000	-1.923315	-22.433774
161	1	0.000000	4.073825	-18.705188
162	1	0.000000	4.061865	-21.121166
163	6	0.000000	3.103770	-5.940585
164	1	0.000000	4.066480	-5.440839

Table S18. The optimized Cartesian coordinates of the zigzag biphenylene ribbon (n×m = 2×2) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.733252	1.898606
2	6	0.000000	-0.733252	1.898606
3	6	0.000000	-1.522108	3.060826
4	6	0.000000	-2.934733	3.066187
5	6	0.000000	1.522108	3.060826
6	6	0.000000	3.725214	1.912190
7	6	0.000000	2.934733	3.066187
8	6	0.000000	-3.725214	1.912190
9	6	0.000000	-0.740123	5.720383
10	6	0.000000	-1.505988	4.570795
11	6	0.000000	-3.665448	5.729260
12	6	0.000000	-2.902506	6.931984
13	6	0.000000	-1.518732	6.927074
14	6	0.000000	0.740123	5.720383
15	6	0.000000	1.518732	6.927074
16	6	0.000000	1.505988	4.570795
17	6	0.000000	2.902506	6.931984
18	6	0.000000	2.929163	4.575451
19	6	0.000000	3.665448	5.729260
20	6	0.000000	-2.929163	4.575451
21	1	0.000000	4.810201	1.920348
22	1	0.000000	-3.423476	7.885483
23	1	0.000000	-1.010241	7.884837
24	1	0.000000	1.010241	7.884837
25	1	0.000000	3.423476	7.885483
26	1	0.000000	4.750758	5.754211
27	6	0.000000	-0.733252	-1.898606
28	6	0.000000	-1.522108	-3.060826

29	6	0.000000	-3.725214	-1.912190
30	6	0.000000	-2.952104	-0.756114
31	6	0.000000	-1.532696	-0.752726
32	6	0.000000	0.733252	-1.898606
33	6	0.000000	-1.532696	0.752726
34	6	0.000000	1.532696	-0.752726
35	6	0.000000	1.532696	0.752726
36	6	0.000000	-2.952104	0.756114
37	6	0.000000	1.522108	-3.060826
38	6	0.000000	2.952104	0.756114
39	6	0.000000	2.952104	-0.756114
40	6	0.000000	2.934733	-3.066187
41	6	0.000000	3.725214	-1.912190
42	6	0.000000	-2.934733	-3.066187
43	1	0.000000	4.810201	-1.920348
44	6	0.000000	-0.740123	-5.720383
45	6	0.000000	-1.518732	-6.927074
46	6	0.000000	-3.665448	-5.729260
47	6	0.000000	-2.929163	-4.575451
48	6	0.000000	-1.505988	-4.570795
49	6	0.000000	0.740123	-5.720383
50	6	0.000000	1.505988	-4.570795
51	6	0.000000	1.518732	-6.927074
52	6	0.000000	2.929163	-4.575451
53	6	0.000000	2.902506	-6.931984
54	6	0.000000	3.665448	-5.729260
55	1	0.000000	3.423476	-7.885483
56	1	0.000000	-1.010241	-7.884837
57	1	0.000000	1.010241	-7.884837
58	6	0.000000	-2.902506	-6.931984
59	1	0.000000	-3.423476	-7.885483
60	1	0.000000	4.750758	-5.754211
61	1	0.000000	-4.810201	1.920348
62	1	0.000000	-4.750758	5.754211
63	1	0.000000	-4.810201	-1.920348
64	1	0.000000	-4.750758	-5.754211

Table S19. The optimized Cartesian coordinates of the zigzag biphenylene ribbon (n×m = 2×3) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.530223	4.568494
2	6	0.000000	2.902901	10.748827
3	6	0.000000	3.665282	9.545950
4	6	0.000000	1.519117	10.744256
5	6	0.000000	0.739808	9.537888
6	6	0.000000	1.505391	8.387546
7	6	0.000000	2.928737	8.392254
8	6	0.000000	2.933691	6.883131
9	6	0.000000	1.521744	6.877950
10	6	0.000000	0.732224	5.714313
11	6	0.000000	2.950290	4.573341
12	6	0.000000	3.723717	5.727664
13	1	0.000000	4.750750	9.569338
14	1	0.000000	3.423325	11.702798
15	1	0.000000	1.011073	11.702425
16	6	0.000000	-0.739808	9.537888
17	6	0.000000	-1.505391	8.387546
18	6	0.000000	-1.521744	6.877950
19	6	0.000000	-0.732224	5.714313
20	6	0.000000	-1.530223	4.568494
21	6	0.000000	-3.723717	5.727664
22	6	0.000000	-2.933691	6.883131
23	6	0.000000	-2.928737	8.392254
24	6	0.000000	-3.665282	9.545950
25	6	0.000000	-2.902901	10.748827
26	6	0.000000	-1.519117	10.744256
27	1	0.000000	-3.423325	11.702798
28	1	0.000000	-1.011073	11.702425

29	1	0.000000	4.808805	5.734963
30	1	0.000000	-4.750750	9.569338
31	6	0.000000	2.949077	3.062346
32	6	0.000000	1.533520	3.061853
33	6	0.000000	0.733880	1.907263
34	6	0.000000	1.531592	0.754084
35	6	0.000000	2.948695	0.754938
36	6	0.000000	3.731559	1.907254
37	6	0.000000	-1.533520	3.061853
38	6	0.000000	-0.733880	1.907263
39	6	0.000000	-1.531592	0.754084
40	6	0.000000	-2.948695	0.754938
41	6	0.000000	-3.731559	1.907254
42	6	0.000000	-2.949077	3.062346
43	6	0.000000	-2.950290	4.573341
44	1	0.000000	4.816575	1.906760
45	1	0.000000	-4.816575	1.906760
46	1	0.000000	-4.808805	5.734963
47	6	0.000000	1.521744	-6.877950
48	6	0.000000	2.948695	-0.754938
49	6	0.000000	3.731559	-1.907254
50	6	0.000000	1.531592	-0.754084
51	6	0.000000	0.733880	-1.907263
52	6	0.000000	1.533520	-3.061853
53	6	0.000000	2.949077	-3.062346
54	6	0.000000	2.950290	-4.573341
55	6	0.000000	1.530223	-4.568494
56	6	0.000000	0.732224	-5.714313
57	6	0.000000	2.933691	-6.883131
58	6	0.000000	3.723717	-5.727664
59	1	0.000000	4.816575	-1.906760
60	6	0.000000	-0.733880	-1.907263
61	6	0.000000	-1.533520	-3.061853
62	6	0.000000	-1.530223	-4.568494
63	6	0.000000	-0.732224	-5.714313
64	6	0.000000	-1.521744	-6.877950
65	6	0.000000	-3.723717	-5.727664
66	6	0.000000	-2.950290	-4.573341
67	6	0.000000	-2.949077	-3.062346
68	6	0.000000	-3.731559	-1.907254
69	6	0.000000	-2.948695	-0.754938
70	6	0.000000	-1.531592	-0.754084
71	1	0.000000	4.808805	-5.734963
72	1	0.000000	-4.816575	-1.906760
73	6	0.000000	-2.933691	-6.883131
74	1	0.000000	-4.808805	-5.734963
75	6	0.000000	2.928737	-8.392254
76	6	0.000000	3.665282	-9.545950
77	6	0.000000	1.505391	-8.387546
78	6	0.000000	0.739808	-9.537888
79	6	0.000000	1.519117	-10.744256
80	6	0.000000	2.902901	-10.748827
81	1	0.000000	4.750750	-9.569338
82	6	0.000000	-0.739808	-9.537888
83	6	0.000000	-1.519117	-10.744256
84	6	0.000000	-2.902901	-10.748827
85	6	0.000000	-3.665282	-9.545950
86	6	0.000000	-2.928737	-8.392254
87	6	0.000000	-1.505391	-8.387546
88	1	0.000000	-4.750750	-9.569338
89	1	0.000000	1.011073	-11.702425
90	1	0.000000	3.423325	-11.702798
91	1	0.000000	-1.011073	-11.702425
92	1	0.000000	-3.423325	-11.702798

Table S20. The optimized Cartesian coordinates of the zigzag biphenylene ribbon (n×m = 2×4) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.530167	8.385273
2	6	0.000000	2.902542	14.565867
3	6	0.000000	3.665285	13.362772

4	6	0.000000	1.518966	14.561202
5	6	0.000000	0.739664	13.354503
6	6	0.000000	1.505387	12.204388
7	6	0.000000	2.928852	12.209186
8	6	0.000000	2.933470	10.699933
9	6	0.000000	1.521976	10.694784
10	6	0.000000	0.732034	9.530729
11	6	0.000000	2.950536	8.390175
12	6	0.000000	3.723936	9.544201
13	1	0.000000	4.750726	13.386508
14	1	0.000000	3.423051	15.519818
15	1	0.000000	1.010816	15.519393
16	6	0.000000	-0.739664	13.354503
17	6	0.000000	-1.505387	12.204388
18	6	0.000000	-1.521976	10.694784
19	6	0.000000	-0.732034	9.530729
20	6	0.000000	-1.530167	8.385273
21	6	0.000000	-3.723936	9.544201
22	6	0.000000	-2.933470	10.699933
23	6	0.000000	-2.928852	12.209186
24	6	0.000000	-3.665285	13.362772
25	6	0.000000	-2.902542	14.565867
26	6	0.000000	-1.518966	14.561202
27	1	0.000000	-3.423051	15.519818
28	1	0.000000	-1.010816	15.519393
29	1	0.000000	4.808991	9.551625
30	1	0.000000	-4.750726	13.386508
31	6	0.000000	2.948772	6.879082
32	6	0.000000	1.533884	6.878691
33	6	0.000000	0.733518	5.723584
34	6	0.000000	1.531199	4.570821
35	6	0.000000	2.948725	4.571770
36	6	0.000000	3.731658	5.723406
37	6	0.000000	-1.533884	6.878691
38	6	0.000000	-0.733518	5.723584
39	6	0.000000	-1.531199	4.570821
40	6	0.000000	-2.948725	4.571770
41	6	0.000000	-3.731658	5.723406
42	6	0.000000	-2.948772	6.879082
43	6	0.000000	-2.950536	8.390175
44	1	0.000000	4.816616	5.722859
45	1	0.000000	-4.816616	5.722859
46	1	0.000000	-4.808991	9.551625
47	6	0.000000	1.531893	-3.062730
48	6	0.000000	2.947417	3.061736
49	6	0.000000	3.730570	1.907882
50	6	0.000000	1.531893	3.062730
51	6	0.000000	0.732966	1.908118
52	6	0.000000	1.531258	0.754067
53	6	0.000000	2.947529	0.754957
54	6	0.000000	2.947529	-0.754957
55	6	0.000000	1.531258	-0.754067
56	6	0.000000	0.732966	-1.908118
57	6	0.000000	2.947417	-3.061736
58	6	0.000000	3.730570	-1.907882
59	1	0.000000	4.815497	1.907852
60	6	0.000000	-0.732966	1.908118
61	6	0.000000	-1.531258	0.754067
62	6	0.000000	-1.531258	-0.754067
63	6	0.000000	-0.732966	-1.908118
64	6	0.000000	-1.531893	-3.062730
65	6	0.000000	-3.730570	-1.907882
66	6	0.000000	-2.947529	-0.754957
67	6	0.000000	-2.947529	0.754957
68	6	0.000000	-3.730570	1.907882
69	6	0.000000	-2.947417	3.061736
70	6	0.000000	-1.531893	3.062730
71	1	0.000000	4.815497	-1.907852
72	1	0.000000	-4.815497	1.907852
73	6	0.000000	-2.947417	-3.061736
74	1	0.000000	-4.815497	-1.907852
75	6	0.000000	1.521976	-10.694784
76	6	0.000000	2.948725	-4.571770
77	6	0.000000	3.731658	-5.723406
78	6	0.000000	1.531199	-4.570821
79	6	0.000000	0.733518	-5.723584
80	6	0.000000	1.533884	-6.878691
81	6	0.000000	2.948772	-6.879082
82	6	0.000000	2.950536	-8.390175

83	6	0.000000	1.530167	-8.385273
84	6	0.000000	0.732034	-9.530729
85	6	0.000000	2.933470	-10.699933
86	6	0.000000	3.723936	-9.544201
87	1	0.000000	4.816616	-5.722859
88	6	0.000000	-0.733518	-5.723584
89	6	0.000000	-1.533884	-6.878691
90	6	0.000000	-1.530167	-8.385273
91	6	0.000000	-0.732034	-9.530729
92	6	0.000000	-1.521976	-10.694784
93	6	0.000000	-3.723936	-9.544201
94	6	0.000000	-2.950536	-8.390175
95	6	0.000000	-2.948772	-6.879082
96	6	0.000000	-3.731658	-5.723406
97	6	0.000000	-2.948725	-4.571770
98	6	0.000000	-1.531199	-4.570821
99	1	0.000000	4.808991	-9.551625
100	1	0.000000	-4.816616	-5.722859
101	6	0.000000	2.928852	-12.209186
102	6	0.000000	1.505387	-12.204388
103	6	0.000000	0.739664	-13.354503
104	6	0.000000	1.518966	-14.561202
105	6	0.000000	2.902542	-14.565867
106	6	0.000000	3.665285	-13.362772
107	6	0.000000	-1.505387	-12.204388
108	6	0.000000	-0.739664	-13.354503
109	6	0.000000	-1.518966	-14.561202
110	6	0.000000	-2.902542	-14.565867
111	6	0.000000	-3.665285	-13.362772
112	6	0.000000	-2.928852	-12.209186
113	6	0.000000	-2.933470	-10.699933
114	1	0.000000	4.750726	-13.386508
115	1	0.000000	-4.750726	-13.386508
116	1	0.000000	-4.808991	-9.551625
117	1	0.000000	1.010816	-15.519393
118	1	0.000000	3.423051	-15.519818
119	1	0.000000	-1.010816	-15.519393
120	1	0.000000	-3.423051	-15.519818

Table S21. The optimized Cartesian coordinates of the zigzag biphenylene ribbon (n×m = 2×5) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.530110	12.201819
2	6	0.000000	2.902556	18.382457
3	6	0.000000	3.665342	17.179268
4	6	0.000000	1.519075	18.377808
5	6	0.000000	0.739659	17.171026
6	6	0.000000	1.505373	16.020920
7	6	0.000000	2.928950	16.025744
8	6	0.000000	2.933480	14.516523
9	6	0.000000	1.522049	14.511404
10	6	0.000000	0.731989	13.347279
11	6	0.000000	2.950560	12.206744
12	6	0.000000	3.723952	13.360694
13	1	0.000000	4.750788	17.203123
14	1	0.000000	3.423158	19.336372
15	1	0.000000	1.010910	19.335986
16	6	0.000000	-0.739659	17.171026
17	6	0.000000	-1.505373	16.020920
18	6	0.000000	-1.522049	14.511404
19	6	0.000000	-0.731989	13.347279
20	6	0.000000	-1.530110	12.201819
21	6	0.000000	-3.723952	13.360694
22	6	0.000000	-2.933480	14.516523
23	6	0.000000	-2.928950	16.025744
24	6	0.000000	-3.665342	17.179268
25	6	0.000000	-2.902556	18.382457
26	6	0.000000	-1.519075	18.377808

27	1	0.000000	-3.423158	19.336372
28	1	0.000000	-1.010910	19.335986
29	1	0.000000	4.809013	13.368078
30	1	0.000000	-4.750788	17.203123
31	6	0.000000	2.948708	10.695687
32	6	0.000000	1.533931	10.695307
33	6	0.000000	0.733443	9.540055
34	6	0.000000	1.531137	8.387355
35	6	0.000000	2.948800	8.388368
36	6	0.000000	3.731688	9.539893
37	6	0.000000	-1.533931	10.695307
38	6	0.000000	-0.733443	9.540055
39	6	0.000000	-1.531137	8.387355
40	6	0.000000	-2.948800	8.388368
41	6	0.000000	-3.731688	9.539893
42	6	0.000000	-2.948708	10.695687
43	6	0.000000	-2.950560	12.206744
44	1	0.000000	4.816649	9.539363
45	1	0.000000	-4.816649	9.539363
46	1	0.000000	-4.809013	13.368078
47	6	0.000000	1.531452	0.753931
48	6	0.000000	2.947302	6.878366
49	6	0.000000	3.730677	5.724320
50	6	0.000000	1.532001	6.879390
51	6	0.000000	0.732848	5.724498
52	6	0.000000	1.531206	4.570648
53	6	0.000000	2.947740	4.571608
54	6	0.000000	2.947273	3.061685
55	6	0.000000	1.531556	3.062737
56	6	0.000000	0.732669	1.908167
57	6	0.000000	2.947487	0.754991
58	6	0.000000	3.730612	1.908195
59	1	0.000000	4.815603	5.724409
60	6	0.000000	-0.732848	5.724498
61	6	0.000000	-1.531206	4.570648
62	6	0.000000	-1.531556	3.062737
63	6	0.000000	-0.732669	1.908167
64	6	0.000000	-1.531452	0.753931
65	6	0.000000	-3.730612	1.908195
66	6	0.000000	-2.947273	3.061685
67	6	0.000000	-2.947740	4.571608
68	6	0.000000	-3.730677	5.724320
69	6	0.000000	-2.947302	6.878366
70	6	0.000000	-1.532001	6.879390
71	1	0.000000	4.815529	1.908265
72	1	0.000000	-4.815603	5.724409
73	6	0.000000	-2.947487	0.754991
74	1	0.000000	-4.815529	1.908265
75	6	0.000000	1.532001	-6.879390
76	6	0.000000	2.947487	-0.754991
77	6	0.000000	3.730612	-1.908195
78	6	0.000000	1.531452	-0.753931
79	6	0.000000	0.732669	-1.908167
80	6	0.000000	1.531556	-3.062737
81	6	0.000000	2.947273	-3.061685
82	6	0.000000	2.947740	-4.571608
83	6	0.000000	1.531206	-4.570648
84	6	0.000000	0.732848	-5.724498
85	6	0.000000	2.947302	-6.878366
86	6	0.000000	3.730677	-5.724320
87	1	0.000000	4.815529	-1.908265
88	6	0.000000	-0.732669	-1.908167
89	6	0.000000	-1.531556	-3.062737
90	6	0.000000	-1.531206	-4.570648
91	6	0.000000	-0.732848	-5.724498
92	6	0.000000	-1.532001	-6.879390
93	6	0.000000	-3.730677	-5.724320
94	6	0.000000	-2.947740	-4.571608
95	6	0.000000	-2.947273	-3.061685
96	6	0.000000	-3.730612	-1.908195
97	6	0.000000	-2.947487	-0.754991
98	6	0.000000	-1.531452	-0.753931
99	1	0.000000	4.815603	-5.724409
100	1	0.000000	-4.815529	-1.908265
101	6	0.000000	2.948800	-8.388368
102	6	0.000000	1.531137	-8.387355
103	6	0.000000	0.733443	-9.540055
104	6	0.000000	1.533931	-10.695307
105	6	0.000000	2.948708	-10.695687

106	6	0.000000	3.731688	-9.539893
107	6	0.000000	-1.531137	-8.387355
108	6	0.000000	-0.733443	-9.540055
109	6	0.000000	-1.533931	-10.695307
110	6	0.000000	-2.948708	-10.695687
111	6	0.000000	-3.731688	-9.539893
112	6	0.000000	-2.948800	-8.388368
113	6	0.000000	-2.947302	-6.878366
114	1	0.000000	4.816649	-9.539363
115	1	0.000000	-4.816649	-9.539363
116	1	0.000000	-4.815603	-5.724409
117	6	0.000000	1.519075	-18.377808
118	6	0.000000	2.950560	-12.206744
119	6	0.000000	3.723952	-13.360694
120	6	0.000000	1.530110	-12.201819
121	6	0.000000	0.731989	-13.347279
122	6	0.000000	1.522049	-14.511404
123	6	0.000000	2.933480	-14.516523
124	6	0.000000	2.928950	-16.025744
125	6	0.000000	1.505373	-16.020920
126	6	0.000000	0.739659	-17.171026
127	6	0.000000	2.902556	-18.382457
128	6	0.000000	3.665342	-17.179268
129	1	0.000000	4.809013	-13.368078
130	6	0.000000	-0.731989	-13.347279
131	6	0.000000	-1.522049	-14.511404
132	6	0.000000	-1.505373	-16.020920
133	6	0.000000	-0.739659	-17.171026
134	6	0.000000	-1.519075	-18.377808
135	6	0.000000	-3.665342	-17.179268
136	6	0.000000	-2.928950	-16.025744
137	6	0.000000	-2.933480	-14.516523
138	6	0.000000	-3.723952	-13.360694
139	6	0.000000	-2.950560	-12.206744
140	6	0.000000	-1.530110	-12.201819
141	1	0.000000	4.750788	-17.203123
142	1	0.000000	-4.809013	-13.368078
143	6	0.000000	-2.902556	-18.382457
144	1	0.000000	-4.750788	-17.203123
145	1	0.000000	1.010910	-19.335986
146	1	0.000000	3.423158	-19.336372
147	1	0.000000	-1.010910	-19.335986
148	1	0.000000	-3.423158	-19.336372

Table S22. The optimized Cartesian coordinates of the boron nitride sheet **1** (n×m = 3×1.5) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	0.000000	5.087560	-5.144331
2	7	0.000000	3.856746	-5.897150
3	7	0.000000	5.038945	-3.714676
4	5	0.000000	3.822464	-2.925314
5	7	0.000000	2.626873	-3.702762
6	5	0.000000	2.640571	-5.173867
7	7	0.000000	1.193609	-5.372582
8	5	0.000000	1.185539	-3.899991
9	7	0.000000	0.000000	-3.096196
10	5	0.000000	-1.185539	-3.899991
11	7	0.000000	-1.193609	-5.372582
12	5	0.000000	0.000000	-6.163503
13	1	0.000000	3.884866	-6.908156
14	1	0.000000	6.139437	-5.716239
15	1	0.000000	5.926449	-3.229471
16	1	0.000000	0.000000	-7.361773
17	7	0.000000	3.843675	-1.455513
18	5	0.000000	2.646344	-0.674155
19	7	0.000000	1.197388	-0.858305
20	5	0.000000	0.000000	-1.644061
21	7	0.000000	-1.197388	-0.858305
22	5	0.000000	-1.185925	0.607409

23	7	0.000000	0.000000	1.413566
24	5	0.000000	1.185925	0.607409
25	7	0.000000	2.629560	0.797757
26	5	0.000000	3.820807	1.573122
27	7	0.000000	5.027951	0.769021
28	5	0.000000	5.061393	-0.658033
29	1	0.000000	5.923589	1.239375
30	1	0.000000	6.134510	-1.191518
31	7	0.000000	3.846865	3.041333
32	5	0.000000	2.648386	3.825141
33	7	0.000000	1.198227	3.652850
34	5	0.000000	0.000000	2.866712
35	7	0.000000	-1.198227	3.652850
36	5	0.000000	-1.196206	5.121887
37	7	0.000000	0.000000	5.900734
38	5	0.000000	1.196206	5.121887
39	7	0.000000	2.643046	5.298601
40	5	0.000000	3.838675	6.054204
41	7	0.000000	5.042897	5.255237
42	5	0.000000	5.072536	3.825697
43	1	0.000000	5.935746	5.731587
44	1	0.000000	6.140056	3.282041
45	5	0.000000	-2.640571	-5.173867
46	7	0.000000	-3.856746	-5.897150
47	7	0.000000	-2.626873	-3.702762
48	5	0.000000	-3.822464	-2.925314
49	7	0.000000	-5.038945	-3.714676
50	5	0.000000	-5.087560	-5.144331
51	1	0.000000	-3.884866	-6.908156
52	7	0.000000	-3.843675	-1.455513
53	5	0.000000	-5.061393	-0.658033
54	7	0.000000	-5.027951	0.769021
55	5	0.000000	-3.820807	1.573122
56	7	0.000000	-2.629560	0.797757
57	5	0.000000	-2.646344	-0.674155
58	7	0.000000	-3.846865	3.041333
59	5	0.000000	-5.072536	3.825697
60	7	0.000000	-5.042897	5.255237
61	5	0.000000	-3.838675	6.054204
62	7	0.000000	-2.643046	5.298601
63	5	0.000000	-2.648386	3.825141
64	1	0.000000	0.000000	6.912889
65	1	0.000000	3.890526	7.250067
66	1	0.000000	-5.926449	-3.229471
67	1	0.000000	-6.139437	-5.716239
68	1	0.000000	-6.134510	-1.191518
69	1	0.000000	-5.923589	1.239375
70	1	0.000000	-6.140056	3.282041
71	1	0.000000	-5.935746	5.731587
72	1	0.000000	-3.890526	7.250067

Table S23. The optimized Cartesian coordinates of the boron nitride sheet **2** (n×m = 3×2) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-3.388218	3.988839	0.000000
2	7	-3.157602	5.399736	0.000000
3	7	-2.287427	3.007064	0.000000
4	5	-0.900354	3.366188	0.000000
5	7	-0.681932	4.782728	0.000000
6	5	-1.778717	5.762849	0.000000
7	7	-0.941478	6.957361	0.000000
8	5	0.157313	5.976405	0.000000
9	7	1.542070	6.343244	0.000000
10	5	1.778717	7.779333	0.000000
11	7	0.696020	8.712662	0.000000
12	5	-0.703614	8.351439	0.000000
13	1	-3.906443	6.080470	0.000000
14	1	2.896873	8.209748	0.000000
15	1	0.938367	9.695136	0.000000

16	1	-1.557565	9.190281	0.000000
17	5	-8.472609	-1.822969	0.000000
18	7	-8.218091	-0.402580	0.000000
19	7	-7.370221	-2.734002	0.000000
20	5	-5.972175	-2.349844	0.000000
21	7	-5.758463	-0.938186	0.000000
22	5	-6.869998	0.024732	0.000000
23	7	-6.060293	1.241121	0.000000
24	5	-4.950007	0.270903	0.000000
25	7	-3.561246	0.625255	0.000000
26	5	-3.381899	2.048034	0.000000
27	7	-4.484434	3.032095	0.000000
28	5	-5.868668	2.657478	0.000000
29	1	-8.991683	0.248734	0.000000
30	1	-9.598133	-2.230743	0.000000
31	1	-7.595140	-3.720147	0.000000
32	1	-6.766959	3.450331	0.000000
33	7	0.185938	2.392863	0.000000
34	5	1.579071	2.735078	0.000000
35	7	2.400367	3.937832	0.000000
36	5	2.616450	5.343670	0.000000
37	7	4.020945	5.707203	0.000000
38	5	5.107566	4.782802	0.000000
39	7	4.890165	3.342954	0.000000
40	5	3.509659	2.971563	0.000000
41	7	2.685092	1.766397	0.000000
42	5	2.478133	0.349482	0.000000
43	7	1.094463	-0.014771	0.000000
44	5	0.000448	0.970391	0.000000
45	1	6.220550	5.227265	0.000000
46	1	4.265510	6.688802	0.000000
47	7	-4.890165	-3.342954	0.000000
48	5	-3.509659	-2.971563	0.000000
49	7	-2.685092	-1.766397	0.000000
50	5	-2.478133	-0.349482	0.000000
51	7	-1.094463	0.014771	0.000000
52	5	-0.000448	-0.970391	0.000000
53	7	-0.185938	-2.392863	0.000000
54	5	-1.579071	-2.735078	0.000000
55	7	-2.400367	-3.937832	0.000000
56	5	-2.616450	-5.343670	0.000000
57	7	-4.020945	-5.707203	0.000000
58	5	-5.107566	-4.782802	0.000000
59	1	-4.265510	-6.688802	0.000000
60	1	-6.220550	-5.227265	0.000000
61	7	3.561246	-0.625255	0.000000
62	5	4.950007	-0.270903	0.000000
63	7	5.758463	0.938186	0.000000
64	5	5.972175	2.349844	0.000000
65	7	7.370221	2.734002	0.000000
66	5	8.472609	1.822969	0.000000
67	7	8.218091	0.402580	0.000000
68	5	6.869998	-0.024732	0.000000
69	7	6.060293	-1.241121	0.000000
70	5	5.868668	-2.657478	0.000000
71	7	4.484434	-3.032095	0.000000
72	5	3.381899	-2.048034	0.000000
73	1	9.598133	2.230743	0.000000
74	1	7.595140	3.720147	0.000000
75	7	-1.542070	-6.343244	0.000000
76	5	-0.157313	-5.976405	0.000000
77	7	0.681932	-4.782728	0.000000
78	5	0.900354	-3.366188	0.000000
79	7	2.287427	-3.007064	0.000000
80	5	3.388218	-3.988839	0.000000
81	7	3.157602	-5.399736	0.000000
82	5	1.778717	-5.762849	0.000000
83	7	0.941478	-6.957361	0.000000
84	5	0.703614	-8.351439	0.000000
85	7	-0.696020	-8.712662	0.000000
86	5	-1.778717	-7.779333	0.000000
87	1	-0.938367	-9.695136	0.000000
88	1	-2.896873	-8.209748	0.000000
89	1	8.991683	-0.248734	0.000000
90	1	6.766959	-3.450331	0.000000
91	1	3.906443	-6.080470	0.000000
92	1	1.557565	-9.190281	0.000000

Table S24. The optimized Cartesian coordinates of the boron nitride sheet **3** (n×m = 3×3) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	3.399027	11.480509	0.000000
2	7	2.016589	11.067763	0.000000
3	7	4.428397	10.487753	0.000000
4	5	4.203381	9.055402	0.000000
5	7	2.825725	8.683830	0.000000
6	5	1.744002	9.679887	0.000000
7	7	0.627558	8.737991	0.000000
8	5	1.716020	7.743201	0.000000
9	7	1.519898	6.322662	0.000000
10	5	0.125724	5.986218	0.000000
11	7	-0.973687	6.972374	0.000000
12	5	-0.758079	8.389562	0.000000
13	1	1.282160	11.762941	0.000000
14	1	3.677416	12.644834	0.000000
15	1	5.382760	10.822704	0.000000
16	1	-1.646883	9.193051	0.000000
17	7	5.310882	8.091256	0.000000
18	5	5.096539	6.677477	0.000000
19	7	3.992944	5.720148	0.000000
20	5	2.608348	5.354338	0.000000
21	7	2.401514	3.936796	0.000000
22	5	3.504978	2.962619	0.000000
23	7	4.897683	3.308745	0.000000
24	5	5.080884	4.732107	0.000000
25	7	6.182623	5.685081	0.000000
26	5	7.554581	6.060444	0.000000
27	7	7.757602	7.496403	0.000000
28	5	6.716090	8.470712	0.000000
29	1	8.705241	7.850263	0.000000
30	1	7.031726	9.626875	0.000000
31	7	8.670506	5.107936	0.000000
32	5	8.462495	3.691094	0.000000
33	7	7.372070	2.720592	0.000000
34	5	5.989387	2.342127	0.000000
35	7	5.791039	0.921953	0.000000
36	5	6.895682	-0.054640	0.000000
37	7	8.270127	0.333396	0.000000
38	5	8.472710	1.744422	0.000000
39	7	9.562686	2.712003	0.000000
40	5	10.920888	3.105810	0.000000
41	7	11.120993	4.537175	0.000000
42	5	10.070171	5.506260	0.000000
43	1	12.069377	4.890091	0.000000
44	1	10.370679	6.666127	0.000000
45	1	9.031086	-0.333699	0.000000
46	1	11.850599	2.351928	0.000000
47	5	-1.802970	5.777735	0.000000
48	7	-3.180164	5.402272	0.000000
49	7	-0.704717	4.791345	0.000000
50	5	-0.911087	3.372868	0.000000
51	7	-2.298845	3.008309	0.000000
52	5	-3.399027	3.992575	0.000000
53	7	-4.494693	3.034697	0.000000
54	5	-3.391850	2.049258	0.000000
55	7	-3.573324	0.624259	0.000000
56	5	-4.966427	0.277653	0.000000
57	7	-6.076085	1.255528	0.000000
58	5	-5.877883	2.672951	0.000000
59	1	-3.934502	6.076858	0.000000
60	1	-6.773636	3.468424	0.000000
61	7	0.179731	2.398160	0.000000
62	5	-0.000683	0.973064	0.000000
63	7	-1.095229	0.015368	0.000000
64	5	-2.481085	-0.346456	0.000000
65	7	-2.681476	-1.764211	0.000000
66	5	-1.574615	-2.740268	0.000000
67	7	-0.179731	-2.398160	0.000000
68	5	0.000683	-0.973064	0.000000
69	7	1.095229	-0.015368	0.000000
70	5	2.481085	0.346456	0.000000

71	7	2.681476	1.764211	0.000000
72	5	1.574615	2.740268	0.000000
73	7	3.573324	-0.624259	0.000000
74	5	3.391850	-2.049258	0.000000
75	7	2.298845	-3.008309	0.000000
76	5	0.911087	-3.372868	0.000000
77	7	0.704717	-4.791345	0.000000
78	5	1.802970	-5.777735	0.000000
79	7	3.180164	-5.402272	0.000000
80	5	3.399027	-3.992575	0.000000
81	7	4.494693	-3.034697	0.000000
82	5	5.877883	-2.672951	0.000000
83	7	6.076085	-1.255528	0.000000
84	5	4.966427	-0.277653	0.000000
85	1	3.934502	-6.076858	0.000000
86	1	6.773636	-3.468424	0.000000
87	5	-6.895682	0.054640	0.000000
88	7	-8.270127	-0.333396	0.000000
89	7	-5.791039	-0.921953	0.000000
90	5	-5.989387	-2.342127	0.000000
91	7	-7.372070	-2.720592	0.000000
92	5	-8.472710	-1.744422	0.000000
93	7	-9.562686	-2.712003	0.000000
94	5	-8.462495	-3.691094	0.000000
95	7	-8.670506	-5.107936	0.000000
96	5	-10.070171	-5.506260	0.000000
97	7	-11.120993	-4.537175	0.000000
98	5	-10.920888	-3.105810	0.000000
99	1	-9.031086	0.333699	0.000000
100	1	-10.370679	-6.666127	0.000000
101	1	-12.069377	-4.890091	0.000000
102	1	-11.850599	-2.351928	0.000000
103	7	-4.897683	-3.308745	0.000000
104	5	-5.080884	-4.732107	0.000000
105	7	-6.182623	-5.685081	0.000000
106	5	-7.554581	-6.060444	0.000000
107	7	-7.757602	-7.496403	0.000000
108	5	-6.716090	-8.470712	0.000000
109	7	-5.310882	-8.091256	0.000000
110	5	-5.096539	-6.677477	0.000000
111	7	-3.992944	-5.720148	0.000000
112	5	-2.608348	-5.354338	0.000000
113	7	-2.401514	-3.936796	0.000000
114	5	-3.504978	-2.962619	0.000000
115	1	-7.031726	-9.626875	0.000000
116	1	-8.705241	-7.850263	0.000000
117	7	-1.519898	-6.322662	0.000000
118	5	-1.716020	-7.743201	0.000000
119	7	-2.825725	-8.683830	0.000000
120	5	-4.203381	-9.055402	0.000000
121	7	-4.428397	-10.487753	0.000000
122	5	-3.399027	-11.480509	0.000000
123	7	-2.016589	-11.067763	0.000000
124	5	-1.744002	-9.679887	0.000000
125	7	-0.627558	-8.737991	0.000000
126	5	0.758079	-8.389562	0.000000
127	7	0.973687	-6.972374	0.000000
128	5	-0.125724	-5.986218	0.000000
129	1	-3.677416	-12.644834	0.000000
130	1	-5.382760	-10.822704	0.000000
131	1	-1.282160	-11.762941	0.000000
132	1	1.646883	-9.193051	0.000000

Table S25. The optimized Cartesian coordinates of the boron nitride sheet **4** (n×m = 4×2) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	9.558423	-3.443524	0.000000
2	7	8.798569	-4.670433	0.000000
3	7	8.869703	-2.190290	0.000000
4	5	7.428242	-2.031787	0.000000
5	7	6.709725	-3.266677	0.000000

6	5	7.387808	-4.571841	0.000000
7	7	6.186591	-5.404781	0.000000
8	5	5.512958	-4.093813	0.000000
9	7	4.091049	-3.913789	0.000000
10	5	3.398633	-5.169708	0.000000
11	7	4.060359	-6.490722	0.000000
12	5	5.486195	-6.651013	0.000000
13	1	9.278605	-5.560665	0.000000
14	1	10.755062	-3.480135	0.000000
15	1	9.442423	-1.356455	0.000000
16	1	6.029321	-7.718986	0.000000
17	7	6.789911	-0.708707	0.000000
18	5	5.369809	-0.547723	0.000000
19	7	4.160932	-1.368271	0.000000
20	5	3.444827	-2.608527	0.000000
21	7	2.023174	-2.439893	0.000000
22	5	1.370401	-1.121404	0.000000
23	7	2.069892	0.129837	0.000000
24	5	3.490176	-0.061158	0.000000
25	7	4.692532	0.758313	0.000000
26	5	5.405311	1.991134	0.000000
27	7	6.846243	1.812402	0.000000
28	5	7.518260	0.553311	0.000000
29	1	7.434173	2.635921	0.000000
30	1	8.716938	0.558597	0.000000
31	7	4.771436	3.314295	0.000000
32	5	3.349810	3.482990	0.000000
33	7	2.137148	2.672018	0.000000
34	5	1.421446	1.432588	0.000000
35	7	0.000848	1.604016	0.000000
36	5	-0.652341	2.922957	0.000000
37	7	0.047192	4.175830	0.000000
38	5	1.468546	3.980688	0.000000
39	7	2.678984	4.791966	0.000000
40	5	3.398633	6.018154	0.000000
41	7	4.839194	5.834074	0.000000
42	5	5.506110	4.572635	0.000000
43	1	5.430926	6.654698	0.000000
44	1	6.704887	4.570566	0.000000
45	5	2.687888	-6.975949	0.000000
46	7	1.951173	-8.201765	0.000000
47	7	2.026805	-5.657373	0.000000
48	5	0.604769	-5.479987	0.000000
49	7	-0.121776	-6.715524	0.000000
50	5	0.535029	-8.031090	0.000000
51	7	-0.685579	-8.831002	0.000000
52	5	-1.343865	-7.513245	0.000000
53	7	-2.767413	-7.342839	0.000000
54	5	-3.516880	-8.590658	0.000000
55	7	-2.855525	-9.857813	0.000000
56	5	-1.420954	-10.038634	0.000000
57	1	2.395885	-9.111260	0.000000
58	1	-0.937382	-11.133651	0.000000
59	7	-0.047192	-4.175830	0.000000
60	5	-1.468546	-3.980688	0.000000
61	7	-2.678984	-4.791966	0.000000
62	5	-3.398633	-6.018154	0.000000
63	7	-4.839194	-5.834074	0.000000
64	5	-5.506110	-4.572635	0.000000
65	7	-4.771436	-3.314295	0.000000
66	5	-3.349810	-3.482990	0.000000
67	7	-2.137148	-2.672018	0.000000
68	5	-1.421446	-1.432588	0.000000
69	7	-0.000848	-1.604016	0.000000
70	5	0.652341	-2.922957	0.000000
71	7	-2.069892	-0.129837	0.000000
72	5	-3.490176	0.061158	0.000000
73	7	-4.692532	-0.758313	0.000000
74	5	-5.405311	-1.991134	0.000000
75	7	-6.846243	-1.812402	0.000000
76	5	-7.518260	-0.553311	0.000000
77	7	-6.789911	0.708707	0.000000
78	5	-5.369809	0.547723	0.000000
79	7	-4.160932	1.368271	0.000000
80	5	-3.444827	2.608527	0.000000
81	7	-2.023174	2.439893	0.000000
82	5	-1.370401	1.121404	0.000000
83	5	3.516880	8.590658	0.000000
84	7	2.767413	7.342839	0.000000

85	7	2.855525	9.857813	0.000000
86	5	1.420954	10.038634	0.000000
87	7	0.685579	8.831002	0.000000
88	5	1.343865	7.513245	0.000000
89	7	0.121776	6.715524	0.000000
90	5	-0.535029	8.031090	0.000000
91	7	-1.951173	8.201765	0.000000
92	5	-2.687888	6.975949	0.000000
93	7	-2.026805	5.657373	0.000000
94	5	-0.604769	5.479987	0.000000
95	1	4.715124	8.577209	0.000000
96	1	3.443727	10.681316	0.000000
97	5	-3.398633	5.169708	0.000000
98	7	-4.091049	3.913789	0.000000
99	7	-4.060359	6.490722	0.000000
100	5	-5.486195	6.651013	0.000000
101	7	-6.186591	5.404781	0.000000
102	5	-5.512958	4.093813	0.000000
103	7	-6.709725	3.266677	0.000000
104	5	-7.387808	4.571841	0.000000
105	7	-8.798569	4.670433	0.000000
106	5	-9.558423	3.443524	0.000000
107	7	-8.869703	2.190290	0.000000
108	5	-7.428242	2.031787	0.000000
109	1	-4.715124	-8.577209	0.000000
110	1	-3.443727	-10.681316	0.000000
111	1	-5.430926	-6.654698	0.000000
112	1	-6.704887	-4.570566	0.000000
113	1	-7.434173	-2.635921	0.000000
114	1	-8.716938	-0.558597	0.000000
115	1	0.937382	11.133651	0.000000
116	1	-2.395885	9.111260	0.000000
117	1	-6.029321	7.718986	0.000000
118	1	-9.278605	5.560665	0.000000
119	1	-10.755062	3.480135	0.000000
120	1	-9.442423	1.356455	0.000000

Table S26. The optimized Cartesian coordinates of the zigzag boron nitride ribbon (n×m = 2×2) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-0.654252	2.936122	0.000000
2	7	0.081937	4.160076	0.000000
3	7	0.001249	1.615011	0.000000
4	5	1.422079	1.432183	0.000000
5	7	2.151234	2.666359	0.000000
6	5	1.496670	3.983940	0.000000
7	7	2.714889	4.783358	0.000000
8	5	3.373558	3.465741	0.000000
9	7	4.794637	3.296686	0.000000
10	5	5.543765	4.543916	0.000000
11	7	4.882686	5.811936	0.000000
12	5	3.449110	5.992071	0.000000
13	1	-0.360340	5.070242	0.000000
14	7	2.065922	0.122556	0.000000
15	5	3.487149	-0.070449	0.000000
16	7	4.693410	0.744841	0.000000
17	5	5.425008	1.969012	0.000000
18	7	6.864500	1.799199	0.000000
19	5	7.542473	0.539692	0.000000
20	7	6.770742	-0.678913	0.000000
21	5	5.361041	-0.565418	0.000000
22	7	4.153900	-1.386020	0.000000
23	5	3.449110	-2.628823	0.000000
24	7	2.026917	-2.456946	0.000000
25	5	1.370632	-1.132330	0.000000
26	1	8.738607	0.493553	0.000000
27	1	7.445208	2.627258	0.000000
28	1	6.741813	4.533341	0.000000
29	1	5.471161	6.635116	0.000000

30	1	2.963469	7.086252	0.000000
31	5	-7.542473	-0.539692	0.000000
32	7	-6.770742	0.678913	0.000000
33	7	-6.864500	-1.799199	0.000000
34	5	-5.425008	-1.969012	0.000000
35	7	-4.693410	-0.744841	0.000000
36	5	-5.361041	0.565418	0.000000
37	7	-4.153900	1.386020	0.000000
38	5	-3.487149	0.070449	0.000000
39	7	-2.065922	-0.122556	0.000000
40	5	-1.370632	1.132330	0.000000
41	7	-2.026917	2.456946	0.000000
42	5	-3.449110	2.628823	0.000000
43	1	-7.240306	1.574550	0.000000
44	1	-8.738607	-0.493553	0.000000
45	1	-7.445208	-2.627258	0.000000
46	7	-4.794637	-3.296686	0.000000
47	5	-3.373558	-3.465741	0.000000
48	7	-2.151234	-2.666359	0.000000
49	5	-1.422079	-1.432183	0.000000
50	7	-0.001249	-1.615011	0.000000
51	5	0.654252	-2.936122	0.000000
52	7	-0.081937	-4.160076	0.000000
53	5	-1.496670	-3.983940	0.000000
54	7	-2.714889	-4.783358	0.000000
55	5	-3.449110	-5.992071	0.000000
56	7	-4.882686	-5.811936	0.000000
57	5	-5.543765	-4.543916	0.000000
58	1	-5.471161	-6.635116	0.000000
59	1	-6.741813	-4.533341	0.000000
60	1	-3.986817	3.699506	0.000000
61	1	7.240306	-1.574550	0.000000
62	1	3.986817	-3.699506	0.000000
63	1	0.360340	-5.070242	0.000000
64	1	-2.963469	-7.086252	0.000000

Table S27. The optimized Cartesian coordinates of the zigzag boron nitride ribbon (n×m = 2×3) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	3.364781	3.467175	0.000000
2	5	8.442092	7.356661	0.000000
3	7	7.005404	7.483525	0.000000
4	7	9.030842	6.053064	0.000000
5	5	8.291276	4.806524	0.000000
6	7	6.874579	4.968326	0.000000
7	5	6.239289	6.294647	0.000000
8	7	4.854382	5.833894	0.000000
9	5	5.494239	4.505241	0.000000
10	7	4.784209	3.258753	0.000000
11	7	2.712992	4.792962	0.000000
12	5	3.438905	6.027713	0.000000
13	1	6.579154	8.400581	0.000000
14	1	9.131878	8.334924	0.000000
15	1	10.041379	6.011231	0.000000
16	7	8.962911	3.499200	0.000000
17	5	8.233753	2.267807	0.000000
18	7	6.856000	1.781864	0.000000
19	5	5.432692	1.952609	0.000000
20	7	4.712997	0.712820	0.000000
21	7	6.785874	-0.768213	0.000000
22	5	7.505914	0.462199	0.000000
23	7	8.880523	0.944216	0.000000
24	5	10.286799	0.793307	0.000000
25	7	11.014391	2.041473	0.000000
26	5	10.408526	3.336776	0.000000
27	1	12.025769	2.009039	0.000000
28	1	11.127544	4.295101	0.000000
29	1	2.913827	7.104607	0.000000
30	1	10.861046	-0.257094	0.000000

31	5	1.497622	3.995858	0.000000
32	7	2.147737	2.670282	0.000000
33	5	1.426205	1.432007	0.000000
34	7	0.003076	1.611373	0.000000
35	5	-0.648018	2.936246	0.000000
36	7	0.080740	4.162282	0.000000
37	5	3.495783	-0.084836	0.000000
38	7	2.074251	0.120353	0.000000
39	5	1.370686	-1.132132	0.000000
40	7	2.021656	-2.460319	0.000000
41	5	3.438905	-2.647649	0.000000
42	7	4.154686	-1.409654	0.000000
43	5	5.367170	-0.608156	0.000000
44	1	-0.367634	5.069479	0.000000
45	1	3.968511	-3.722240	0.000000
46	1	7.239083	-1.672985	0.000000
47	7	-6.856000	-1.781864	0.000000
48	7	-2.021656	2.460319	0.000000
49	5	-3.438905	2.647649	0.000000
50	5	-1.370686	1.132132	0.000000
51	7	-2.074251	-0.120353	0.000000
52	5	-3.495783	0.084836	0.000000
53	7	-4.154686	1.409654	0.000000
54	5	-5.367170	0.608156	0.000000
55	7	-4.712997	-0.712820	0.000000
56	5	-5.432692	-1.952609	0.000000
57	5	-7.505914	-0.462199	0.000000
58	7	-6.785874	0.768213	0.000000
59	1	-3.968511	3.722240	0.000000
60	5	-1.426205	-1.432007	0.000000
61	7	-2.147737	-2.670282	0.000000
62	5	-3.364781	-3.467175	0.000000
63	7	-4.784209	-3.258753	0.000000
64	5	-5.494239	-4.505241	0.000000
65	5	-3.438905	-6.027713	0.000000
66	7	-2.712992	-4.792962	0.000000
67	5	-1.497622	-3.995858	0.000000
68	7	-0.080740	-4.162282	0.000000
69	5	0.648018	-2.936246	0.000000
70	7	-0.003076	-1.611373	0.000000
71	1	-7.239083	1.672985	0.000000
72	1	0.367634	-5.069479	0.000000
73	7	-8.880523	-0.944216	0.000000
74	5	-8.233753	-2.267807	0.000000
75	7	-8.962911	-3.499200	0.000000
76	5	-10.408526	-3.336776	0.000000
77	7	-11.014391	-2.041473	0.000000
78	5	-10.286799	-0.793307	0.000000
79	7	-6.874579	-4.968326	0.000000
80	5	-8.291276	-4.806524	0.000000
81	7	-9.030842	-6.053064	0.000000
82	5	-8.442092	-7.356661	0.000000
83	7	-7.005404	-7.483525	0.000000
84	5	-6.239289	-6.294647	0.000000
85	7	-4.854382	-5.833894	0.000000
86	1	-9.131878	-8.334924	0.000000
87	1	-10.041379	-6.011231	0.000000
88	1	-11.127544	-4.295101	0.000000
89	1	-12.025769	-2.009039	0.000000
90	1	-10.861046	0.257094	0.000000
91	1	-6.579154	-8.400581	0.000000
92	1	-2.913827	-7.104607	0.000000

Table S28. The optimized Cartesian coordinates of the zigzag boron nitride ribbon (n×m = 2×4) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	8.225586	-2.271471	0.000000
2	5	14.397307	-3.947954	0.000000
3	7	13.626510	-2.728782	0.000000
4	7	13.718271	-5.206905	0.000000

5	5	12.278721	-5.375294	0.000000
6	7	11.547922	-4.150841	0.000000
7	5	12.216740	-2.841133	0.000000
8	7	11.010293	-2.019725	0.000000
9	5	10.342399	-3.334457	0.000000
10	7	8.920891	-3.526400	0.000000
11	7	8.883668	-0.948839	0.000000
12	5	10.305744	-0.776804	0.000000
13	1	14.096671	-1.833457	0.000000
14	1	15.593446	-3.902832	0.000000
15	1	14.298131	-6.035546	0.000000
16	7	11.646896	-6.702351	0.000000
17	5	10.225831	-6.869692	0.000000
18	7	9.003576	-6.069279	0.000000
19	5	8.275840	-4.834269	0.000000
20	7	6.853574	-5.014289	0.000000
21	7	6.934248	-7.560916	0.000000
22	5	8.349067	-7.386603	0.000000
23	7	9.566128	-8.186807	0.000000
24	5	10.299150	-9.396455	0.000000
25	7	11.732701	-9.217684	0.000000
26	5	12.394920	-7.950271	0.000000
27	1	12.320447	-10.041400	0.000000
28	1	13.592921	-7.940693	0.000000
29	1	10.843373	0.293863	0.000000
30	1	9.812130	-10.489972	0.000000
31	5	7.512522	-0.466607	0.000000
32	7	6.853574	-1.787975	0.000000
33	5	5.431590	-1.965562	0.000000
34	7	4.710517	-0.725817	0.000000
35	5	5.368318	0.595658	0.000000
36	7	6.784921	0.760625	0.000000
37	5	5.480937	-4.530966	0.000000
38	7	4.781634	-3.276348	0.000000
39	5	3.359403	-3.476649	0.000000
40	7	2.698918	-4.800039	0.000000
41	5	3.409572	-6.040666	0.000000
42	7	4.827835	-5.858688	0.000000
43	5	6.200798	-6.335999	0.000000
44	1	7.233708	1.667582	0.000000
45	1	2.876092	-7.113308	0.000000
46	1	6.490138	-8.470152	0.000000
47	7	-2.144182	2.675616	0.000000
48	7	4.156468	1.398337	0.000000
49	5	3.444780	2.638130	0.000000
50	5	3.495859	0.075262	0.000000
51	7	2.073426	-0.125682	0.000000
52	5	1.372792	1.128280	0.000000
53	7	2.026698	2.454620	0.000000
54	5	0.654950	2.933839	0.000000
55	7	-0.000371	1.611398	0.000000
56	5	-1.423631	1.435351	0.000000
57	5	-1.487515	3.997302	0.000000
58	7	-0.070973	4.161491	0.000000
59	1	3.976903	3.711430	0.000000
60	5	1.423631	-1.435351	0.000000
61	7	0.000371	-1.611398	0.000000
62	5	-1.372792	-1.128280	0.000000
63	7	-2.073426	0.125682	0.000000
64	5	-3.495859	-0.075262	0.000000
65	5	-3.444780	-2.638130	0.000000
66	7	-2.026698	-2.454620	0.000000
67	5	-0.654950	-2.933839	0.000000
68	7	0.070973	-4.161491	0.000000
69	5	1.487515	-3.997302	0.000000
70	7	2.144182	-2.675616	0.000000
71	1	0.378945	5.067862	0.000000
72	1	-0.378945	-5.067862	0.000000
73	7	-4.156468	-1.398337	0.000000
74	1	-3.976903	-3.711430	0.000000
75	7	-9.003576	6.069279	0.000000
76	7	-2.698918	4.800039	0.000000
77	5	-3.409572	6.040666	0.000000
78	5	-3.359403	3.476649	0.000000
79	7	-4.781634	3.276348	0.000000
80	5	-5.480937	4.530966	0.000000
81	7	-4.827835	5.858688	0.000000
82	5	-6.200798	6.335999	0.000000
83	7	-6.853574	5.014289	0.000000

84	5	-8.275840	4.834269	0.000000
85	5	-8.349067	7.386603	0.000000
86	7	-6.934248	7.560916	0.000000
87	1	-2.876092	7.113308	0.000000
88	5	-5.431590	1.965562	0.000000
89	7	-6.853574	1.787975	0.000000
90	5	-8.225586	2.271471	0.000000
91	7	-8.920891	3.526400	0.000000
92	5	-10.342399	3.334457	0.000000
93	5	-10.305744	0.776804	0.000000
94	7	-8.883668	0.948839	0.000000
95	5	-7.512522	0.466607	0.000000
96	7	-6.784921	-0.760625	0.000000
97	5	-5.368318	-0.595658	0.000000
98	7	-4.710517	0.725817	0.000000
99	1	-6.490138	8.470152	0.000000
100	1	-7.233708	-1.667582	0.000000
101	7	-9.566128	8.186807	0.000000
102	5	-10.225831	6.869692	0.000000
103	7	-11.646896	6.702351	0.000000
104	5	-12.394920	7.950271	0.000000
105	7	-11.732701	9.217684	0.000000
106	5	-10.299150	9.396455	0.000000
107	7	-11.547922	4.150841	0.000000
108	5	-12.278721	5.375294	0.000000
109	7	-13.718271	5.206905	0.000000
110	5	-14.397307	3.947954	0.000000
111	7	-13.626510	2.728782	0.000000
112	5	-12.216740	2.841133	0.000000
113	7	-11.010293	2.019725	0.000000
114	1	-9.812130	10.489972	0.000000
115	1	-14.096671	1.833457	0.000000
116	1	-10.843373	-0.293863	0.000000
117	1	-13.592921	7.940693	0.000000
118	1	-12.320447	10.041400	0.000000
119	1	-14.298131	6.035546	0.000000
120	1	-15.593446	3.902832	0.000000

Table S29. The optimized Cartesian coordinates of the zigzag boron nitride ribbon (n×m = 2×5) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-0.093135	12.311351	0.000000
2	5	-0.546317	18.690923	0.000000
3	7	-1.442843	17.561047	0.000000
4	7	0.866161	18.465058	0.000000
5	5	1.500070	17.161575	0.000000
6	7	0.585352	16.067714	0.000000
7	5	-0.871619	16.267269	0.000000
8	7	-1.249335	14.857417	0.000000
9	5	0.212022	14.660428	0.000000
10	7	0.862072	13.381721	0.000000
11	7	-1.558839	12.496586	0.000000
12	5	-2.190259	13.782370	0.000000
13	1	-2.443159	17.709507	0.000000
14	1	-0.983503	19.805215	0.000000
15	1	1.456913	19.286007	0.000000
16	7	2.961155	17.002882	0.000000
17	5	3.587894	15.716507	0.000000
18	7	3.235157	14.298671	0.000000
19	5	2.309435	13.204279	0.000000
20	7	2.948547	11.920899	0.000000
21	7	5.325856	12.836922	0.000000
22	5	4.694574	14.115145	0.000000
23	7	5.048784	15.528011	0.000000
24	5	5.948898	16.618968	0.000000
25	7	5.307345	17.913410	0.000000
26	5	3.892406	18.120666	0.000000
27	1	5.891167	18.739906	0.000000

28	1	3.488067	19.248439	0.000000
29	1	-3.378292	13.936982	0.000000
30	1	7.141828	16.519580	0.000000
31	5	-1.561896	11.043182	0.000000
32	7	-0.097137	10.856705	0.000000
33	5	0.539548	9.572832	0.000000
34	7	-0.392858	8.483154	0.000000
35	5	-1.857300	8.668510	0.000000
36	7	-2.480311	9.951451	0.000000
37	5	2.944914	10.465762	0.000000
38	7	1.991293	9.391697	0.000000
39	5	2.649395	8.115095	0.000000
40	7	4.116468	7.927842	0.000000
41	5	5.053242	9.007937	0.000000
42	7	4.413781	10.286846	0.000000
43	5	4.411591	11.740415	0.000000
44	1	-3.484581	10.075857	0.000000
45	1	6.241761	8.857771	0.000000
46	1	6.330741	12.717739	0.000000
47	7	-1.342928	0.890102	0.000000
48	7	-2.215648	7.259735	0.000000
49	5	-3.151294	6.179016	0.000000
50	5	-0.748834	7.072347	0.000000
51	7	-0.090026	5.795722	0.000000
52	5	-1.042621	4.720687	0.000000
53	7	-2.510418	4.900737	0.000000
54	5	-2.510418	3.447740	0.000000
55	7	-1.045809	3.265114	0.000000
56	5	-0.410256	1.979555	0.000000
57	5	-2.807220	1.074236	0.000000
58	7	-3.429610	2.357324	0.000000
59	1	-4.339979	6.327633	0.000000
60	5	1.360554	5.614395	0.000000
61	7	1.996229	4.328670	0.000000
62	5	1.992937	2.873133	0.000000
63	7	1.040353	1.798005	0.000000
64	5	1.698641	0.521335	0.000000
65	5	4.101371	1.414795	0.000000
66	7	3.460769	2.692984	0.000000
67	5	3.460769	4.146102	0.000000
68	7	4.380160	5.236302	0.000000
69	5	3.757909	6.519527	0.000000
70	7	2.293656	6.703667	0.000000
71	1	-4.433726	2.482815	0.000000
72	1	5.384248	5.110625	0.000000
73	7	3.165451	0.334100	0.000000
74	1	5.289999	1.265716	0.000000
75	7	-2.293656	-6.703667	0.000000
76	7	-3.165451	-0.334100	0.000000
77	5	-4.101371	-1.414795	0.000000
78	5	-1.698641	-0.521335	0.000000
79	7	-1.040353	-1.798005	0.000000
80	5	-1.992937	-2.873133	0.000000
81	7	-3.460769	-2.692984	0.000000
82	5	-3.460769	-4.146102	0.000000
83	7	-1.996229	-4.328670	0.000000
84	5	-1.360554	-5.614395	0.000000
85	5	-3.757909	-6.519527	0.000000
86	7	-4.380160	-5.236302	0.000000
87	1	-5.289999	-1.265716	0.000000
88	5	0.410256	-1.979555	0.000000
89	7	1.045809	-3.265114	0.000000
90	5	1.042621	-4.720687	0.000000
91	7	0.090026	-5.795722	0.000000
92	5	0.748834	-7.072347	0.000000
93	5	3.151294	-6.179016	0.000000
94	7	2.510418	-4.900737	0.000000
95	5	2.510418	-3.447740	0.000000
96	7	3.429610	-2.357324	0.000000
97	5	2.807220	-1.074236	0.000000
98	7	1.342928	-0.890102	0.000000
99	1	-5.384248	-5.110625	0.000000
100	1	4.433726	-2.482815	0.000000
101	7	-4.116468	-7.927842	0.000000
102	5	-2.649395	-8.115095	0.000000
103	7	-1.991293	-9.391697	0.000000
104	5	-2.944914	-10.465762	0.000000
105	7	-4.413781	-10.286846	0.000000
106	5	-5.053242	-9.007937	0.000000

107	7	0.392858	-8.483154	0.000000
108	5	-0.539548	-9.572832	0.000000
109	7	0.097137	-10.856705	0.000000
110	5	1.561896	-11.043182	0.000000
111	7	2.480311	-9.951451	0.000000
112	5	1.857300	-8.668510	0.000000
113	7	2.215648	-7.259735	0.000000
114	1	-6.241761	-8.857771	0.000000
115	1	3.484581	-10.075857	0.000000
116	1	4.339979	-6.327633	0.000000
117	5	-3.892406	-18.120666	0.000000
118	5	-4.411591	-11.740415	0.000000
119	7	-5.325856	-12.836922	0.000000
120	7	-2.948547	-11.920899	0.000000
121	5	-2.309435	-13.204279	0.000000
122	7	-3.235157	-14.298671	0.000000
123	5	-4.694574	-14.115145	0.000000
124	7	-5.048784	-15.528011	0.000000
125	5	-3.587894	-15.716507	0.000000
126	7	-2.961155	-17.002882	0.000000
127	7	-5.307345	-17.913410	0.000000
128	5	-5.948898	-16.618968	0.000000
129	1	-6.330741	-12.717739	0.000000
130	7	-0.862072	-13.381721	0.000000
131	5	-0.212022	-14.660428	0.000000
132	7	-0.585352	-16.067714	0.000000
133	5	-1.500070	-17.161575	0.000000
134	7	-0.866161	-18.465058	0.000000
135	7	1.442843	-17.561047	0.000000
136	5	0.871619	-16.267269	0.000000
137	7	1.249335	-14.857417	0.000000
138	5	2.190259	-13.782370	0.000000
139	7	1.558839	-12.496586	0.000000
140	5	0.093135	-12.311351	0.000000
141	1	-7.141828	-16.519580	0.000000
142	1	3.378292	-13.936982	0.000000
143	5	0.546317	-18.690923	0.000000
144	1	2.443159	-17.709507	0.000000
145	1	-3.488067	-19.248439	0.000000
146	1	-5.891167	-18.739906	0.000000
147	1	-1.456913	-19.286007	0.000000
148	1	0.983503	-19.805215	0.000000

Table S30. The optimized Cartesian coordinates of the boron nitride compound (n×m = 1×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	1.407946	2.919405	0.000000
2	7	0.071415	2.374912	0.000000
3	7	2.524845	2.021223	0.000000
4	5	2.420910	0.579227	0.000000
5	7	1.096218	0.076702	0.000000
6	5	-0.071415	0.966897	0.000000
7	7	-1.096218	-0.076702	0.000000
8	5	0.071415	-0.966897	0.000000
9	7	-0.071415	-2.374912	0.000000
10	5	-1.407946	-2.919405	0.000000
11	7	-2.524845	-2.021223	0.000000
12	5	-2.420910	-0.579227	0.000000
13	1	-0.724448	2.998602	0.000000
14	1	1.573379	4.104867	0.000000
15	1	3.448882	2.433363	0.000000
16	1	-1.573379	-4.104867	0.000000
17	1	-3.448882	-2.433363	0.000000
18	1	-3.404363	0.104542	0.000000
19	1	3.404363	-0.104542	0.000000
20	1	0.724448	-2.998602	0.000000

Table S31. The optimized Cartesian coordinates of the armchair boron nitride ribbon (n×m = 2×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-1.482117	4.008001	0.000000
2	7	-0.041352	4.091529	0.000000
3	7	-2.105241	2.721934	0.000000
4	5	-1.399994	1.455054	0.000000
5	7	0.021044	1.572452	0.000000
6	5	0.684809	2.879257	0.000000
7	7	2.059375	2.382234	0.000000
8	5	1.395599	1.071889	0.000000
9	7	2.105241	-0.169403	0.000000
10	5	3.553388	-0.033248	0.000000
11	7	4.177918	1.251975	0.000000
12	5	3.466463	2.511320	0.000000
13	1	0.413399	4.994575	0.000000
14	1	-2.142246	5.006258	0.000000
15	1	-3.116576	2.705230	0.000000
16	7	-2.105241	0.169403	0.000000
17	5	-1.395599	-1.071889	0.000000
18	7	-0.021044	-1.572452	0.000000
19	5	1.399994	-1.455054	0.000000
20	7	2.105241	-2.721934	0.000000
21	5	1.482117	-4.008001	0.000000
22	7	0.041352	-4.091529	0.000000
23	5	-0.684809	-2.879257	0.000000
24	7	-2.059375	-2.382234	0.000000
25	5	-3.466463	-2.511320	0.000000
26	7	-4.177918	-1.251975	0.000000
27	5	-3.553388	0.033248	0.000000
28	1	-5.189539	-1.271040	0.000000
29	1	-4.254421	1.005052	0.000000
30	1	2.142246	-5.006258	0.000000
31	1	3.116576	-2.705230	0.000000
32	1	4.254421	-1.005052	0.000000
33	1	5.189539	1.271040	0.000000
34	1	4.058034	3.552233	0.000000
35	1	-0.413399	-4.994575	0.000000
36	1	-4.058034	-3.552233	0.000000

Table S32. The optimized Cartesian coordinates of the armchair boron nitride ribbon (n×m = 3×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	6.038049	-1.103074	0.000000
2	5	5.838226	-2.536335	0.000000
3	5	4.985794	-0.136756	0.000000
4	7	4.482407	-2.932688	0.000000
5	7	3.588474	-0.542032	0.000000
6	5	3.384225	-1.957591	0.000000
7	7	3.148469	-5.291395	0.000000
8	5	1.775322	-5.736998	0.000000
9	5	3.384225	-3.898248	0.000000
10	7	0.726938	-4.765984	0.000000
11	7	2.289300	-2.924026	0.000000
12	5	0.921788	-3.328724	0.000000
13	1	1.524000	-6.907210	0.000000
14	1	-0.221026	-5.118869	0.000000
15	5	1.599059	2.791125	0.000000
16	7	-0.726938	4.765984	0.000000
17	5	-0.921788	3.328724	0.000000
18	7	0.200817	2.388211	0.000000
19	5	0.003389	0.972696	0.000000

20	7	1.094879	-0.005594	0.000000
21	7	2.649833	1.830153	0.000000
22	5	-1.775322	5.736998	0.000000
23	7	-2.289300	2.924026	0.000000
24	7	-3.148469	5.291395	0.000000
25	5	-3.384225	3.898248	0.000000
26	5	2.461013	0.391882	0.000000
27	5	-2.461013	-0.391882	0.000000
28	7	-1.094879	0.005594	0.000000
29	7	-0.200817	-2.388211	0.000000
30	5	-1.599059	-2.791125	0.000000
31	7	-2.649833	-1.830153	0.000000
32	7	-3.588474	0.542032	0.000000
33	5	-4.985794	0.136756	0.000000
34	5	-3.384225	1.957591	0.000000
35	7	-6.038049	1.103074	0.000000
36	7	-4.482407	2.932688	0.000000
37	5	-5.838226	2.536335	0.000000
38	5	-0.003389	-0.972696	0.000000
39	1	-3.899919	5.968190	0.000000
40	1	-1.895593	-3.952429	0.000000
41	1	-3.594941	-2.190869	0.000000
42	1	-5.280522	-1.025055	0.000000
43	1	-6.986231	0.749700	0.000000
44	1	-6.771157	3.286729	0.000000
45	1	6.986231	-0.749700	0.000000
46	1	6.771157	-3.286729	0.000000
47	1	5.280522	1.025055	0.000000
48	1	3.899919	-5.968190	0.000000
49	1	1.895593	3.952429	0.000000
50	1	0.221026	5.118869	0.000000
51	1	3.594941	2.190869	0.000000
52	1	-1.524000	6.907210	0.000000

Table S33. The optimized Cartesian coordinates of the armchair boron nitride ribbon (n×m = 4×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	0.482353	7.979241	0.000000
2	7	1.922045	8.086388	0.000000
3	7	-0.120402	6.683710	0.000000
4	5	0.604050	5.427239	0.000000
5	7	2.023398	5.569405	0.000000
6	5	2.667109	6.886035	0.000000
7	7	4.049700	6.408811	0.000000
8	5	3.403163	5.090137	0.000000
9	7	4.128565	3.857375	0.000000
10	5	5.575221	4.011383	0.000000
11	7	6.182572	5.304324	0.000000
12	5	5.454821	6.555167	0.000000
13	1	2.361814	8.996786	0.000000
14	1	-0.193361	8.967084	0.000000
15	1	-1.131368	6.651270	0.000000
16	7	-0.079359	4.132111	0.000000
17	5	0.639757	2.897783	0.000000
18	7	2.023398	2.419391	0.000000
19	5	3.438100	2.566640	0.000000
20	7	4.156700	1.305706	0.000000
21	5	3.547294	0.019113	0.000000
22	7	2.099990	-0.135161	0.000000
23	5	1.383128	1.101327	0.000000
24	7	0.001754	1.578419	0.000000
25	5	-1.413087	1.425963	0.000000
26	7	-2.133349	2.685830	0.000000
27	5	-1.526263	3.973702	0.000000
28	1	-3.144589	2.660624	0.000000
29	1	-2.241057	4.935675	0.000000
30	7	-2.099990	0.135161	0.000000
31	5	-1.383128	-1.101327	0.000000

32	7	-0.001754	-1.578419	0.000000
33	5	1.413087	-1.425963	0.000000
34	1	4.259690	-0.944703	0.000000
35	7	2.133349	-2.685830	0.000000
36	5	1.526263	-3.973702	0.000000
37	7	0.079359	-4.132111	0.000000
38	5	-0.639757	-2.897783	0.000000
39	7	-2.023398	-2.419391	0.000000
40	5	-3.438100	-2.566640	0.000000
41	7	-4.156700	-1.305706	0.000000
42	5	-3.547294	-0.019113	0.000000
43	1	-4.259690	0.944703	0.000000
44	1	-5.168005	-1.329316	0.000000
45	1	2.241057	-4.935675	0.000000
46	1	3.144589	-2.660624	0.000000
47	1	5.168005	1.329316	0.000000
48	1	6.287992	3.047873	0.000000
49	1	7.193846	5.336724	0.000000
50	1	6.034040	7.602926	0.000000
51	5	-5.575221	-4.011383	0.000000
52	7	-4.128565	-3.857375	0.000000
53	7	-6.182572	-5.304324	0.000000
54	5	-5.454821	-6.555167	0.000000
55	7	-4.049700	-6.408811	0.000000
56	5	-3.403163	-5.090137	0.000000
57	7	-2.023398	-5.569405	0.000000
58	5	-2.667109	-6.886035	0.000000
59	7	-1.922045	-8.086388	0.000000
60	5	-0.482353	-7.979241	0.000000
61	7	0.120402	-6.683710	0.000000
62	5	-0.604050	-5.427239	0.000000
63	1	-6.287992	-3.047873	0.000000
64	1	-7.193846	-5.336724	0.000000
65	1	0.193361	-8.967084	0.000000
66	1	1.131368	-6.651270	0.000000
67	1	-6.034040	-7.602926	0.000000
68	1	-2.361814	-8.996786	0.000000

Table S34. The optimized Cartesian coordinates of the armchair boron nitride ribbon (n×m = 5×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-3.175753	9.574753	0.000000
2	7	-1.939901	10.320974	0.000000
3	7	-3.127890	8.146696	0.000000
4	5	-1.913755	7.353383	0.000000
5	7	-0.711962	8.121552	0.000000
6	5	-0.732575	9.587072	0.000000
7	7	0.716382	9.785983	0.000000
8	5	0.735464	8.317450	0.000000
9	7	1.939901	7.545891	0.000000
10	5	3.160691	8.337406	0.000000
11	7	3.117955	9.765250	0.000000
12	5	1.903313	10.551928	0.000000
13	1	-1.958907	11.332022	0.000000
14	1	-4.224992	10.150631	0.000000
15	1	-4.015004	7.660653	0.000000
16	7	-1.938123	5.889150	0.000000
17	5	-0.738808	5.113090	0.000000
18	7	0.711962	5.311531	0.000000
19	5	1.907270	6.082379	0.000000
20	7	3.118368	5.282509	0.000000
21	5	3.156343	3.859494	0.000000
22	7	1.934997	3.067693	0.000000
23	5	0.736220	3.846445	0.000000
24	7	-0.711845	3.647854	0.000000
25	5	-1.905385	2.872508	0.000000
26	7	-3.117085	3.670909	0.000000
27	5	-3.157386	5.094056	0.000000

28	1	-4.007783	3.191244	0.000000
29	1	-4.229864	5.629083	0.000000
30	7	-1.935247	1.410751	0.000000
31	5	-0.736901	0.632828	0.000000
32	7	0.711546	0.831899	0.000000
33	5	1.905032	1.606010	0.000000
34	1	4.227547	3.321653	0.000000
35	7	3.116651	0.805984	0.000000
36	5	3.155902	-0.616971	0.000000
37	7	1.935247	-1.410751	0.000000
38	5	0.736901	-0.632828	0.000000
39	7	-0.711546	-0.831899	0.000000
40	5	-1.905032	-1.606010	0.000000
41	7	-3.116651	-0.805984	0.000000
42	5	-3.155902	0.616971	0.000000
43	1	-4.227543	1.153928	0.000000
44	1	-4.007787	-1.284849	0.000000
45	1	4.227543	-1.153928	0.000000
46	1	4.007787	1.284849	0.000000
47	1	4.009758	5.760887	0.000000
48	1	4.232265	7.800440	0.000000
49	1	4.005442	10.251373	0.000000
50	1	1.945681	11.748420	0.000000
51	5	-3.156343	-3.859494	0.000000
52	7	-1.934997	-3.067693	0.000000
53	7	-3.118368	-5.282509	0.000000
54	5	-1.907270	-6.082379	0.000000
55	7	-0.711962	-5.311531	0.000000
56	5	-0.736220	-3.846445	0.000000
57	7	0.711845	-3.647854	0.000000
58	5	0.738808	-5.113090	0.000000
59	7	1.938123	-5.889150	0.000000
60	5	3.157386	-5.094056	0.000000
61	7	3.117085	-3.670909	0.000000
62	5	1.905385	-2.872508	0.000000
63	1	-4.227547	-3.321653	0.000000
64	1	-4.009758	-5.760887	0.000000
65	7	-1.939901	-7.545891	0.000000
66	5	-0.735464	-8.317450	0.000000
67	7	0.711962	-8.121552	0.000000
68	5	1.913755	-7.353383	0.000000
69	7	3.127890	-8.146696	0.000000
70	5	3.175753	-9.574753	0.000000
71	7	1.939901	-10.320974	0.000000
72	5	0.732575	-9.587072	0.000000
73	7	-0.716382	-9.785983	0.000000
74	5	-1.903313	-10.551928	0.000000
75	7	-3.117955	-9.765250	0.000000
76	5	-3.160691	-8.337406	0.000000
77	1	-4.005442	-10.251373	0.000000
78	1	-4.232265	-7.800440	0.000000
79	1	4.224992	-10.150631	0.000000
80	1	4.015004	-7.660653	0.000000
81	1	4.229864	-5.629083	0.000000
82	1	4.007783	-3.191244	0.000000
83	1	1.958907	-11.332022	0.000000
84	1	-1.945681	-11.748420	0.000000

Table S35. The optimized Cartesian coordinates of the armchair boron nitride ribbon (n×m = 6×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-3.179178	11.813580	0.000000
2	7	-1.943216	12.559773	0.000000
3	7	-3.131388	10.385504	0.000000
4	5	-1.917212	9.592056	0.000000
5	7	-0.715519	10.360362	0.000000
6	5	-0.735969	11.825895	0.000000
7	7	0.712894	12.024996	0.000000
8	5	0.731957	10.556590	0.000000
9	7	1.936705	9.785381	0.000000

10	5	3.157163	10.577445	0.000000
11	7	3.114417	12.005247	0.000000
12	5	1.899411	12.791347	0.000000
13	1	-1.962415	13.570918	0.000000
14	1	-4.228234	12.389834	0.000000
15	1	-4.018751	9.899836	0.000000
16	7	-1.941122	8.127757	0.000000
17	5	-0.741442	7.352029	0.000000
18	7	0.709236	7.550871	0.000000
19	5	1.904337	8.321991	0.000000
20	7	3.115649	7.522478	0.000000
21	5	3.153874	6.099626	0.000000
22	7	1.932787	5.307328	0.000000
23	5	0.733625	6.085741	0.000000
24	7	-0.714252	5.886643	0.000000
25	5	-1.907504	5.110903	0.000000
26	7	-3.119448	5.908967	0.000000
27	5	-3.160108	7.332039	0.000000
28	1	-4.010151	5.429237	0.000000
29	1	-4.232791	7.866375	0.000000
30	7	-1.936776	3.649100	0.000000
31	5	-0.737985	2.871582	0.000000
32	7	0.710406	3.071129	0.000000
33	5	1.903436	3.845756	0.000000
34	1	4.225242	5.562320	0.000000
35	7	3.115638	3.046451	0.000000
36	5	3.155557	1.623729	0.000000
37	7	1.935308	0.829198	0.000000
38	5	0.735969	1.606308	0.000000
39	7	-0.712386	1.406796	0.000000
40	5	-1.905874	0.632264	0.000000
41	7	-3.117642	1.431901	0.000000
42	5	-3.157164	2.854753	0.000000
43	1	-4.228982	3.391080	0.000000
44	1	-4.008752	0.952875	0.000000
45	1	4.227379	1.087283	0.000000
46	1	4.006611	3.525704	0.000000
47	1	4.007064	8.000879	0.000000
48	1	4.228964	10.041082	0.000000
49	1	4.001712	12.491795	0.000000
50	1	1.941475	13.987849	0.000000
51	5	-3.155557	-1.623729	0.000000
52	7	-1.935308	-0.829198	0.000000
53	7	-3.115638	-3.046451	0.000000
54	5	-1.903436	-3.845756	0.000000
55	7	-0.710406	-3.071129	0.000000
56	5	-0.735969	-1.606308	0.000000
57	7	0.712386	-1.406796	0.000000
58	5	0.737985	-2.871582	0.000000
59	7	1.936776	-3.649100	0.000000
60	5	3.157164	-2.854753	0.000000
61	7	3.117642	-1.431901	0.000000
62	5	1.905874	-0.632264	0.000000
63	1	-4.227379	-1.087283	0.000000
64	1	-4.006611	-3.525704	0.000000
65	7	-1.932787	-5.307328	0.000000
66	5	-0.733625	-6.085741	0.000000
67	7	0.714252	-5.886643	0.000000
68	5	1.907504	-5.110903	0.000000
69	7	3.119448	-5.908967	0.000000
70	5	3.160108	-7.332039	0.000000
71	7	1.941122	-8.127757	0.000000
72	5	0.741442	-7.352029	0.000000
73	7	-0.709236	-7.550871	0.000000
74	5	-1.904337	-8.321991	0.000000
75	7	-3.115649	-7.522478	0.000000
76	5	-3.153874	-6.099626	0.000000
77	1	-4.007064	-8.000879	0.000000
78	1	-4.225242	-5.562320	0.000000
79	7	-1.936705	-9.785381	0.000000
80	5	-0.731957	-10.556590	0.000000
81	7	0.715519	-10.360362	0.000000
82	5	1.917212	-9.592056	0.000000
83	1	4.232791	-7.866375	0.000000
84	7	3.131388	-10.385504	0.000000
85	5	3.179178	-11.813580	0.000000
86	7	1.943216	-12.559773	0.000000
87	5	0.735969	-11.825895	0.000000
88	7	-0.712894	-12.024996	0.000000

89	5	-1.899411	-12.791347	0.000000
90	7	-3.114417	-12.005247	0.000000
91	5	-3.157163	-10.577445	0.000000
92	1	-4.228964	-10.041082	0.000000
93	1	-4.001712	-12.491795	0.000000
94	1	-1.941475	-13.987849	0.000000
95	1	1.962415	-13.570918	0.000000
96	1	4.228234	-12.389834	0.000000
97	1	4.018751	-9.899836	0.000000
98	1	4.010151	-5.429237	0.000000
99	1	4.228982	-3.391080	0.000000
100	1	4.008752	-0.952875	0.000000

Table S36. The optimized Cartesian coordinates of the armchair boron nitride ribbon (n×m = 7×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-3.173781	14.053905	0.000000
2	7	-1.937763	14.799572	0.000000
3	7	-3.126435	12.625629	0.000000
4	5	-1.912548	11.831962	0.000000
5	7	-0.710584	12.600062	0.000000
6	5	-0.730424	14.065629	0.000000
7	7	0.718347	14.264141	0.000000
8	5	0.736850	12.795523	0.000000
9	7	1.941179	12.023645	0.000000
10	5	3.162135	12.815078	0.000000
11	7	3.119878	14.242860	0.000000
12	5	1.905433	15.029819	0.000000
13	1	-1.956607	15.810416	0.000000
14	1	-4.222960	14.629916	0.000000
15	1	-4.013870	12.140179	0.000000
16	7	-1.936936	10.367701	0.000000
17	5	-0.737664	9.591377	0.000000
18	7	0.713007	9.789211	0.000000
19	5	1.908438	10.560019	0.000000
20	7	3.119355	9.759920	0.000000
21	5	3.156848	8.336857	0.000000
22	7	1.935598	7.545328	0.000000
23	5	0.736601	8.324099	0.000000
24	7	-0.711201	8.125800	0.000000
25	5	-1.904952	7.350913	0.000000
26	7	-3.116457	8.149590	0.000000
27	5	-3.156394	9.572725	0.000000
28	1	-4.007326	7.670262	0.000000
29	1	-4.228748	10.107878	0.000000
30	7	-1.934852	5.889034	0.000000
31	5	-0.736600	5.110947	0.000000
32	7	0.712005	5.309699	0.000000
33	5	1.905470	6.083676	0.000000
34	1	4.228196	7.799310	0.000000
35	7	3.117283	5.283761	0.000000
36	5	3.156575	3.860990	0.000000
37	7	1.935884	3.067184	0.000000
38	5	0.736982	3.844919	0.000000
39	7	-0.711472	3.646119	0.000000
40	5	-1.905433	2.872289	0.000000
41	7	-3.116816	3.672565	0.000000
42	5	-3.155735	5.095483	0.000000
43	1	-4.227269	5.632493	0.000000
44	1	-4.008038	3.193828	0.000000
45	1	4.228136	3.323909	0.000000
46	1	4.008364	5.762722	0.000000
47	1	4.010977	10.237809	0.000000
48	1	4.233618	12.278036	0.000000
49	1	4.007452	14.728758	0.000000
50	1	1.948053	16.226293	0.000000
51	5	-3.156474	0.617111	0.000000
52	7	-1.935669	1.410778	0.000000
53	7	-3.117307	-0.805673	0.000000
54	5	-1.905666	-1.605730	0.000000

55	7	-0.711819	-0.831766	0.000000
56	5	-0.736813	0.633012	0.000000
57	7	0.711819	0.831766	0.000000
58	5	0.736813	-0.633012	0.000000
59	7	1.935669	-1.410778	0.000000
60	5	3.156474	-0.617111	0.000000
61	7	3.117307	0.805673	0.000000
62	5	1.905666	1.605730	0.000000
63	1	-4.227938	1.154346	0.000000
64	1	-4.008387	-1.284675	0.000000
65	7	-1.935884	-3.067184	0.000000
66	5	-0.736982	-3.844919	0.000000
67	7	0.711472	-3.646119	0.000000
68	5	1.905433	-2.872289	0.000000
69	7	3.116816	-3.672565	0.000000
70	5	3.155735	-5.095483	0.000000
71	7	1.934852	-5.889034	0.000000
72	5	0.736600	-5.110947	0.000000
73	7	-0.712005	-5.309699	0.000000
74	5	-1.905470	-6.083676	0.000000
75	7	-3.117283	-5.283761	0.000000
76	5	-3.156575	-3.860990	0.000000
77	1	-4.008364	-5.762722	0.000000
78	1	-4.228136	-3.323909	0.000000
79	7	-1.935598	-7.545328	0.000000
80	5	-0.736601	-8.324099	0.000000
81	7	0.711201	-8.125800	0.000000
82	5	1.904952	-7.350913	0.000000
83	1	4.227269	-5.632493	0.000000
84	7	3.116457	-8.149590	0.000000
85	5	3.156394	-9.572725	0.000000
86	7	1.936936	-10.367701	0.000000
87	5	0.737664	-9.591377	0.000000
88	7	-0.713007	-9.789211	0.000000
89	5	-1.908438	-10.560019	0.000000
90	7	-3.119355	-9.759920	0.000000
91	5	-3.156848	-8.336857	0.000000
92	1	-4.228196	-7.799310	0.000000
93	1	-4.010977	-10.237809	0.000000
94	1	4.228748	-10.107878	0.000000
95	1	4.007326	-7.670262	0.000000
96	1	4.008038	-3.193828	0.000000
97	1	4.227938	-1.154346	0.000000
98	1	4.008387	1.284675	0.000000
99	5	-3.162135	-12.815078	0.000000
100	7	-1.941179	-12.023645	0.000000
101	7	-3.119878	-14.242860	0.000000
102	5	-1.905433	-15.029819	0.000000
103	7	-0.718347	-14.264141	0.000000
104	5	-0.736850	-12.795523	0.000000
105	7	0.710584	-12.600062	0.000000
106	5	0.730424	-14.065629	0.000000
107	7	1.937763	-14.799572	0.000000
108	5	3.173781	-14.053905	0.000000
109	7	3.126435	-12.625629	0.000000
110	5	1.912548	-11.831962	0.000000
111	1	-4.233618	-12.278036	0.000000
112	1	-4.007452	-14.728758	0.000000
113	1	4.222960	-14.629916	0.000000
114	1	4.013870	-12.140179	0.000000
115	1	-1.948053	-16.226293	0.000000
116	1	1.956607	-15.810416	0.000000

Table S37. The optimized Cartesian coordinates of the armchair boron nitride ribbon (n×m = 8×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-3.175598	16.291337	0.000000
2	7	-1.939653	17.037443	0.000000
3	7	-3.127800	14.863296	0.000000

4	5	-1.913762	14.069846	0.000000
5	7	-0.711806	14.837839	0.000000
6	5	-0.732534	16.303341	0.000000
7	7	0.716444	16.502373	0.000000
8	5	0.735593	15.033874	0.000000
9	7	1.939850	14.262246	0.000000
10	5	3.160907	15.053455	0.000000
11	7	3.118133	16.481257	0.000000
12	5	1.903627	17.268099	0.000000
13	1	-1.958464	18.048466	0.000000
14	1	-4.224874	16.867135	0.000000
15	1	-4.014926	14.377284	0.000000
16	7	-1.938227	12.605554	0.000000
17	5	-0.739153	11.829364	0.000000
18	7	0.711707	12.028078	0.000000
19	5	1.907176	12.798767	0.000000
20	7	3.118243	11.998868	0.000000
21	5	3.156351	10.575906	0.000000
22	7	1.934838	9.784294	0.000000
23	5	0.736208	10.563107	0.000000
24	7	-0.711870	10.364218	0.000000
25	5	-1.905554	9.589020	0.000000
26	7	-3.117194	10.387458	0.000000
27	5	-3.157688	11.810590	0.000000
28	1	-4.007904	9.907781	0.000000
29	1	-4.230117	12.345657	0.000000
30	7	-1.935274	8.127220	0.000000
31	5	-0.737178	7.349193	0.000000
32	7	0.711464	7.548568	0.000000
33	5	1.904993	8.322661	0.000000
34	1	4.227511	10.037984	0.000000
35	7	3.116826	7.522815	0.000000
36	5	3.156521	6.100000	0.000000
37	7	1.935777	5.306247	0.000000
38	5	0.737077	6.084027	0.000000
39	7	-0.711464	5.884544	0.000000
40	5	-1.905557	5.110770	0.000000
41	7	-3.116956	5.910878	0.000000
42	5	-3.156267	7.333778	0.000000
43	1	-4.227742	7.870958	0.000000
44	1	-4.008025	5.431801	0.000000
45	1	4.228103	5.562823	0.000000
46	1	4.007780	8.002061	0.000000
47	1	4.009590	12.477355	0.000000
48	1	4.232347	14.516255	0.000000
49	1	4.005609	16.967446	0.000000
50	1	1.946059	18.464584	0.000000
51	5	-3.156678	2.855756	0.000000
52	7	-1.935760	3.649261	0.000000
53	7	-3.117156	1.432950	0.000000
54	5	-1.905549	0.632993	0.000000
55	7	-0.711513	1.406862	0.000000
56	5	-0.737163	2.871440	0.000000
57	7	0.711536	3.070915	0.000000
58	5	0.737142	1.606352	0.000000
59	7	1.935758	0.828494	0.000000
60	5	3.156679	1.622012	0.000000
61	7	3.117193	3.044803	0.000000
62	5	1.905554	3.844782	0.000000
63	1	-4.228126	3.393129	0.000000
64	1	-4.008083	0.953611	0.000000
65	7	-1.935758	-0.828494	0.000000
66	5	-0.737142	-1.606352	0.000000
67	7	0.711513	-1.406862	0.000000
68	5	1.905549	-0.632993	0.000000
69	7	3.117156	-1.432950	0.000000
70	5	3.156678	-2.855756	0.000000
71	7	1.935760	-3.649261	0.000000
72	5	0.737163	-2.871440	0.000000
73	7	-0.711536	-3.070915	0.000000
74	5	-1.905554	-3.844782	0.000000
75	7	-3.117193	-3.044803	0.000000
76	5	-3.156679	-1.622012	0.000000
77	1	-4.008107	-3.524169	0.000000
78	1	-4.228149	-1.084644	0.000000
79	7	-1.935777	-5.306247	0.000000
80	5	-0.737077	-6.084027	0.000000
81	7	0.711464	-5.884544	0.000000
82	5	1.905557	-5.110770	0.000000

83	1	4.228126	-3.393129	0.000000
84	7	3.116956	-5.910878	0.000000
85	5	3.156267	-7.333778	0.000000
86	7	1.935274	-8.127220	0.000000
87	5	0.737178	-7.349193	0.000000
88	7	-0.711464	-7.548568	0.000000
89	5	-1.904993	-8.322661	0.000000
90	7	-3.116826	-7.522815	0.000000
91	5	-3.156521	-6.100000	0.000000
92	1	-4.228103	-5.562823	0.000000
93	1	-4.007780	-8.002061	0.000000
94	1	4.227742	-7.870958	0.000000
95	1	4.008025	-5.431801	0.000000
96	1	4.008083	-0.953611	0.000000
97	1	4.228149	1.084644	0.000000
98	1	4.008107	3.524169	0.000000
99	5	-3.156351	-10.575906	0.000000
100	7	-1.934838	-9.784294	0.000000
101	7	-3.118243	-11.998868	0.000000
102	5	-1.907176	-12.798767	0.000000
103	7	-0.711707	-12.028078	0.000000
104	5	-0.736208	-10.563107	0.000000
105	7	0.711870	-10.364218	0.000000
106	5	0.739153	-11.829364	0.000000
107	7	1.938227	-12.605554	0.000000
108	5	3.157688	-11.810590	0.000000
109	7	3.117194	-10.387458	0.000000
110	5	1.905554	-9.589020	0.000000
111	1	-4.227511	-10.037984	0.000000
112	1	-4.009590	-12.477355	0.000000
113	7	-1.939850	-14.262246	0.000000
114	5	-0.735593	-15.033874	0.000000
115	7	0.711806	-14.837839	0.000000
116	5	1.913762	-14.069846	0.000000
117	7	3.127800	-14.863296	0.000000
118	5	3.175598	-16.291337	0.000000
119	7	1.939653	-17.037443	0.000000
120	5	0.732534	-16.303341	0.000000
121	7	-0.716444	-16.502373	0.000000
122	5	-1.903627	-17.268099	0.000000
123	7	-3.118133	-16.481257	0.000000
124	5	-3.160907	-15.053455	0.000000
125	1	-4.005609	-16.967446	0.000000
126	1	-4.232347	-14.516255	0.000000
127	1	4.224874	-16.867135	0.000000
128	1	4.014926	-14.377284	0.000000
129	1	4.230117	-12.345657	0.000000
130	1	4.007904	-9.907781	0.000000
131	1	1.958464	-18.048466	0.000000
132	1	-1.946059	-18.464584	0.000000

Table S38. The optimized Cartesian coordinates of the armchair boron nitride ribbon (n×m = 9×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-3.175094	18.530734	0.000000
2	7	-1.939021	19.276616	0.000000
3	7	-3.127423	17.102623	0.000000
4	5	-1.913443	16.308968	0.000000
5	7	-0.711493	17.076878	0.000000
6	5	-0.732010	18.542393	0.000000
7	7	0.716991	18.741354	0.000000
8	5	0.735953	17.272904	0.000000
9	7	1.940094	16.501170	0.000000
10	5	3.161224	17.292232	0.000000
11	7	3.118643	18.720052	0.000000
12	5	1.904170	19.506963	0.000000
13	1	-1.957606	20.287761	0.000000
14	1	-4.224280	19.106689	0.000000
15	1	-4.014638	16.616753	0.000000

16	7	-1.938025	14.844608	0.000000
17	5	-0.739038	14.068320	0.000000
18	7	0.711805	14.267108	0.000000
19	5	1.907266	15.037693	0.000000
20	7	3.118316	14.237688	0.000000
21	5	3.156307	12.814728	0.000000
22	7	1.934762	12.023227	0.000000
23	5	0.736215	12.802150	0.000000
24	7	-0.711844	12.603126	0.000000
25	5	-1.905516	11.827996	0.000000
26	7	-3.117144	12.626574	0.000000
27	5	-3.157499	14.049752	0.000000
28	1	-4.007864	12.146920	0.000000
29	1	-4.229779	14.584946	0.000000
30	7	-1.935358	10.366112	0.000000
31	5	-0.737289	9.588025	0.000000
32	7	0.711303	9.787535	0.000000
33	5	1.904805	10.561562	0.000000
34	1	4.227313	12.276668	0.000000
35	7	3.116676	9.761690	0.000000
36	5	3.156306	8.338867	0.000000
37	7	1.935572	7.545207	0.000000
38	5	0.736893	8.322961	0.000000
39	7	-0.711614	8.123359	0.000000
40	5	-1.905655	7.349605	0.000000
41	7	-3.117074	8.149747	0.000000
42	5	-3.156306	9.572696	0.000000
43	1	-4.227669	10.109938	0.000000
44	1	-4.008155	7.670702	0.000000
45	1	4.227786	7.801643	0.000000
46	1	4.007603	10.240976	0.000000
47	1	4.009686	14.716137	0.000000
48	1	4.232489	16.754858	0.000000
49	1	4.006117	19.206239	0.000000
50	1	1.946786	20.703443	0.000000
51	5	-3.156714	5.094667	0.000000
52	7	-1.935816	5.888154	0.000000
53	7	-3.117194	3.671832	0.000000
54	5	-1.905538	2.871864	0.000000
55	7	-0.711581	3.645725	0.000000
56	5	-0.737251	5.110358	0.000000
57	7	0.711440	5.309941	0.000000
58	5	0.737014	3.845378	0.000000
59	7	1.935655	3.067548	0.000000
60	5	3.156518	3.861038	0.000000
61	7	3.117082	5.283849	0.000000
62	5	1.905392	6.083816	0.000000
63	1	-4.228065	5.632065	0.000000
64	1	-4.008104	3.192455	0.000000
65	7	-1.935724	1.410308	0.000000
66	5	-0.737151	0.632453	0.000000
67	7	0.711493	0.832139	0.000000
68	5	1.905431	1.606020	0.000000
69	7	3.117103	0.806012	0.000000
70	5	3.156608	-0.616794	0.000000
71	7	1.935724	-1.410308	0.000000
72	5	0.737151	-0.632453	0.000000
73	7	-0.711493	-0.832139	0.000000
74	5	-1.905431	-1.606020	0.000000
75	7	-3.117103	-0.806012	0.000000
76	5	-3.156608	0.616794	0.000000
77	1	-4.008005	-1.285401	0.000000
78	1	-4.227960	1.154205	0.000000
79	7	-1.935655	-3.067548	0.000000
80	5	-0.737014	-3.845378	0.000000
81	7	0.711581	-3.645725	0.000000
82	5	1.905538	-2.871864	0.000000
83	1	4.227960	-1.154205	0.000000
84	7	3.117194	-3.671832	0.000000
85	5	3.156714	-5.094667	0.000000
86	7	1.935816	-5.888154	0.000000
87	5	0.737251	-5.110358	0.000000
88	7	-0.711440	-5.309941	0.000000
89	5	-1.905392	-6.083816	0.000000
90	7	-3.117082	-5.283849	0.000000
91	5	-3.156518	-3.861038	0.000000
92	1	-4.227876	-3.323616	0.000000
93	1	-4.007995	-5.763201	0.000000
94	1	4.228065	-5.632065	0.000000

95	1	4.008104	-3.192455	0.000000
96	1	4.008005	1.285401	0.000000
97	1	4.227876	3.323616	0.000000
98	1	4.007995	5.763201	0.000000
99	5	-3.156306	-8.338867	0.000000
100	7	-1.935572	-7.545207	0.000000
101	7	-3.116676	-9.761690	0.000000
102	5	-1.904805	-10.561562	0.000000
103	7	-0.711303	-9.787535	0.000000
104	5	-0.736893	-8.322961	0.000000
105	7	0.711614	-8.123359	0.000000
106	5	0.737289	-9.588025	0.000000
107	7	1.935358	-10.366112	0.000000
108	5	3.156306	-9.572696	0.000000
109	7	3.117074	-8.149747	0.000000
110	5	1.905655	-7.349605	0.000000
111	1	-4.227786	-7.801643	0.000000
112	1	-4.007603	-10.240976	0.000000
113	7	-1.934762	-12.023227	0.000000
114	5	-0.736215	-12.802150	0.000000
115	7	0.711844	-12.603126	0.000000
116	5	1.905516	-11.827996	0.000000
117	7	3.117144	-12.626574	0.000000
118	5	3.157499	-14.049752	0.000000
119	7	1.938025	-14.844608	0.000000
120	5	0.739038	-14.068320	0.000000
121	7	-0.711805	-14.267108	0.000000
122	5	-1.907266	-15.037693	0.000000
123	7	-3.118316	-14.237688	0.000000
124	5	-3.156307	-12.814728	0.000000
125	1	-4.009686	-14.716137	0.000000
126	1	-4.227313	-12.276668	0.000000
127	7	-1.940094	-16.501170	0.000000
128	5	-0.735953	-17.272904	0.000000
129	7	0.711493	-17.076878	0.000000
130	5	1.913443	-16.308968	0.000000
131	1	4.229779	-14.584946	0.000000
132	7	3.127423	-17.102623	0.000000
133	5	3.175094	-18.530734	0.000000
134	7	1.939021	-19.276616	0.000000
135	5	0.732010	-18.542393	0.000000
136	7	-0.716991	-18.741354	0.000000
137	5	-1.904170	-19.506963	0.000000
138	7	-3.118643	-18.720052	0.000000
139	5	-3.161224	-17.292232	0.000000
140	1	-4.232489	-16.754858	0.000000
141	1	-4.006117	-19.206239	0.000000
142	1	4.224280	-19.106689	0.000000
143	1	4.014638	-16.616753	0.000000
144	1	4.007864	-12.146920	0.000000
145	1	4.227669	-10.109938	0.000000
146	1	4.008155	-7.670702	0.000000
147	1	1.957606	-20.287761	0.000000
148	1	-1.946786	-20.703443	0.000000

Table S39. The optimized Cartesian coordinates of the armchair boron nitride ribbon (n×m = 10×1) calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-3.174047	20.771434	0.000000
2	7	-1.937772	21.516976	0.000000
3	7	-3.126662	19.343259	0.000000
4	5	-1.912827	18.549388	0.000000
5	7	-0.710764	19.317278	0.000000
6	5	-0.730641	20.782883	0.000000
7	7	0.718332	20.981196	0.000000
8	5	0.736720	19.512642	0.000000
9	7	1.940995	18.740748	0.000000
10	5	3.162047	19.531946	0.000000
11	7	3.119926	20.959762	0.000000
12	5	1.905461	21.746771	0.000000
13	1	-1.956375	22.527994	0.000000

14	1	-4.222982	21.347858	0.000000
15	1	-4.014094	18.857831	0.000000
16	7	-1.937407	17.085081	0.000000
17	5	-0.738173	16.308825	0.000000
18	7	0.712588	16.506748	0.000000
19	5	1.908027	17.277400	0.000000
20	7	3.119013	16.477267	0.000000
21	5	3.156632	15.054344	0.000000
22	7	1.935151	14.262703	0.000000
23	5	0.736343	15.041624	0.000000
24	7	-0.711628	14.843381	0.000000
25	5	-1.905266	14.068186	0.000000
26	7	-3.116838	14.866892	0.000000
27	5	-3.156852	16.290032	0.000000
28	1	-4.007719	14.387632	0.000000
29	1	-4.229207	16.825161	0.000000
30	7	-1.935181	12.606373	0.000000
31	5	-0.736865	11.828292	0.000000
32	7	0.711627	12.027103	0.000000
33	5	1.905104	12.801189	0.000000
34	1	4.227728	14.516331	0.000000
35	7	3.116965	12.001239	0.000000
36	5	3.156263	10.578457	0.000000
37	7	1.935611	9.784643	0.000000
38	5	0.736686	10.562337	0.000000
39	7	-0.711749	10.363413	0.000000
40	5	-1.905722	9.589563	0.000000
41	7	-3.117093	10.389792	0.000000
42	5	-3.156047	11.812715	0.000000
43	1	-4.227548	12.349797	0.000000
44	1	-4.008329	9.911106	0.000000
45	1	4.227850	10.041306	0.000000
46	1	4.008062	12.480116	0.000000
47	1	4.010580	16.955255	0.000000
48	1	4.233433	18.994648	0.000000
49	1	4.007535	21.445540	0.000000
50	1	1.948529	22.943223	0.000000
51	5	-3.156378	7.334278	0.000000
52	7	-1.935898	8.127992	0.000000
53	7	-3.117220	5.911333	0.000000
54	5	-1.905619	5.111288	0.000000
55	7	-0.711802	5.885606	0.000000
56	5	-0.736787	7.350445	0.000000
57	7	0.711558	7.549441	0.000000
58	5	0.736535	6.084521	0.000000
59	7	1.935541	5.306636	0.000000
60	5	3.156269	6.100460	0.000000
61	7	3.117128	7.523198	0.000000
62	5	1.905503	8.323240	0.000000
63	1	-4.228126	7.871118	0.000000
64	1	-4.008338	5.432480	0.000000
65	7	-1.935664	3.649703	0.000000
66	5	-0.736719	2.871818	0.000000
67	7	0.711620	3.070772	0.000000
68	5	1.905461	3.845078	0.000000
69	7	3.117093	3.045017	0.000000
70	5	3.156232	1.622093	0.000000
71	7	1.935758	0.828420	0.000000
72	5	0.736659	1.605998	0.000000
73	7	-0.711658	1.406827	0.000000
74	5	-1.905642	0.633108	0.000000
75	7	-3.117235	1.433102	0.000000
76	5	-3.156411	2.855862	0.000000
77	1	-4.008320	0.954136	0.000000
78	1	-4.227913	3.393158	0.000000
79	7	-1.935758	-0.828420	0.000000
80	5	-0.736659	-1.605998	0.000000
81	7	0.711658	-1.406827	0.000000
82	5	1.905642	-0.633108	0.000000
83	1	4.228039	1.085292	0.000000
84	7	3.117235	-1.433102	0.000000
85	5	3.156411	-2.855862	0.000000
86	7	1.935664	-3.649703	0.000000
87	5	0.736719	-2.871818	0.000000
88	7	-0.711620	-3.070772	0.000000
89	5	-1.905461	-3.845078	0.000000
90	7	-3.117093	-3.045017	0.000000
91	5	-3.156232	-1.622093	0.000000
92	1	-4.228039	-1.085292	0.000000

93	1	-4.008186	-3.523912	0.000000
94	1	4.227913	-3.393158	0.000000
95	1	4.008320	-0.954136	0.000000
96	1	4.008186	3.523912	0.000000
97	1	4.227781	5.563150	0.000000
98	1	4.008223	8.002130	0.000000
99	5	-3.156269	-6.100460	0.000000
100	7	-1.935541	-5.306636	0.000000
101	7	-3.117128	-7.523198	0.000000
102	5	-1.905503	-8.323240	0.000000
103	7	-0.711558	-7.549441	0.000000
104	5	-0.736535	-6.084521	0.000000
105	7	0.711802	-5.885606	0.000000
106	5	0.736787	-7.350445	0.000000
107	7	1.935898	-8.127992	0.000000
108	5	3.156378	-7.334278	0.000000
109	7	3.117220	-5.911333	0.000000
110	5	1.905619	-5.111288	0.000000
111	1	-4.227781	-5.563150	0.000000
112	1	-4.008223	-8.002130	0.000000
113	7	-1.935611	-9.784643	0.000000
114	5	-0.736686	-10.562337	0.000000
115	7	0.711749	-10.363413	0.000000
116	5	1.905722	-9.589563	0.000000
117	7	3.117093	-10.389792	0.000000
118	5	3.156047	-11.812715	0.000000
119	7	1.935181	-12.606373	0.000000
120	5	0.736865	-11.828292	0.000000
121	7	-0.711627	-12.027103	0.000000
122	5	-1.905104	-12.801189	0.000000
123	7	-3.116965	-12.001239	0.000000
124	5	-3.156263	-10.578457	0.000000
125	1	-4.008062	-12.480116	0.000000
126	1	-4.227850	-10.041306	0.000000
127	7	-1.935151	-14.262703	0.000000
128	5	-0.736343	-15.041624	0.000000
129	7	0.711628	-14.843381	0.000000
130	5	1.905266	-14.068186	0.000000
131	1	4.227548	-12.349797	0.000000
132	7	3.116838	-14.866892	0.000000
133	5	3.156852	-16.290032	0.000000
134	7	1.937407	-17.085081	0.000000
135	5	0.738173	-16.308825	0.000000
136	7	-0.712588	-16.506748	0.000000
137	5	-1.908027	-17.277400	0.000000
138	7	-3.119013	-16.477267	0.000000
139	5	-3.156632	-15.054344	0.000000
140	1	-4.227728	-14.516331	0.000000
141	1	-4.010580	-16.955255	0.000000
142	1	4.229207	-16.825161	0.000000
143	1	4.007719	-14.387632	0.000000
144	1	4.008329	-9.911106	0.000000
145	1	4.228126	-7.871118	0.000000
146	1	4.008338	-5.432480	0.000000
147	5	-3.162047	-19.531946	0.000000
148	7	-1.940995	-18.740748	0.000000
149	7	-3.119926	-20.959762	0.000000
150	5	-1.905461	-21.746771	0.000000
151	7	-0.718332	-20.981196	0.000000
152	5	-0.736720	-19.512642	0.000000
153	7	0.710764	-19.317278	0.000000
154	5	0.730641	-20.782883	0.000000
155	7	1.937772	-21.516976	0.000000
156	5	3.174047	-20.771434	0.000000
157	7	3.126662	-19.343259	0.000000
158	5	1.912827	-18.549388	0.000000
159	1	-4.233433	-18.994648	0.000000
160	1	-4.007535	-21.445540	0.000000
161	1	4.222982	-21.347858	0.000000
162	1	4.014094	-18.857831	0.000000
163	1	-1.948529	-22.943223	0.000000
164	1	1.956375	-22.527994	0.000000

Table S40. The optimized Cartesian coordinates of the tunnel-like carbon allotrope calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.778565	1.991306	0.845496
2	6	-1.521765	0.798158	1.358840
3	6	-2.886375	3.173130	1.388499
4	6	-3.642717	1.971235	0.818127
5	6	-2.862440	0.783653	1.321660
6	6	-1.549499	3.176047	1.413090
7	1	-3.457752	4.010966	1.779854
8	1	-1.010976	4.025189	1.820880
9	6	-0.778565	1.991306	-0.845496
10	6	-3.642717	1.971235	-0.818127
11	6	-1.549499	3.176047	-1.413090
12	6	-2.886375	3.173130	-1.388499
13	6	-1.521765	0.798158	-1.358840
14	6	-2.862440	0.783653	-1.321660
15	1	-1.010976	4.025189	-1.820880
16	1	-3.457752	4.010966	-1.779854
17	1	-4.686370	1.980429	-1.152297
18	1	-4.686370	1.980429	1.152297
19	6	3.642717	1.971235	0.818127
20	6	2.862440	0.783653	1.321660
21	6	1.549499	3.176047	1.413090
22	6	0.778565	1.991306	0.845496
23	6	1.521765	0.798158	1.358840
24	6	2.886375	3.173130	1.388499
25	1	1.010976	4.025189	1.820880
26	1	3.457752	4.010966	1.779854
27	6	3.642717	1.971235	-0.818127
28	6	0.778565	1.991306	-0.845496
29	6	2.886375	3.173130	-1.388499
30	6	1.549499	3.176047	-1.413090
31	6	2.862440	0.783653	-1.321660
32	6	1.521765	0.798158	-1.358840
33	1	3.457752	4.010966	-1.779854
34	1	1.010976	4.025189	-1.820880
35	1	4.686370	1.980429	-1.152297
36	1	4.686370	1.980429	1.152297
37	6	-0.778565	-1.991306	0.845496
38	6	-1.549499	-3.176047	1.413090
39	6	-2.862440	-0.783653	1.321660
40	6	-3.642717	-1.971235	0.818127
41	6	-2.886375	-3.173130	1.388499
42	6	-1.521765	-0.798158	1.358840
43	1	-1.010976	-4.025189	1.820880
44	1	-3.457752	-4.010966	1.779854
45	6	-0.778565	-1.991306	-0.845496
46	6	-3.642717	-1.971235	-0.818127
47	6	-1.521765	-0.798158	-1.358840
48	6	-2.862440	-0.783653	-1.321660
49	6	-1.549499	-3.176047	-1.413090
50	6	-2.886375	-3.173130	-1.388499
51	1	-1.010976	-4.025189	-1.820880
52	1	-3.457752	-4.010966	-1.779854
53	1	-4.686370	-1.980429	-1.152297
54	1	-4.686370	-1.980429	1.152297
55	6	3.642717	-1.971235	0.818127
56	6	2.886375	-3.173130	1.388499
57	6	1.521765	-0.798158	1.358840
58	6	0.778565	-1.991306	0.845496
59	6	1.549499	-3.176047	1.413090
60	6	2.862440	-0.783653	1.321660
61	1	3.457752	-4.010966	1.779854
62	1	1.010976	-4.025189	1.820880
63	6	3.642717	-1.971235	-0.818127
64	6	0.778565	-1.991306	-0.845496
65	6	2.862440	-0.783653	-1.321660
66	6	1.521765	-0.798158	-1.358840
67	6	2.886375	-3.173130	-1.388499
68	6	1.549499	-3.176047	-1.413090
69	1	3.457752	-4.010966	-1.779854
70	1	1.010976	-4.025189	-1.820880

71	1	4.686370	-1.980429	-1.152297
72	1	4.686370	-1.980429	1.152297

Table S41. The optimized Cartesian coordinates of the Li-containing complex with the “tunnel” graphene cluster calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.724918	1.888298	2.021562
2	6	-1.480005	0.730010	1.963510
3	6	-2.795681	3.125712	1.369696
4	6	-3.529991	1.909643	0.837887
5	6	-2.873890	0.695025	1.415690
6	6	-1.531444	3.107763	1.852402
7	1	-3.314665	4.077533	1.297793
8	1	-1.080270	4.056045	2.131998
9	6	-0.724918	1.888298	-2.021562
10	6	-3.529991	1.909643	-0.837887
11	6	-1.531444	3.107763	-1.852402
12	6	-2.795681	3.125712	-1.369696
13	6	-1.480005	0.730010	-1.963510
14	6	-2.873890	0.695025	-1.415690
15	1	-1.080270	4.056045	-2.131998
16	1	-3.314665	4.077533	-1.297793
17	1	-4.588982	1.964699	-1.117168
18	1	-4.588982	1.964699	1.117168
19	6	3.529991	1.909643	0.837887
20	6	2.873890	0.695025	1.415690
21	6	1.531444	3.107763	1.852402
22	6	0.724918	1.888298	2.021562
23	6	1.480005	0.730010	1.963510
24	6	2.795681	3.125712	1.369696
25	1	1.080270	4.056045	2.131998
26	1	3.314665	4.077533	1.297793
27	6	3.529991	1.909643	-0.837887
28	6	0.724918	1.888298	-2.021562
29	6	2.795681	3.125712	-1.369696
30	6	1.531444	3.107763	-1.852402
31	6	2.873890	0.695025	-1.415690
32	6	1.480005	0.730010	-1.963510
33	1	3.314665	4.077533	-1.297793
34	1	1.080270	4.056045	-2.131998
35	1	4.588982	1.964699	-1.117168
36	1	4.588982	1.964699	1.117168
37	6	-0.724918	-1.888298	2.021562
38	6	-1.531444	-3.107763	1.852402
39	6	-2.873890	-0.695025	1.415690
40	6	-3.529991	-1.909643	0.837887
41	6	-2.795681	-3.125712	1.369696
42	6	-1.480005	-0.730010	1.963510
43	1	-1.080270	-4.056045	2.131998
44	1	-3.314665	-4.077533	1.297793
45	6	-0.724918	-1.888298	-2.021562
46	6	-3.529991	-1.909643	-0.837887
47	6	-1.480005	-0.730010	-1.963510
48	6	-2.873890	-0.695025	-1.415690
49	6	-1.531444	-3.107763	-1.852402
50	6	-2.795681	-3.125712	-1.369696
51	1	-1.080270	-4.056045	-2.131998
52	1	-3.314665	-4.077533	-1.297793
53	1	-4.588982	-1.964699	-1.117168
54	1	-4.588982	-1.964699	1.117168
55	6	3.529991	-1.909643	0.837887
56	6	2.795681	-3.125712	1.369696
57	6	1.480005	-0.730010	1.963510
58	6	0.724918	-1.888298	2.021562
59	6	1.531444	-3.107763	1.852402
60	6	2.873890	-0.695025	1.415690
61	1	3.314665	-4.077533	1.297793
62	1	1.080270	-4.056045	2.131998
63	6	3.529991	-1.909643	-0.837887
64	6	0.724918	-1.888298	-2.021562

65	6	2.873890	-0.695025	-1.415690
66	6	1.480005	-0.730010	-1.963510
67	6	2.795681	-3.125712	-1.369696
68	6	1.531444	-3.107763	-1.852402
69	1	3.314665	-4.077533	-1.297793
70	1	1.080270	-4.056045	-2.131998
71	1	4.588982	-1.964699	-1.117168
72	1	4.588982	-1.964699	1.117168
73	3	-1.357603	0.000000	0.000000
74	3	1.357603	0.000000	0.000000