

Design of nanoscaled materials based on tetraoxa[8]circulene

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Electronic Supplementary Information

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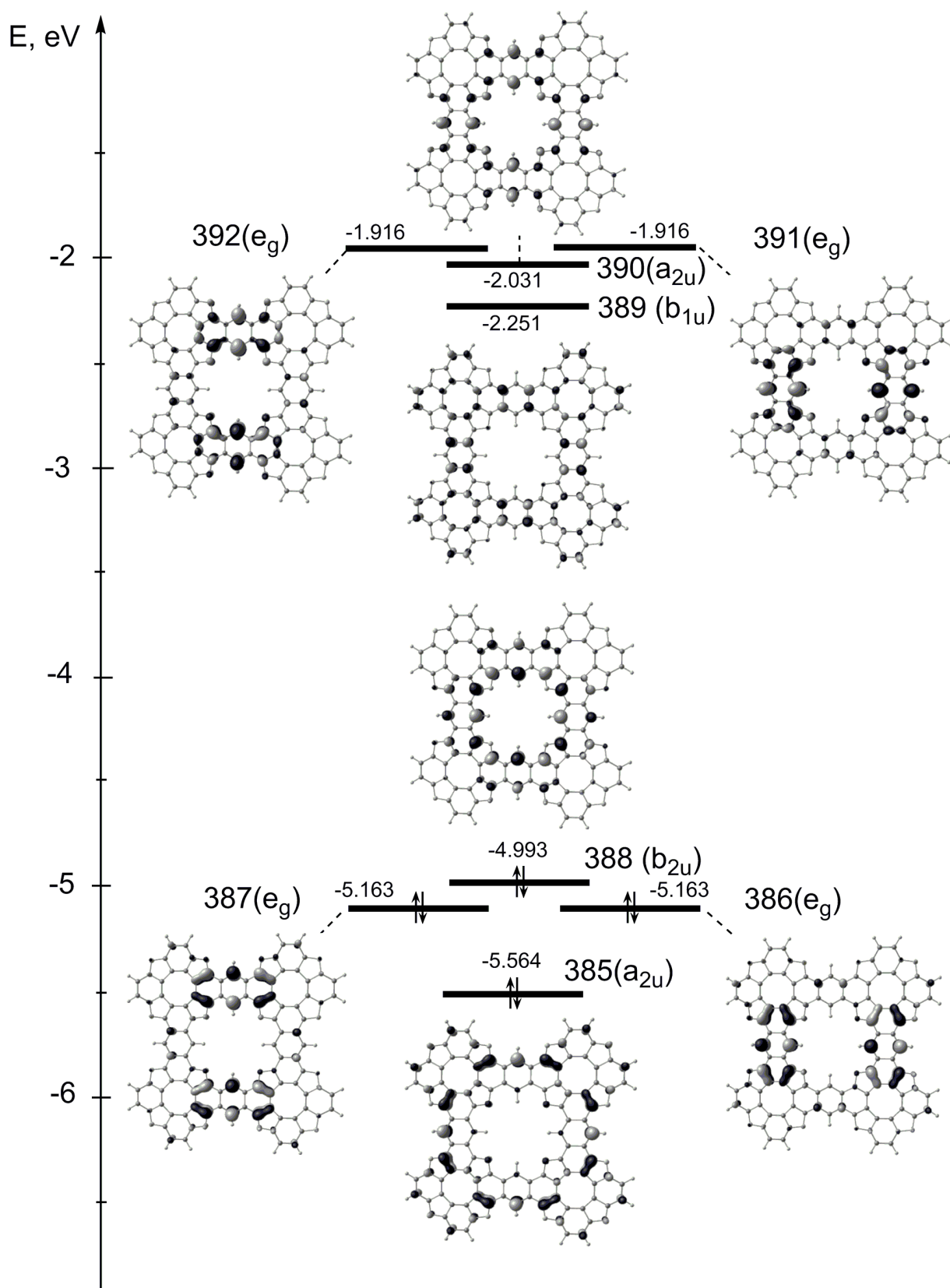


Figure S1. Molecular orbitals diagram of the compound 1 calculated at the B3LYP/6-21G(d) level of theory

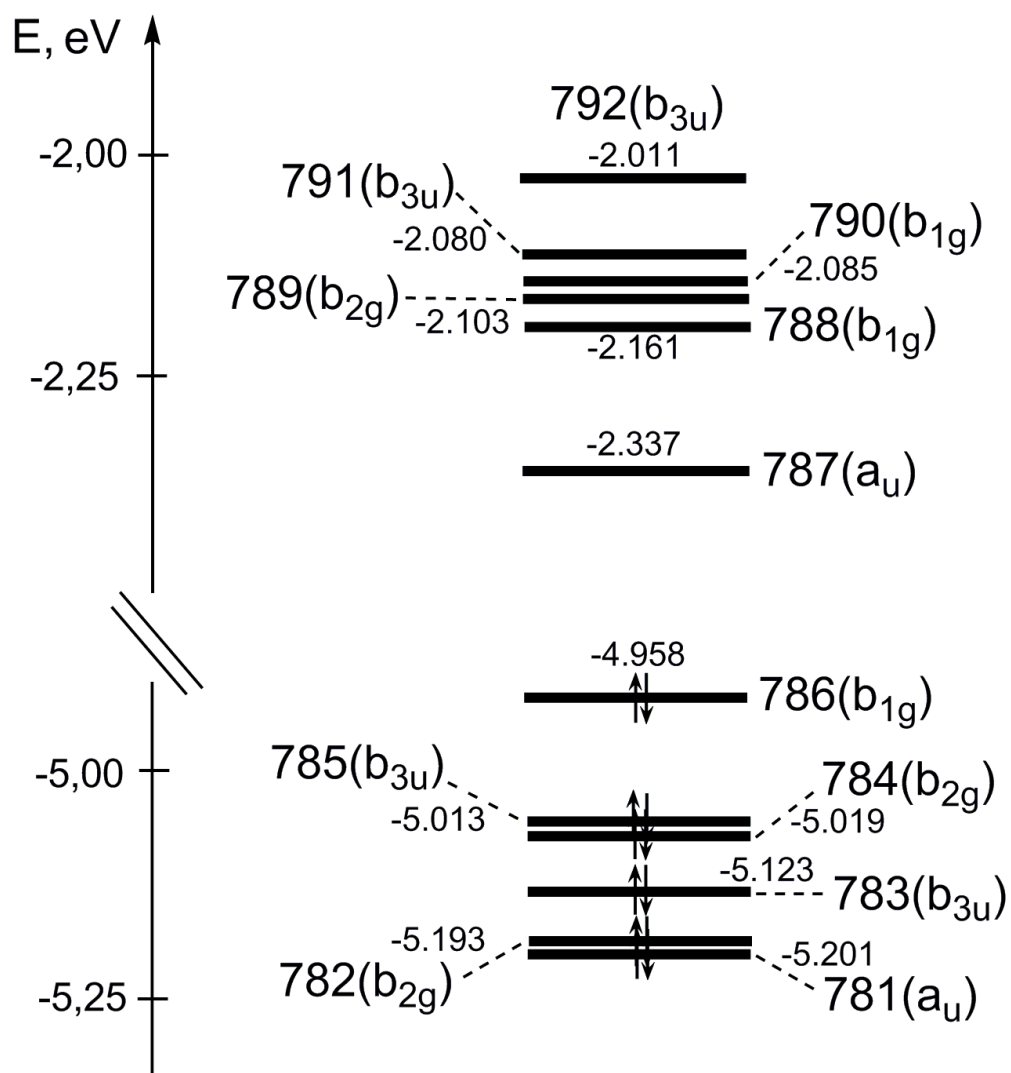


Figure S2. Molecular orbitals diagram of the compound **2** calculated at the B3LYP/6-21G(d) level of theory

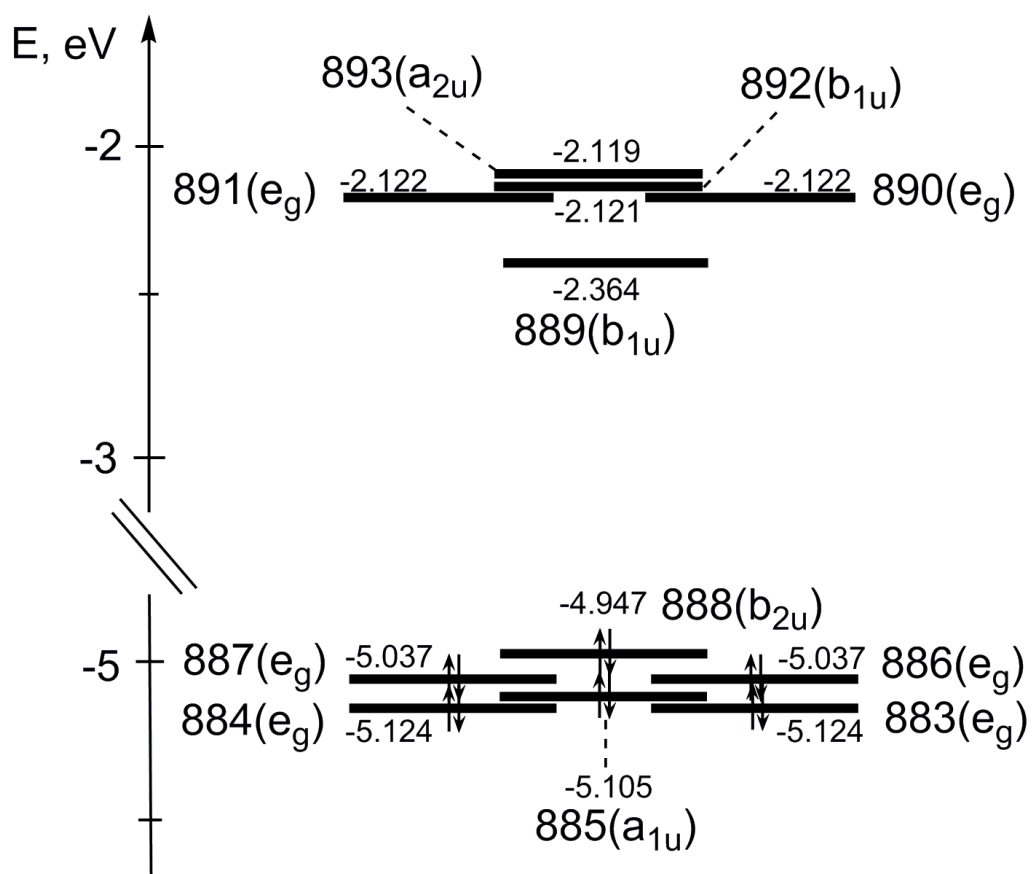


Figure S3. Molecular orbitals diagram of the compound **3** calculated at the B3LYP/6-21G(d) level of theory

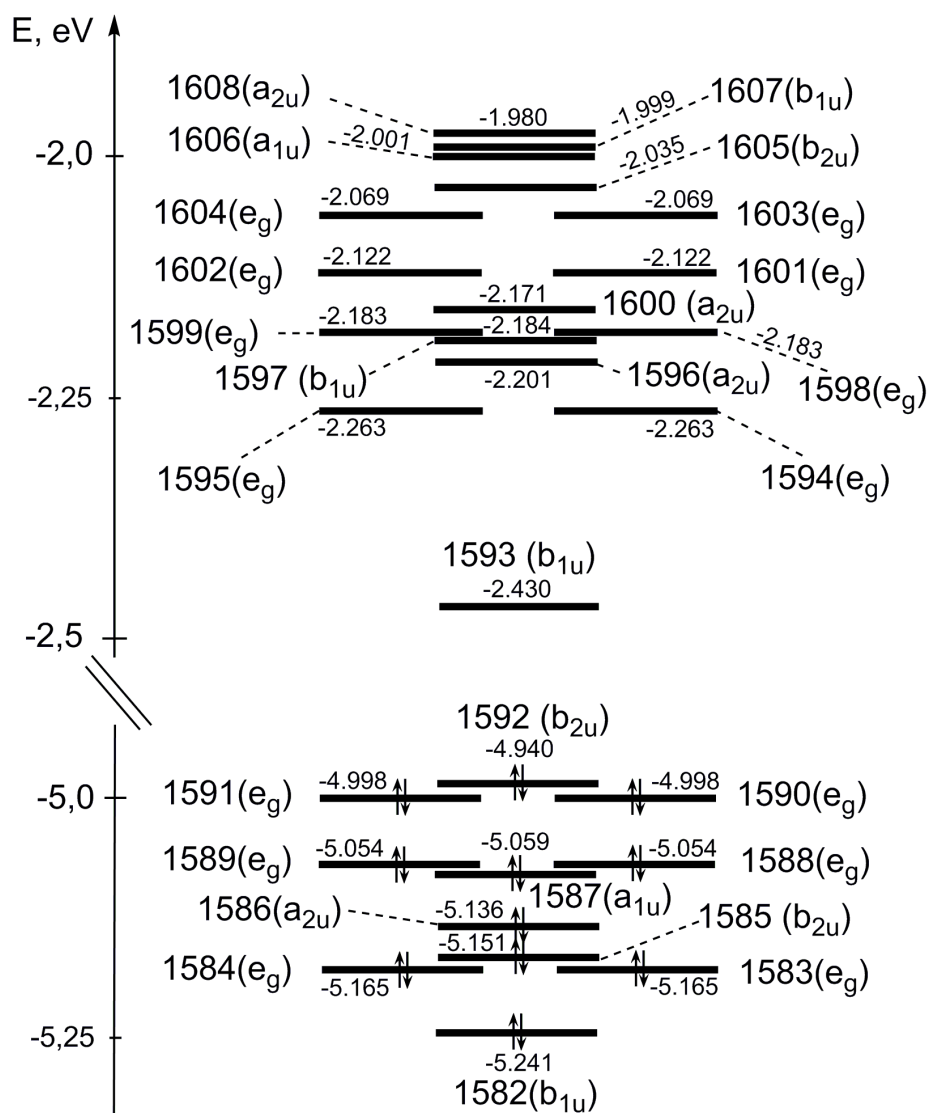


Figure S4. Molecular orbitals diagram of the compound **4** calculated at the B3LYP/6-21G(d) level of theory

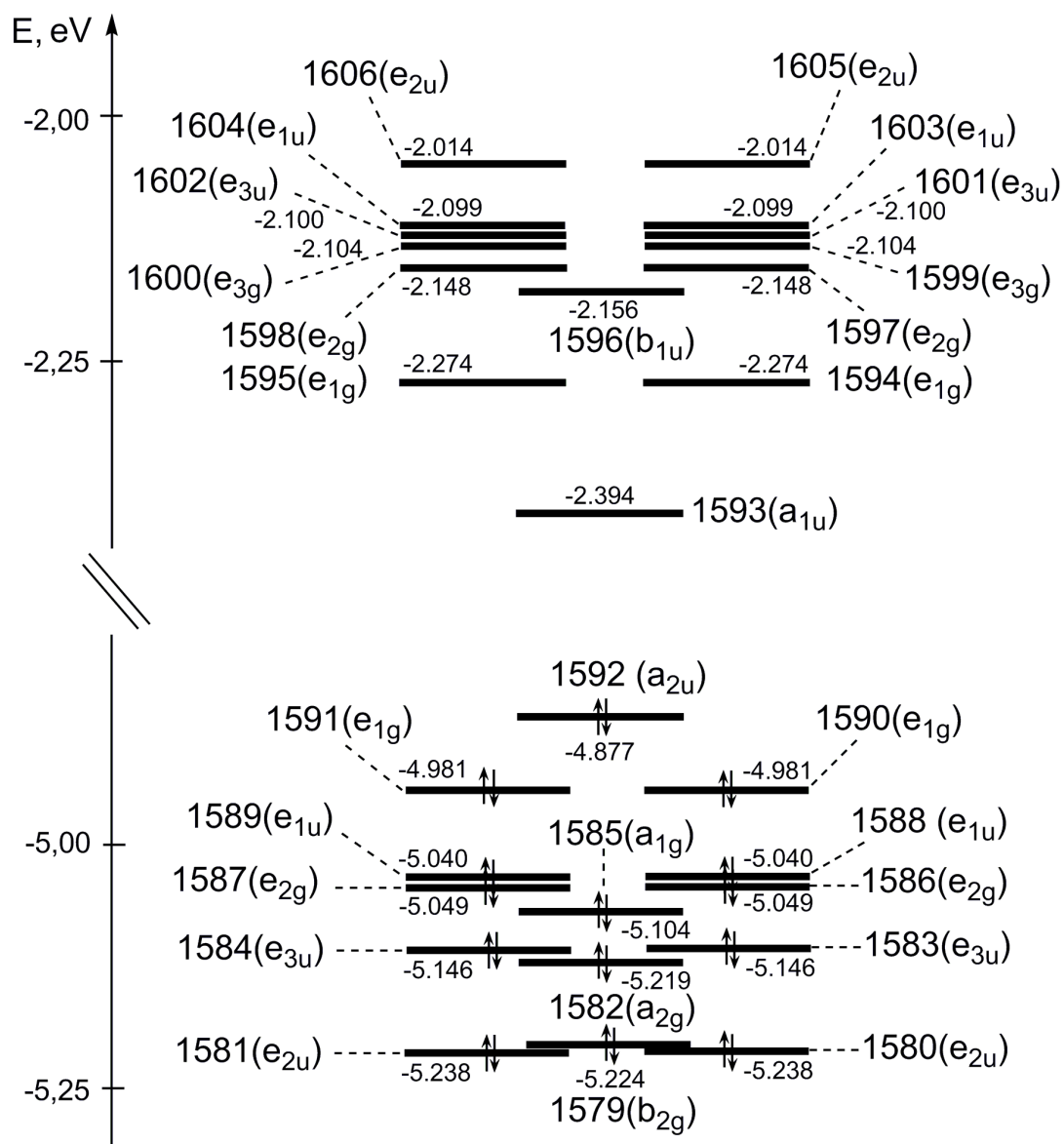


Figure S5. Molecular orbitals diagram of the compound **5** calculated at the B3LYP/6-21G(d) level of theory

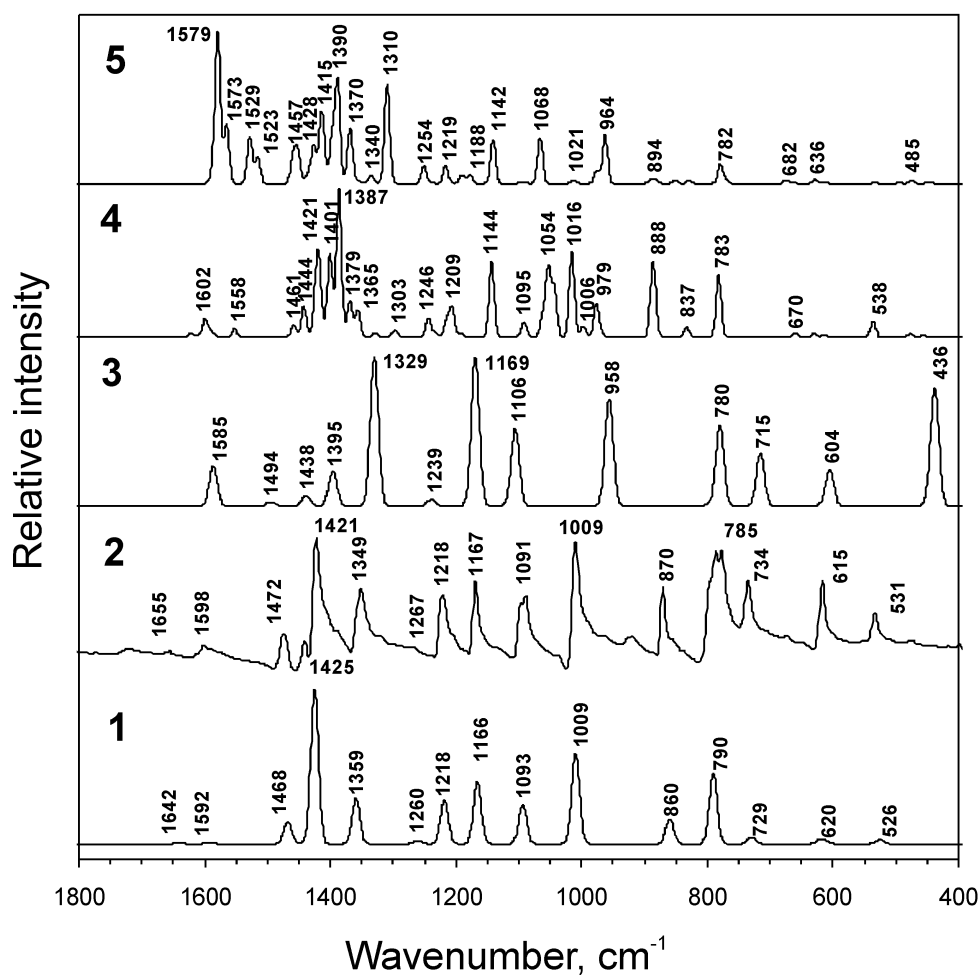


Figure S6. The FTIR spectra for compounds **4B** and **1** Calculated by the B3LYP/6-21G(d) method in the ground singlet (S₀) and excited triplet (T₁) electronic states: 1 – **4B** (S₀); 2 – experimental spectrum for **4B**; 3 – **4B** (T₁); 4 – compound **1** (S₀); 5 – compound **1** (T₁).

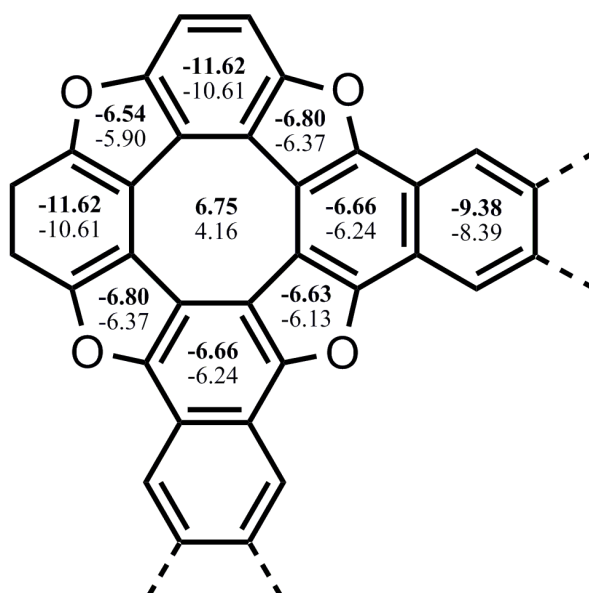


Figure S7. The NICS(0) (top) and NICS (1) (bottom) indexes for the compound **1** calculated at the GIAO B3LYP/6-311++G(d,p) level of theory.

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

State	Transition	λ , nm	M_{xy} , a.u.	μ_z, β	f	Assignment (in vacuum approximation)
Compound 1						
T ₁	X ¹ A _{1g} →1 ³ B _{1g}	641	0	0	0.000	0.44(388→390) + 0.30[(386→391) – (387→392)] – 0.18(385→395) + 0.15(384→389)
T ₂₍₃₎	X ¹ A _{1g} →1 ³ E _u	605	0	0	0.000	0.33(388→392) – 0.28(387→390) – 0.26(388→391) – 0.22(386→390) + 0.18(387→395) – 0.14(386→395) + 0.13(385→392) – 0.12(386→389) + 0.10(385→391)
T ₄	X ¹ A _{1g} →1 ³ A _{2g}	545	0	0	0.000	0.63(388→389) + 0.14[(387→391) – (386→392)] + 0.11[(386→393) – (387→394)]
S ₁	X ¹ A _{1g} →1 ¹ A _{2g}	508	0	8.30	0.000	0.68(388→389)
S ₂₍₃₎	X ¹ A _{1g} →1 ¹ E _u	454	3.23	0	0.700	0.63(386, 387→389) – 0.15[(386→389) + (387→389)] – 0.13[(386,387→390) + (388→392) – (388→391)] + 0.10[(384→391) – (384→392)]
S ₄	X ¹ A _{1g} →1 ¹ B _{1g}	448	0	0	0.000	0.69(388→390) + 0.12 (384→389)
S ₅₍₆₎	X ¹ A _{1g} →2 ¹ E _u	431	0.34	0	0.008	0.62(388→391,392) + 0.25[(386→390) – (387→390)] + 0.20[(387→389) – (386→389)]
S ₇	X ¹ A _{1g} →1 ¹ B _{2g}	430	0	0	0.000	0.46[(386→392) + (387→391)] + 0.21(385→389)
S ₈₍₉₎	X ¹ A _{1g} →3 ¹ E _u	423	1.89	0	0.136	0.55(386,387→390) + 0.25[(388→392, 394) – (388→391, 393)] + 0.19[(386→390) – (387→390)]
S ₁₀	X ¹ A _{1g} →2 ¹ A _{2g}	420	0	7.30	0.000	0.48[(386→392) – (387→391)] – 0.11[(388→389) + (384→390)]
Compound 3						
T ₁	X ¹ A _{1g} →1 ³ A _{2g}	663	0	0	0.000	0.25(885→893) + 0.24(888→892) + 0.18[(887→894) – (886→895)] – 0.16[(884→896) – (883→897)]
T ₂₍₃₎	X ¹ A _{1g} →1 ³ E _u	638	0	0	0.000	–0.22[(888→896) – (887→892)] – 0.18(883→893) – 0.16[(888→894) + (887→898) + (885→897)] + 0.15(884→892)
T ₄	X ¹ A _{1g} →1 ³ A _{2g}	613	0	0	0.000	–0.26(888→892) + 0.19(884→894) – 0.18(883→895) + 0.16[(888→889) + (885→893)] – 0.15[(885→900) – (887→896)] – 0.14[(886→890) + (887→891) – (886→897)]
S ₁	X ¹ A _{1g} →1 ¹ A _{2g}	518	0	18.79	0.000	0.64(888→889) + 0.14[(887→891) – (886→890)]
S ₂	X ¹ A _{1g} →1 ¹ B _{1g}	495	0	0	0.000	0.59(885→889) – 0.17[(884→890) + (883→891) + (888→893)]
S ₃₍₄₎	X ¹ A _{1g} →1 ¹ E _u	491	0.33	0	0.007	0.57(883,884→889) – 0.19(888→894,895) + 0.18[(885→891) + (888→890) – (885→890, 891)] + 0.11[(883→889) – (884→889)]
S ₅₍₆₎	X ¹ A _{1g} →2 ¹ E _u	484	5.60	0	1.965	0.51(886, 887→889) + 0.42[(886→889) – (887→889)]
S ₇	X ¹ A _{1g} →2 ¹ B _{1g}	466	0	0	0.000	0.53(888→893) – 0.26(885→889) + 0.18[(886→895) – (887→894)]
S ₈	X ¹ A _{1g} →1 ¹ A _{1g}	462	0	0	0.000	0.35[(886→891) + (887→890)] + 0.24[(886→895) + (887→894)] + 0.16[(883→891) + (884→890)]
S ₉₍₁₀₎	X ¹ A _{1g} →3 ¹ E _u	462	1.43	0	0.135	0.36(888→894,895) + 0.34(888→890, 891) +

						+ 0.27 (886,887→893) – 0.21[(888→895) + (888→894)] – 0.20[(888→891) + (888→890)] – 0.16(886, 887→893)
Compound 4						
T ₁₍₂₎	X ¹ A _{1g} →1 ³ E _u	655	0	0	0.000	0.13[(1592→1602) – (1592→1601)] – 0.12(1587→1603,1604) + 0.11(1590,1591→1600) – 0.10(1592→1601,1602)
T ₃	X ¹ A _{1g} →1 ³ A _{2g}	640	0	0	0.000	– 0.19(1587→1608) + 0.16(1585→1599) – 0.15(1592→1607) – 0.14(1582→1605) + 0.13[(1588→1604) – (1589→1603) + (1583→1603) – (1584→1604)] – 0.12(1586→1606)
S ₁	X ¹ A _{1g} →1 ¹ A _{2g}	522	0	32.49	0.000	0.59(1592→1593) + 0.21[(1590→1594) + (1591→1595)]
S ₂₍₃₎	X ¹ A _{1g} →1 ¹ E _u	504	1.57	0	0.149	0.46(1588,1589→1593) – 0.25[(1592→1594) + (1592→1595)] + 0.23[(1588→1593) – (1589→1593)] + 0.16[(1587→1594) – (1587→1595)] + 0.13(1592→1594,1595) + 0.10[(1591→1593) – (1590→1593)]
S ₄₍₅₎	X ¹ A _{1g} →2 ¹ E _u	500	6.95	0	2.311	0.53(1590,1591→1593) – 0.26(1592→1594,1595) + 0.21[(1590→1593) – (1591→1593)] + 0.13[(1589→1593) – (1588→1593)] + 0.12[(1587→1594) – (1587→1595)] + 0.10[(1592→1594) – (1592→1595)]
S ₆	X ¹ A _{1g} →1 ¹ B _{1g}	493	0	0.001	0	0.49(1586→1593) + 0.23[(1588→1594) – (1589→1595)] – 0.16(1592→1599) + 0.13[(1582→1595) – (1583→1594)] – 0.10(1581→1596)
Compound 2						
T ₁	X ¹ A _{1g} →1 ³ B _{1u}	640	0	0	0.000	– 0.30(784→792) + 0.22(783→789) + 0.21(786→794) – 0.19[(785→793) – (781→790)] – 0.16[(782→791) – (785→789)]
T ₂	X ¹ A _{1g} →1 ³ B _{2u}	618	0	0	0.000	0.31(785→790) – 0.28(786→791) – 0.21(786→797) – 0.18(783→798) + 0.16 (780→790) + 0.13(786→792)
T ₃	X ¹ A _{1g} →1 ³ B _{3g}	611	0	0	0.000	0.25[(786→789) + (784→790)] + 0.24(781→792) – 0.21(785→794) + 0.17[(784→798) + (783→794)] – 0.15(786→799)
S ₁	X ¹ A _{1g} →1 ¹ B _{2u}	505	0.23	0	0.003	0.60(784→787) – 0.25(785→788) + 0.18(783→788) – 0.12(786→791)
S ₂	X ¹ A _{1g} →1 ¹ B _{3g}	504	0	16.00	0.000	0.61(785→787) – 0.25(784→788) – 0.13(786→795)
S ₃	X ¹ A _{1g} →1 ¹ B _{1u}	498	6.99	0	2.978	0.68(786→787) – 0.12(781→788)
S ₄	X ¹ A _{1g} →2 ¹ B _{3g}	491	0	1.07	0.000	0.58(783→787) + 0.29(784→788) + 0.15(786→789)
S ₅	X ¹ A _{1g} →3 ¹ B _{3g}	467	0	0.80	0.000	0.60(786→789) – 0.20(786→793) – 0.15(783→787)
S ₆	X ¹ A _{1g} →2 ¹ B _{2u}	465	1.54	0	0.155	0.51(786→791) + 0.27(782→787) + 0.22(785→788) + 0.17(784→787)
S ₇	X ¹ A _{1g} →1 ¹ A _g	462	0	0	0.000	0.53(786→788) – 0.31(781→787) + 0.23(786→790)
S ₈	X ¹ A _{1g} →2 ¹ A _g	457	0	0	0.000	0.53(786→790) + 0.21(784→789) – 0.20(785→791) – 0.18(786→788) + 0.17(781→787)
S ₉	X ¹ A _{1g} →3 ¹ B _{2u}	453	3.38	0	0.764	0.45(782→787) – 0.39(786→791) + 0.24(785→788) + 0.13(786→792)
S ₁₀	X ¹ A _{1g} →2 ¹ B _{1u}	452	0.01	0	0.000	0.51(785→789) + 0.36(784→791) – 0.15(784→792)
Compound 5						

$T_{1(2)}$	$X^1A_{1g} \rightarrow 1^3E_u$	618	0	0	0.000	$0.19[(1579 \rightarrow 1601) - (1579 \rightarrow 1602)] -$ $0.17[(1588, 1589 \rightarrow 1609) - (1583, 1584 \rightarrow 1607)] -$ $0.14[(1582 \rightarrow 1603) + 0.14(1582 \rightarrow 1604)] -$ $- 0.13[(1583, 1584 \rightarrow 1598) - (1584 \rightarrow 1597)] +$ $+ (1583 \rightarrow 1597)]$
T_3	$X^1A_{1g} \rightarrow 1^3A_{2g}$	610	0	0	0.000	$0.21(1592 \rightarrow 1593) - 0.20(1579 \rightarrow 1607) +$ $0.19[(1587 \rightarrow 1598) - (1586 \rightarrow 1597)] +$ $+ 0.18[(1583 \rightarrow 1601) - (1584 \rightarrow 1602)] -$ $- 0.16[(1588 \rightarrow 1603) + (1589 \rightarrow 1604) - (1582 \rightarrow 1609)]$
S_1	$X^1A_{1g} \rightarrow 1^1A_{2g}$	530	0	28.92	0.000	$0.60(1592 \rightarrow 1593) - 0.23[(1590 \rightarrow 1594) +$ $+ (1591 \rightarrow 1595)]$
S_2	$X^1A_{1g} \rightarrow 1^1E_{2u}$	502	0	0	0.000	$0.50(1586 \rightarrow 1593) - 0.22[(1588 \rightarrow 1595) +$ $+ (1589 \rightarrow 1594)] - 0.18(1592 \rightarrow 1597) +$ $0.16[(1583 \rightarrow 1595) + (1584 \rightarrow 1594)]$
$S_{3(4)}$	$X^1A_{1g} \rightarrow 1^1E_u$	499	6.7	0	2.747	$0.38(1590, 1591 \rightarrow 1593) - 0.34[(1590 \rightarrow 1593) +$ $+ (1591 \rightarrow 1593) + (1592 \rightarrow 1595) - (1592 \rightarrow 1594)] +$ $+ 0.30[(1592 \rightarrow 1594, 1595)]$

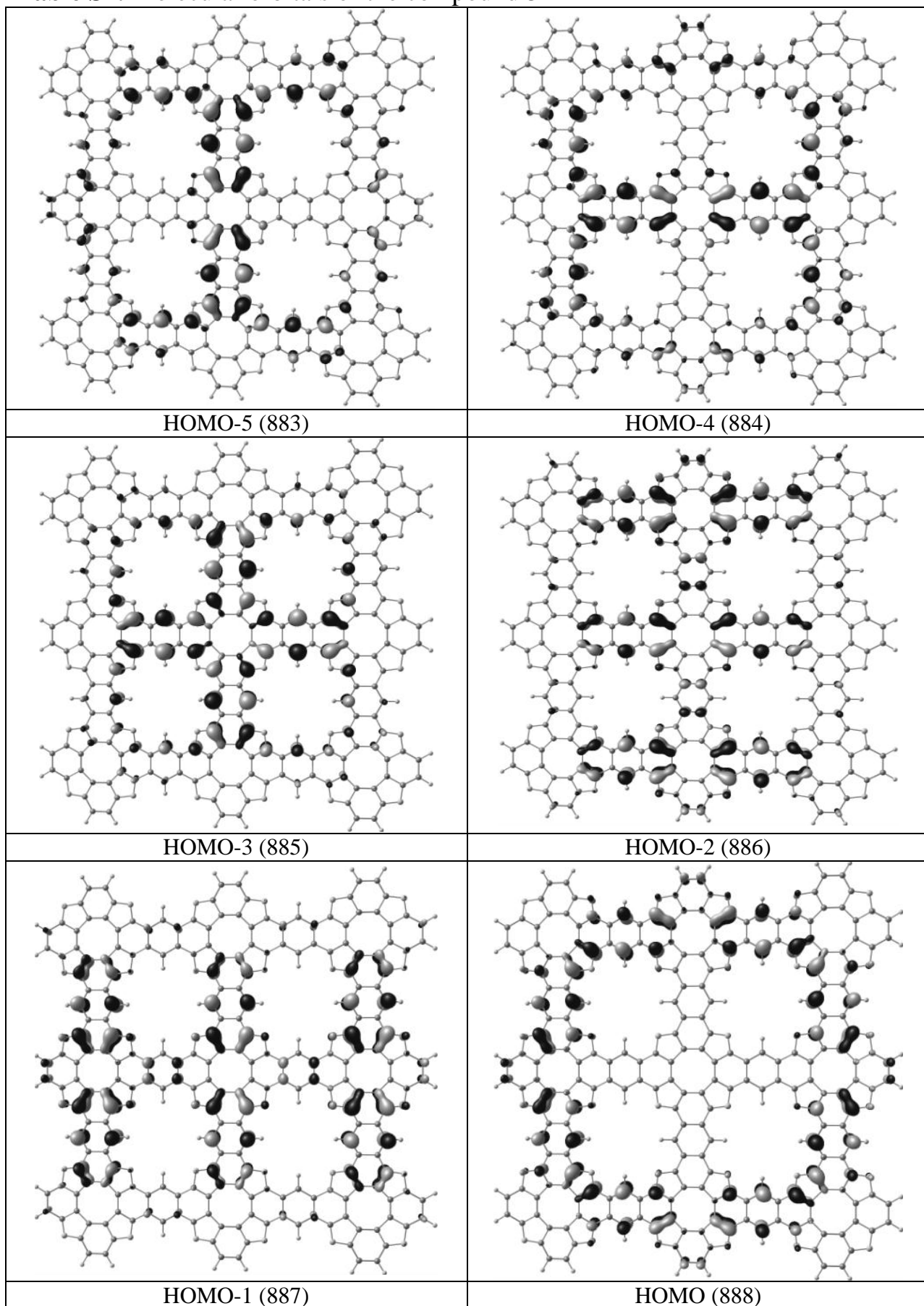
μ_z – magnetic dipole moment along the x axis (β – Bohr magneton);

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

λ – wavelength;

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

Table S2. Molecular orbitals of the compound **3**



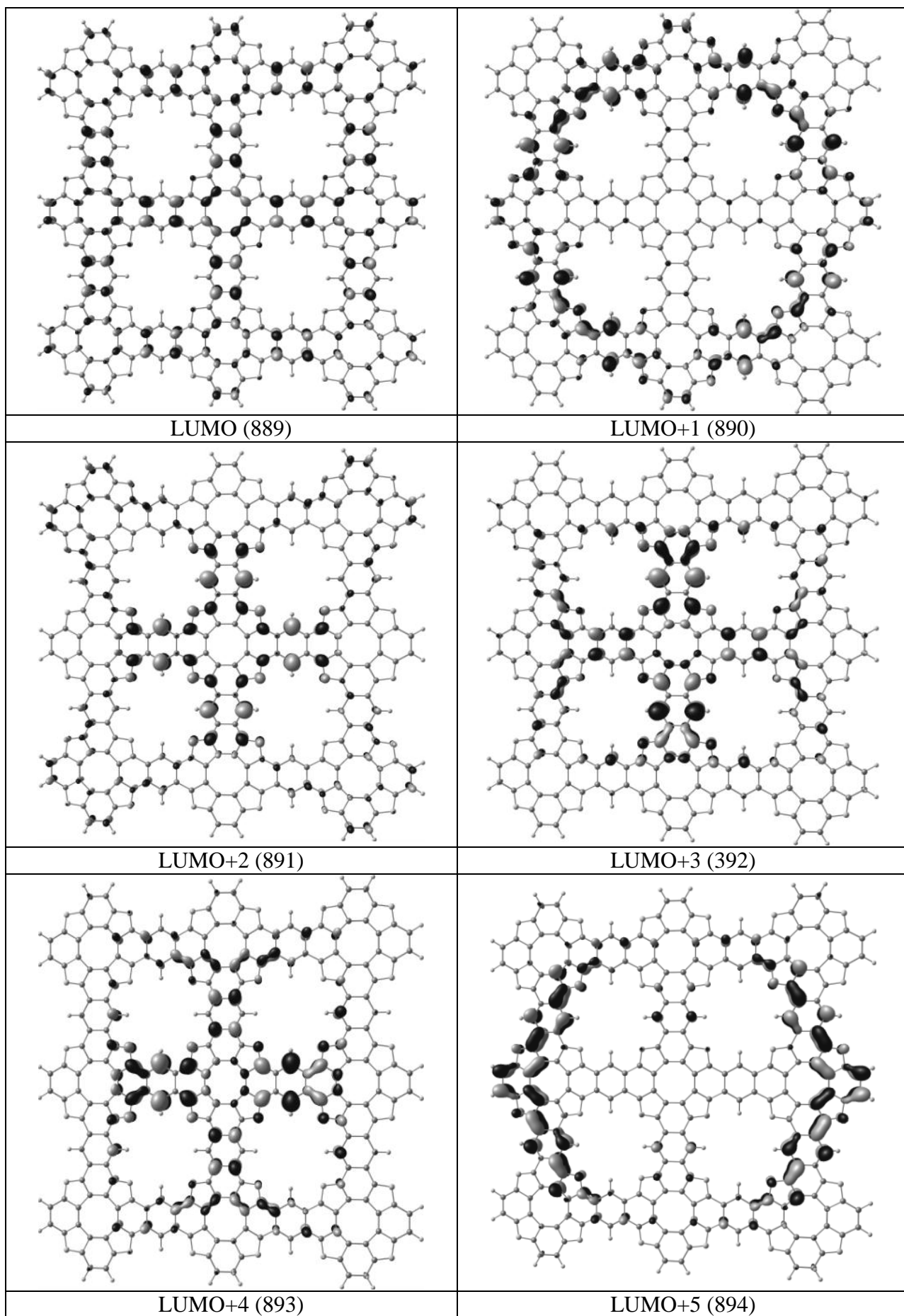


Table S3. Total energy of the ground singlet state ($^1A_{1g}$) of the compounds **1–5** at the B3LYP/6–21G(d) level of theory

Compounds	$E_{tot}, a.u.$
1	-5177.7656
2	-10505.5420
3	-11874.9887
4	-21311.1052
5	-21310.9687

The 6-21G(d) double-valence split basis set affords us to optimize all studied systems which consist at the most of 576 atoms (compound **4**). The extension of the chosen basis set prevents optimization of all studied molecules at the uniform level of accuracy. For comparison we have optimized the sheet **1** with the 6-311++G(d,p) basis. The calculated deviations in the structural parameters are negligible (no more than 0.002 Å for the bond lengths) and all conclusions remain. Thus, the choice of the 6-21G(d) basis set is quite justified by a very big size of the studied systems.

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	6.845423	0.000000
2	8	0	2.675869	8.182648	0.000000
3	6	0	6.811417	2.492841	0.000000
4	6	0	8.376663	4.052849	0.000000
5	6	0	8.366859	6.800122	0.000000
6	6	0	6.800122	8.366859	0.000000
7	6	0	4.052849	8.376663	0.000000
8	6	0	2.492841	6.811417	0.000000
9	6	0	6.135165	3.703715	0.000000
10	6	0	4.714435	3.703408	0.000000
11	6	0	3.703408	4.714435	0.000000
12	6	0	3.703715	6.135165	0.000000
13	6	0	4.722853	7.139689	0.000000
14	6	0	6.122585	7.135792	0.000000
15	6	0	7.135792	6.122585	0.000000
16	6	0	7.139689	4.722853	0.000000
17	6	0	4.044740	2.487337	0.000000
18	6	0	2.487337	4.044740	0.000000
19	6	0	4.698933	1.217878	0.000000
20	6	0	6.158965	1.219173	0.000000
21	6	0	4.727654	9.603604	0.000000
22	6	0	6.130684	9.598431	0.000000
23	6	0	1.219173	6.158965	0.000000
24	6	0	1.217878	4.698933	0.000000
25	6	0	9.598431	6.130684	0.000000
26	6	0	9.603604	4.727654	0.000000
27	8	0	8.182648	2.675869	0.000000
28	8	0	2.673749	2.673749	0.000000
29	8	0	8.176134	8.176134	0.000000
30	1	0	4.177638	10.540021	0.000000
31	1	0	6.687226	10.530937	0.000000
32	1	0	10.530937	6.687226	0.000000
33	1	0	10.540021	4.177638	0.000000
34	6	0	0.000000	4.012398	0.000000
35	8	0	2.673749	-2.673749	0.000000
36	6	0	6.800122	-8.366859	0.000000
37	6	0	8.366859	-6.800122	0.000000
38	6	0	8.376663	-4.052849	0.000000
39	6	0	6.811417	-2.492841	0.000000
40	6	0	4.044740	-2.487337	0.000000
41	6	0	2.487337	-4.044740	0.000000
42	6	0	6.122585	-7.135792	0.000000
43	6	0	4.722853	-7.139689	0.000000
44	6	0	3.703715	-6.135165	0.000000
45	6	0	3.703408	-4.714435	0.000000
46	6	0	4.714435	-3.703408	0.000000
47	6	0	6.135165	-3.703715	0.000000
48	6	0	7.139689	-4.722853	0.000000
49	6	0	7.135792	-6.122585	0.000000
50	6	0	4.052849	-8.376663	0.000000
51	6	0	2.492841	-6.811417	0.000000
52	6	0	4.727654	-9.603604	0.000000
53	6	0	6.130684	-9.598431	0.000000
54	6	0	4.698933	-1.217878	0.000000
55	6	0	6.158965	-1.219173	0.000000
56	6	0	1.217878	-4.698933	0.000000
57	6	0	1.219173	-6.158965	0.000000
58	6	0	9.603604	-4.727654	0.000000
59	6	0	9.598431	-6.130684	0.000000
60	8	0	8.176134	-8.176134	0.000000
61	8	0	2.675869	-8.182648	0.000000
62	8	0	8.182648	-2.675869	0.000000
63	1	0	4.177638	-10.540021	0.000000
64	1	0	6.687226	-10.530937	0.000000
65	1	0	10.540021	-4.177638	0.000000
66	1	0	10.530937	-6.687226	0.000000
67	6	0	0.000000	-4.012398	0.000000
68	8	0	-8.176134	8.176134	0.000000

69	6	0	-4.044740	2.487337	0.000000
70	6	0	-2.487337	4.044740	0.000000
71	6	0	-2.492841	6.811417	0.000000
72	6	0	-4.052849	8.376663	0.000000
73	6	0	-6.800122	8.366859	0.000000
74	6	0	-8.366859	6.800122	0.000000
75	6	0	-4.714435	3.703408	0.000000
76	6	0	-6.135165	3.703715	0.000000
77	6	0	-7.139689	4.722853	0.000000
78	6	0	-7.135792	6.122585	0.000000
79	6	0	-6.122585	7.135792	0.000000
80	6	0	-4.722853	7.139689	0.000000
81	6	0	-3.703715	6.135165	0.000000
82	6	0	-3.703408	4.714435	0.000000
83	6	0	-6.811417	2.492841	0.000000
84	6	0	-8.376663	4.052849	0.000000
85	6	0	-6.158965	1.219173	0.000000
86	6	0	-4.698933	1.217878	0.000000
87	6	0	-6.130684	9.598431	0.000000
88	6	0	-4.727654	9.603604	0.000000
89	6	0	-9.598431	6.130684	0.000000
90	6	0	-9.603604	4.727654	0.000000
91	6	0	-1.219173	6.158965	0.000000
92	6	0	-1.217878	4.698933	0.000000
93	8	0	-2.673749	2.673749	0.000000
94	8	0	-8.182648	2.675869	0.000000
95	8	0	-2.675869	8.182648	0.000000
96	1	0	-6.687226	10.530937	0.000000
97	1	0	-4.177638	10.540021	0.000000
98	1	0	-10.530937	6.687226	0.000000
99	1	0	-10.540021	4.177638	0.000000
100	6	0	-6.845423	0.000000	0.000000
101	8	0	-8.182648	-2.675869	0.000000
102	6	0	-4.052849	-8.376663	0.000000
103	6	0	-2.492841	-6.811417	0.000000
104	6	0	-2.487337	-4.044740	0.000000
105	6	0	-4.044740	-2.487337	0.000000
106	6	0	-6.811417	-2.492841	0.000000
107	6	0	-8.376663	-4.052849	0.000000
108	6	0	-4.722853	-7.139689	0.000000
109	6	0	-6.122585	-7.135792	0.000000
110	6	0	-7.135792	-6.122585	0.000000
111	6	0	-7.139689	-4.722853	0.000000
112	6	0	-6.135165	-3.703715	0.000000
113	6	0	-4.714435	-3.703408	0.000000
114	6	0	-3.703408	-4.714435	0.000000
115	6	0	-3.703715	-6.135165	0.000000
116	6	0	-6.800122	-8.366859	0.000000
117	6	0	-8.366859	-6.800122	0.000000
118	6	0	-6.130684	-9.598431	0.000000
119	6	0	-4.727654	-9.603604	0.000000
120	6	0	-6.158965	-1.219173	0.000000
121	6	0	-4.698933	-1.217878	0.000000
122	6	0	-9.603604	-4.727654	0.000000
123	6	0	-9.598431	-6.130684	0.000000
124	6	0	-1.217878	-4.698933	0.000000
125	6	0	-1.219173	-6.158965	0.000000
126	8	0	-2.675869	-8.182648	0.000000
127	8	0	-8.176134	-8.176134	0.000000
128	8	0	-2.673749	-2.673749	0.000000
129	1	0	-6.687226	-10.530937	0.000000
130	1	0	-4.177638	-10.540021	0.000000
131	1	0	-10.540021	-4.177638	0.000000
132	1	0	-10.530937	-6.687226	0.000000
133	6	0	-4.012398	0.000000	0.000000
134	6	0	0.000000	-6.845423	0.000000
135	6	0	4.012398	0.000000	0.000000
136	6	0	6.845423	0.000000	0.000000
137	1	0	0.000000	7.932189	0.000000
138	1	0	0.000000	2.925650	0.000000
139	1	0	0.000000	-2.925650	0.000000
140	1	0	-7.932189	0.000000	0.000000
141	1	0	-2.925650	0.000000	0.000000
142	1	0	0.000000	-7.932189	0.000000
143	1	0	2.925650	0.000000	0.000000
144	1	0	7.932189	0.000000	0.000000

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

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	6.851387	0.000000
2	6	0.000000	0.000000	4.006471
3	8	0.000000	2.679004	2.672386
4	6	0.000000	6.814643	8.355459
5	6	0.000000	8.380687	6.796451
6	6	0.000000	8.381472	4.053165
7	6	0.000000	6.816354	2.493277
8	6	0.000000	4.050632	2.486575
9	6	0.000000	2.490883	4.042617
10	6	0.000000	6.139177	7.143602
11	6	0.000000	4.718323	7.144256
12	6	0.000000	3.707356	6.134258
13	6	0.000000	3.707586	4.712792
14	6	0.000000	4.719166	3.703408
15	6	0.000000	6.140112	3.704699
16	6	0.000000	7.144858	4.723651
17	6	0.000000	7.144462	6.125158
18	6	0.000000	4.049170	8.360847
19	6	0.000000	2.490376	6.803817
20	6	0.000000	4.702769	9.629927
21	6	0.000000	6.162736	9.628871
22	6	0.000000	4.704973	1.217675
23	6	0.000000	6.165207	1.219205
24	6	0.000000	1.218640	4.693070
25	6	0.000000	1.218552	6.152718
26	6	0.000000	9.611388	4.723981
27	6	0.000000	9.610987	6.126254
28	8	0.000000	8.185605	8.172358
29	8	0.000000	2.677706	8.174260
30	8	0.000000	8.187209	2.677115
31	1	0.000000	10.545484	4.170262
32	1	0.000000	10.544740	6.680554
33	6	0.000000	0.000000	6.839360
34	8	0.000000	2.674914	13.520584
35	6	0.000000	6.799455	19.215468
36	6	0.000000	8.366614	17.649551
37	6	0.000000	8.377538	14.902190
38	6	0.000000	6.813239	13.341534
39	6	0.000000	4.046378	13.334996
40	6	0.000000	2.487928	14.891886
41	6	0.000000	6.122325	17.984214
42	6	0.000000	4.722477	17.987446
43	6	0.000000	3.703767	16.982581
44	6	0.000000	3.703976	15.561876
45	6	0.000000	4.715337	14.551440
46	6	0.000000	6.136208	14.552064
47	6	0.000000	7.140297	15.571589
48	6	0.000000	7.135889	16.971459
49	6	0.000000	4.052106	19.224160
50	6	0.000000	2.492659	17.658538
51	6	0.000000	4.726558	20.451346
52	6	0.000000	6.129481	20.446689
53	6	0.000000	4.701354	12.065838
54	6	0.000000	6.161668	12.067379
55	6	0.000000	1.218172	15.545765
56	6	0.000000	1.219193	17.005879
57	6	0.000000	9.604169	15.577619
58	6	0.000000	9.598369	16.980521
59	8	0.000000	8.175188	19.025111
60	8	0.000000	2.675108	19.029520
61	8	0.000000	8.183973	13.525069
62	1	0.000000	4.176071	21.387515
63	1	0.000000	6.685445	21.379476
64	1	0.000000	10.540778	15.027956
65	1	0.000000	10.530685	17.537269
66	6	0.000000	0.000000	14.859146
67	8	0.000000	-8.187209	2.677115
68	6	0.000000	-4.049170	8.360847

69	6	0.000000	-2.490376	6.803817
70	6	0.000000	-2.490883	4.042617
71	6	0.000000	-4.050632	2.486575
72	6	0.000000	-6.816354	2.493277
73	6	0.000000	-8.381472	4.053165
74	6	0.000000	-4.718323	7.144256
75	6	0.000000	-6.139177	7.143602
76	6	0.000000	-7.144462	6.125158
77	6	0.000000	-7.144858	4.723651
78	6	0.000000	-6.140112	3.704699
79	6	0.000000	-4.719166	3.703408
80	6	0.000000	-3.707586	4.712792
81	6	0.000000	-3.707356	6.134258
82	6	0.000000	-6.814643	8.355459
83	6	0.000000	-8.380687	6.796451
84	6	0.000000	-6.162736	9.628871
85	6	0.000000	-4.702769	9.629927
86	6	0.000000	-6.165207	1.219205
87	6	0.000000	-4.704973	1.217675
88	6	0.000000	-9.611388	4.723981
89	6	0.000000	-9.610987	6.126254
90	6	0.000000	-1.218640	4.693070
91	6	0.000000	-1.218552	6.152718
92	8	0.000000	-2.677706	8.174260
93	8	0.000000	-8.185605	8.172358
94	8	0.000000	-2.679004	2.672386
95	1	0.000000	-10.545484	4.170262
96	1	0.000000	-10.544740	6.680554
97	6	0.000000	-6.848555	10.848668
98	8	0.000000	-8.183973	13.525069
99	6	0.000000	-4.052106	19.224160
100	6	0.000000	-2.492659	17.658538
101	6	0.000000	-2.487928	14.891886
102	6	0.000000	-4.046378	13.334996
103	6	0.000000	-6.813239	13.341534
104	6	0.000000	-8.377538	14.902190
105	6	0.000000	-4.722477	17.987446
106	6	0.000000	-6.122325	17.984214
107	6	0.000000	-7.135889	16.971459
108	6	0.000000	-7.140297	15.571589
109	6	0.000000	-6.136208	14.552064
110	6	0.000000	-4.715337	14.551440
111	6	0.000000	-3.703976	15.561876
112	6	0.000000	-3.703767	16.982581
113	6	0.000000	-6.799455	19.215468
114	6	0.000000	-8.366614	17.649551
115	6	0.000000	-6.129481	20.446689
116	6	0.000000	-4.726558	20.451346
117	6	0.000000	-6.161668	12.067379
118	6	0.000000	-4.701354	12.065838
119	6	0.000000	-9.604169	15.577619
120	6	0.000000	-9.598369	16.980521
121	6	0.000000	-1.218172	15.545765
122	6	0.000000	-1.219193	17.005879
123	8	0.000000	-2.675108	19.029520
124	8	0.000000	-8.175188	19.025111
125	8	0.000000	-2.674914	13.520584
126	1	0.000000	-6.685445	21.379476
127	1	0.000000	-4.176071	21.387515
128	1	0.000000	-10.540778	15.027956
129	1	0.000000	-10.530685	17.537269
130	6	0.000000	-4.015357	10.847718
131	6	0.000000	0.000000	17.692167
132	6	0.000000	4.015357	10.847718
133	6	0.000000	6.848555	10.848668
134	1	0.000000	0.000000	2.919406
135	1	0.000000	0.000000	7.926556
136	1	0.000000	0.000000	13.771805
137	1	0.000000	-7.935056	10.849476
138	1	0.000000	-2.928015	10.847193
139	1	0.000000	0.000000	18.778792
140	1	0.000000	2.928015	10.847193
141	1	0.000000	7.935056	10.849476
142	6	0.000000	0.000000	-17.692167
143	8	0.000000	2.675108	-19.029520
144	6	0.000000	6.813239	-13.341534
145	6	0.000000	8.377538	-14.902190
146	6	0.000000	8.366614	-17.649551
147	6	0.000000	6.799455	-19.215468

148	6	0.000000	4.052106	-19.224160
149	6	0.000000	2.492659	-17.658538
150	6	0.000000	6.136208	-14.552064
151	6	0.000000	4.715337	-14.551440
152	6	0.000000	3.703976	-15.561876
153	6	0.000000	3.703767	-16.982581
154	6	0.000000	4.722477	-17.987446
155	6	0.000000	6.122325	-17.984214
156	6	0.000000	7.135889	-16.971459
157	6	0.000000	7.140297	-15.571589
158	6	0.000000	4.046378	-13.334996
159	6	0.000000	2.487928	-14.891886
160	6	0.000000	4.701354	-12.065838
161	6	0.000000	6.161668	-12.067379
162	6	0.000000	4.726558	-20.451346
163	6	0.000000	6.129481	-20.446689
164	6	0.000000	1.219193	-17.005879
165	6	0.000000	1.218172	-15.545765
166	6	0.000000	9.598369	-16.980521
167	6	0.000000	9.604169	-15.577619
168	8	0.000000	8.183973	-13.525069
169	8	0.000000	2.674914	-13.520584
170	8	0.000000	8.175188	-19.025111
171	1	0.000000	4.176071	-21.387515
172	1	0.000000	6.685445	-21.379476
173	1	0.000000	10.530685	-17.537269
174	1	0.000000	10.540778	-15.027956
175	6	0.000000	0.000000	-14.859146
176	8	0.000000	2.677706	-8.174260
177	6	0.000000	6.816354	-2.493277
178	6	0.000000	8.381472	-4.053165
179	6	0.000000	8.380687	-6.796451
180	6	0.000000	6.814643	-8.355459
181	6	0.000000	4.049170	-8.360847
182	6	0.000000	2.490376	-6.803817
183	6	0.000000	6.140112	-3.704699
184	6	0.000000	4.719166	-3.703408
185	6	0.000000	3.707586	-4.712792
186	6	0.000000	3.707356	-6.134258
187	6	0.000000	4.718323	-7.144256
188	6	0.000000	6.139177	-7.143602
189	6	0.000000	7.144462	-6.125158
190	6	0.000000	7.144858	-4.723651
191	6	0.000000	4.050632	-2.486575
192	6	0.000000	2.490883	-4.042617
193	6	0.000000	4.704973	-1.217675
194	6	0.000000	4.702769	-9.629927
195	6	0.000000	6.162736	-9.628871
196	6	0.000000	1.218552	-6.152718
197	6	0.000000	1.218640	-4.693070
198	6	0.000000	9.610987	-6.126254
199	6	0.000000	9.611388	-4.723981
200	8	0.000000	8.187209	-2.677115
201	8	0.000000	2.679004	-2.672386
202	8	0.000000	8.185605	-8.172358
203	1	0.000000	10.544740	-6.680554
204	1	0.000000	10.545484	-4.170262
205	6	0.000000	0.000000	-6.839360
206	8	0.000000	-8.175188	-19.025111
207	6	0.000000	-4.046378	-13.334996
208	6	0.000000	-2.487928	-14.891886
209	6	0.000000	-2.492659	-17.658538
210	6	0.000000	-4.052106	-19.224160
211	6	0.000000	-6.799455	-19.215468
212	6	0.000000	-8.366614	-17.649551
213	6	0.000000	-4.715337	-14.551440
214	6	0.000000	-6.136208	-14.552064
215	6	0.000000	-7.140297	-15.571589
216	6	0.000000	-7.135889	-16.971459
217	6	0.000000	-6.122325	-17.984214
218	6	0.000000	-4.722477	-17.987446
219	6	0.000000	-3.703767	-16.982581
220	6	0.000000	-3.703976	-15.561876
221	6	0.000000	-6.813239	-13.341534
222	6	0.000000	-8.377538	-14.902190
223	6	0.000000	-6.161668	-12.067379
224	6	0.000000	-4.701354	-12.065838
225	6	0.000000	-6.129481	-20.446689
226	6	0.000000	-4.726558	-20.451346

227	6	0.000000	-9.598369	-16.980521
228	6	0.000000	-9.604169	-15.577619
229	6	0.000000	-1.219193	-17.005879
230	6	0.000000	-1.218172	-15.545765
231	8	0.000000	-2.674914	-13.520584
232	8	0.000000	-8.183973	-13.525069
233	8	0.000000	-2.675108	-19.029520
234	1	0.000000	-6.685445	-21.379476
235	1	0.000000	-4.176071	-21.387515
236	1	0.000000	-10.530685	-17.537269
237	1	0.000000	-10.540778	-15.027956
238	6	0.000000	-6.848555	-10.848668
239	8	0.000000	-8.185605	-8.172358
240	6	0.000000	-4.050632	-2.486575
241	6	0.000000	-2.490883	-4.042617
242	6	0.000000	-2.490376	-6.803817
243	6	0.000000	-4.049170	-8.360847
244	6	0.000000	-6.814643	-8.355459
245	6	0.000000	-8.380687	-6.796451
246	6	0.000000	-4.719166	-3.703408
247	6	0.000000	-6.140112	-3.704699
248	6	0.000000	-7.144858	-4.723651
249	6	0.000000	-7.144462	-6.125158
250	6	0.000000	-6.139177	-7.143602
251	6	0.000000	-4.718323	-7.144256
252	6	0.000000	-3.707356	-6.134258
253	6	0.000000	-3.707586	-4.712792
254	6	0.000000	-6.816354	-2.493277
255	6	0.000000	-8.381472	-4.053165
256	6	0.000000	-6.165207	-1.219205
257	6	0.000000	-4.704973	-1.217675
258	6	0.000000	-6.162736	-9.628871
259	6	0.000000	-4.702769	-9.629927
260	6	0.000000	-9.610987	-6.126254
261	6	0.000000	-9.611388	-4.723981
262	6	0.000000	-1.218552	-6.152718
263	6	0.000000	-1.218640	-4.693070
264	8	0.000000	-2.679004	-2.672386
265	8	0.000000	-8.187209	-2.677115
266	8	0.000000	-2.677706	-8.174260
267	6	0.000000	-6.851387	0.000000
268	6	0.000000	-4.018511	0.000000
269	1	0.000000	-10.544740	-6.680554
270	1	0.000000	-10.545484	-4.170262
271	6	0.000000	-4.015357	-10.847718
272	6	0.000000	0.000000	-4.006471
273	6	0.000000	4.015357	-10.847718
274	6	0.000000	6.848555	-10.848668
275	1	0.000000	0.000000	-18.778792
276	1	0.000000	0.000000	-13.771805
277	1	0.000000	0.000000	-7.926556
278	1	0.000000	-7.935056	-10.849476
279	1	0.000000	-2.928015	-10.847193
280	1	0.000000	0.000000	-2.919406
281	1	0.000000	2.928015	-10.847193
282	1	0.000000	7.935056	-10.849476
283	6	0.000000	6.165207	-1.219205
284	6	0.000000	4.018511	0.000000
285	1	0.000000	7.937927	0.000000
286	1	0.000000	-7.937927	0.000000
287	1	0.000000	-2.931213	0.000000
288	1	0.000000	2.931213	0.000000

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.416685	5.428279	0.000000
2	6	0	-5.424031	9.440472	0.000000
3	8	0	-2.750439	8.104727	0.000000
4	6	0	1.371872	13.806657	0.000000
5	6	0	2.931727	12.241016	0.000000
6	6	0	2.937353	9.475562	0.000000
7	6	0	1.380550	7.917626	0.000000
8	6	0	-1.380550	7.917626	0.000000
9	6	0	-2.937353	9.475562	0.000000
10	6	0	0.700791	12.570287	0.000000
11	6	0	-0.700791	12.570287	0.000000
12	6	0	-1.719934	11.565552	0.000000
13	6	0	-1.720975	10.144995	0.000000
14	6	0	-0.710732	9.134220	0.000000
15	6	0	0.710732	9.134220	0.000000
16	6	0	1.720975	10.144995	0.000000
17	6	0	1.719934	11.565552	0.000000
18	6	0	-1.371872	13.806657	0.000000
19	6	0	-2.931727	12.241016	0.000000
20	6	0	0.701191	15.036700	0.000000
21	6	0	-0.729642	6.646135	0.000000
22	6	0	0.729642	6.646135	0.000000
23	6	0	-4.206571	10.128645	0.000000
24	6	0	-4.205361	11.588552	0.000000
25	6	0	4.206571	10.128645	0.000000
26	6	0	4.205361	11.588552	0.000000
27	8	0	2.747936	13.612169	0.000000
28	8	0	-2.747936	13.612169	0.000000
29	8	0	2.750439	8.104727	0.000000
30	6	0	-5.425813	12.273483	0.000000
31	8	0	-13.608514	8.101486	0.000000
32	6	0	-9.478304	13.802300	0.000000
33	6	0	-7.918342	12.237644	0.000000
34	6	0	-7.912304	9.469951	0.000000
35	6	0	-9.469951	7.912304	0.000000
36	6	0	-12.237644	7.918342	0.000000
37	6	0	-13.802300	9.478304	0.000000
38	6	0	-10.148298	12.565315	0.000000
39	6	0	-11.548232	12.561489	0.000000
40	6	0	-12.561489	11.548232	0.000000
41	6	0	-12.565315	10.148298	0.000000
42	6	0	-11.560755	9.128934	0.000000
43	6	0	-10.139659	9.128445	0.000000
44	6	0	-9.128445	10.139659	0.000000
45	6	0	-9.128934	11.560755	0.000000
46	6	0	-12.225957	13.792455	0.000000
47	6	0	-13.792455	12.225957	0.000000
48	6	0	-11.556329	15.023861	0.000000
49	6	0	-10.153400	15.029073	0.000000
50	6	0	-11.585668	6.644315	0.000000
51	6	0	-10.125285	6.642741	0.000000
52	6	0	-15.029073	10.153400	0.000000
53	6	0	-15.023861	11.556329	0.000000
54	6	0	-6.642741	10.125285	0.000000
55	6	0	-6.644315	11.585668	0.000000
56	8	0	-8.101486	13.608514	0.000000
57	8	0	-13.601666	13.601666	0.000000
58	8	0	-8.098849	8.098849	0.000000
59	1	0	-15.965532	9.603466	0.000000
60	1	0	-15.956393	12.112710	0.000000
61	1	0	-5.422544	8.353681	0.000000
62	1	0	-5.427733	13.360173	0.000000
63	6	0	-5.425813	-12.273483	0.000000
64	8	0	-2.747936	-13.612169	0.000000
65	6	0	1.380550	-7.917626	0.000000
66	6	0	2.937353	-9.475562	0.000000
67	6	0	2.931727	-12.241016	0.000000
68	6	0	1.371872	-13.806657	0.000000

69	6	0	-1.371872	-13.806657	0.000000
70	6	0	-2.931727	-12.241016	0.000000
71	6	0	0.710732	-9.134220	0.000000
72	6	0	-0.710732	-9.134220	0.000000
73	6	0	-1.720975	-10.144995	0.000000
74	6	0	-1.719934	-11.565552	0.000000
75	6	0	-0.700791	-12.570287	0.000000
76	6	0	0.700791	-12.570287	0.000000
77	6	0	1.719934	-11.565552	0.000000
78	6	0	1.720975	-10.144995	0.000000
79	6	0	-1.380550	-7.917626	0.000000
80	6	0	-2.937353	-9.475562	0.000000
81	6	0	-0.729642	-6.646135	0.000000
82	6	0	0.729642	-6.646135	0.000000
83	6	0	-0.701191	-15.036700	0.000000
84	6	0	0.701191	-15.036700	0.000000
85	6	0	-4.205361	-11.588552	0.000000
86	6	0	-4.206571	-10.128645	0.000000
87	6	0	4.205361	-11.588552	0.000000
88	6	0	4.206571	-10.128645	0.000000
89	8	0	2.750439	-8.104727	0.000000
90	8	0	-2.750439	-8.104727	0.000000
91	8	0	2.747936	-13.612169	0.000000
92	1	0	-1.255078	-15.970752	0.000000
93	1	0	1.255078	-15.970752	0.000000
94	6	0	5.425813	-12.273483	0.000000
95	6	0	5.424031	-9.440472	0.000000
96	6	0	-5.424031	-9.440472	0.000000
97	8	0	-2.751292	-2.751292	0.000000
98	6	0	1.381140	2.938609	0.000000
99	6	0	2.938609	1.381140	0.000000
100	6	0	2.938609	-1.381140	0.000000
101	6	0	1.381140	-2.938609	0.000000
102	6	0	-1.381140	-2.938609	0.000000
103	6	0	-2.938609	-1.381140	0.000000
104	6	0	0.711105	1.721809	0.000000
105	6	0	-0.711105	1.721809	0.000000
106	6	0	-1.721809	0.711105	0.000000
107	6	0	-1.721809	-0.711105	0.000000
108	6	0	-0.711105	-1.721809	0.000000
109	6	0	0.711105	-1.721809	0.000000
110	6	0	1.721809	-0.711105	0.000000
111	6	0	1.721809	0.711105	0.000000
112	6	0	-1.381140	2.938609	0.000000
113	6	0	-2.938609	1.381140	0.000000
114	6	0	-0.729781	4.210080	0.000000
115	6	0	-0.729781	-4.210080	0.000000
116	6	0	0.729781	-4.210080	0.000000
117	6	0	-4.210080	-0.729781	0.000000
118	6	0	-4.210080	0.729781	0.000000
119	6	0	4.210080	-0.729781	0.000000
120	6	0	4.210080	0.729781	0.000000
121	8	0	2.751292	2.751292	0.000000
122	8	0	-2.751292	2.751292	0.000000
123	8	0	2.751292	-2.751292	0.000000
124	6	0	-5.428279	-1.416685	0.000000
125	8	0	-13.601666	-13.601666	0.000000
126	6	0	-9.469951	-7.912304	0.000000
127	6	0	-7.912304	-9.469951	0.000000
128	6	0	-7.918342	-12.237644	0.000000
129	6	0	-9.478304	-13.802300	0.000000
130	6	0	-12.225957	-13.792455	0.000000
131	6	0	-13.792455	-12.225957	0.000000
132	6	0	-10.139659	-9.128445	0.000000
133	6	0	-11.560755	-9.128934	0.000000
134	6	0	-12.565315	-10.148298	0.000000
135	6	0	-12.561489	-11.548232	0.000000
136	6	0	-11.548232	-12.561489	0.000000
137	6	0	-10.148298	-12.565315	0.000000
138	6	0	-9.128934	-11.560755	0.000000
139	6	0	-9.128445	-10.139659	0.000000
140	6	0	-12.237644	-7.918342	0.000000
141	6	0	-13.802300	-9.478304	0.000000
142	6	0	-11.585668	-6.644315	0.000000
143	6	0	-10.125285	-6.642741	0.000000
144	6	0	-11.556329	-15.023861	0.000000
145	6	0	-10.153400	-15.029073	0.000000
146	6	0	-15.023861	-11.556329	0.000000
147	6	0	-15.029073	-10.153400	0.000000

148	6	0	-6.644315	-11.585668	0.000000
149	6	0	-6.642741	-10.125285	0.000000
150	8	0	-8.098849	-8.098849	0.000000
151	8	0	-13.608514	-8.101486	0.000000
152	8	0	-8.101486	-13.608514	0.000000
153	1	0	-12.112710	-15.956393	0.000000
154	1	0	-9.603466	-15.965532	0.000000
155	1	0	-15.956393	-12.112710	0.000000
156	1	0	-15.965532	-9.603466	0.000000
157	6	0	-12.273483	-5.425813	0.000000
158	8	0	-13.612169	-2.747936	0.000000
159	6	0	-9.475562	2.937353	0.000000
160	6	0	-7.917626	1.380550	0.000000
161	6	0	-7.917626	-1.380550	0.000000
162	6	0	-9.475562	-2.937353	0.000000
163	6	0	-12.241016	-2.931727	0.000000
164	6	0	-13.806657	-1.371872	0.000000
165	6	0	-10.144995	1.720975	0.000000
166	6	0	-11.565552	1.719934	0.000000
167	6	0	-12.570287	0.700791	0.000000
168	6	0	-12.570287	-0.700791	0.000000
169	6	0	-11.565552	-1.719934	0.000000
170	6	0	-10.144995	-1.720975	0.000000
171	6	0	-9.134220	-0.710732	0.000000
172	6	0	-9.134220	0.710732	0.000000
173	6	0	-12.241016	2.931727	0.000000
174	6	0	-13.806657	1.371872	0.000000
175	6	0	-11.588552	4.205361	0.000000
176	6	0	-10.128645	4.206571	0.000000
177	6	0	-11.588552	-4.205361	0.000000
178	6	0	-10.128645	-4.206571	0.000000
179	6	0	-15.036700	-0.701191	0.000000
180	6	0	-15.036700	0.701191	0.000000
181	6	0	-6.646135	-0.729642	0.000000
182	6	0	-6.646135	0.729642	0.000000
183	8	0	-8.104727	2.750439	0.000000
184	8	0	-13.612169	2.747936	0.000000
185	8	0	-8.104727	-2.750439	0.000000
186	6	0	-12.273483	5.425813	0.000000
187	6	0	-9.440472	5.424031	0.000000
188	1	0	-15.970752	-1.255078	0.000000
189	1	0	-15.970752	1.255078	0.000000
190	6	0	-9.440472	-5.424031	0.000000
191	6	0	-5.428279	1.416685	0.000000
192	6	0	-1.416685	-5.428279	0.000000
193	6	0	1.416685	-5.428279	0.000000
194	1	0	-5.427733	-13.360173	0.000000
195	1	0	-5.422544	-8.353681	0.000000
196	1	0	-5.428003	-2.503371	0.000000
197	1	0	-13.360173	-5.427733	0.000000
198	1	0	-8.353681	-5.422544	0.000000
199	1	0	-5.428003	2.503371	0.000000
200	1	0	-2.503371	-5.428003	0.000000
201	1	0	2.503371	-5.428003	0.000000
202	6	0	0.729781	4.210080	0.000000
203	6	0	-1.416685	5.428279	0.000000
204	1	0	2.503371	5.428003	0.000000
205	1	0	-13.360173	5.427733	0.000000
206	1	0	-8.353681	5.422544	0.000000
207	1	0	-2.503371	5.428003	0.000000
208	6	0	5.428279	-1.416685	0.000000
209	8	0	8.098849	8.098849	0.000000
210	6	0	12.225957	13.792455	0.000000
211	6	0	13.792455	12.225957	0.000000
212	6	0	13.802300	9.478304	0.000000
213	6	0	12.237644	7.918342	0.000000
214	6	0	9.469951	7.912304	0.000000
215	6	0	7.912304	9.469951	0.000000
216	6	0	11.548232	12.561489	0.000000
217	6	0	10.148298	12.565315	0.000000
218	6	0	9.128934	11.560755	0.000000
219	6	0	9.128445	10.139659	0.000000
220	6	0	10.139659	9.128445	0.000000
221	6	0	11.560755	9.128934	0.000000
222	6	0	12.565315	10.148298	0.000000
223	6	0	12.561489	11.548232	0.000000
224	6	0	9.478304	13.802300	0.000000
225	6	0	7.918342	12.237644	0.000000
226	6	0	10.153400	15.029073	0.000000

227	6	0	11.556329	15.023861	0.000000
228	6	0	10.125285	6.642741	0.000000
229	6	0	11.585668	6.644315	0.000000
230	6	0	6.642741	10.125285	0.000000
231	6	0	6.644315	11.585668	0.000000
232	6	0	15.023861	11.556329	0.000000
233	8	0	13.601666	13.601666	0.000000
234	8	0	8.101486	13.608514	0.000000
235	8	0	13.608514	8.101486	0.000000
236	8	0	8.101486	-13.608514	0.000000
237	6	0	12.237644	-7.918342	0.000000
238	6	0	13.802300	-9.478304	0.000000
239	6	0	13.792455	-12.225957	0.000000
240	6	0	12.225957	-13.792455	0.000000
241	6	0	9.478304	-13.802300	0.000000
242	6	0	7.918342	-12.237644	0.000000
243	6	0	11.560755	-9.128934	0.000000
244	6	0	10.139659	-9.128445	0.000000
245	6	0	9.128445	-10.139659	0.000000
246	6	0	9.128934	-11.560755	0.000000
247	6	0	10.148298	-12.565315	0.000000
248	6	0	11.548232	-12.561489	0.000000
249	6	0	12.561489	-11.548232	0.000000
250	6	0	12.565315	-10.148298	0.000000
251	6	0	9.469951	-7.912304	0.000000
252	6	0	7.912304	-9.469951	0.000000
253	6	0	10.125285	-6.642741	0.000000
254	6	0	11.585668	-6.644315	0.000000
255	6	0	10.153400	-15.029073	0.000000
256	6	0	11.556329	-15.023861	0.000000
257	6	0	6.644315	-11.585668	0.000000
258	6	0	6.642741	-10.125285	0.000000
259	6	0	15.023861	-11.556329	0.000000
260	6	0	15.029073	-10.153400	0.000000
261	8	0	13.608514	-8.101486	0.000000
262	8	0	8.098849	-8.098849	0.000000
263	8	0	13.601666	-13.601666	0.000000
264	1	0	9.603466	-15.965532	0.000000
265	1	0	12.112710	-15.956393	0.000000
266	6	0	9.440472	-5.424031	0.000000
267	8	0	8.104727	-2.750439	0.000000
268	6	0	12.241016	2.931727	0.000000
269	6	0	13.806657	1.371872	0.000000
270	6	0	13.806657	-1.371872	0.000000
271	6	0	12.241016	-2.931727	0.000000
272	6	0	9.475562	-2.937353	0.000000
273	6	0	7.917626	-1.380550	0.000000
274	6	0	11.565552	1.719934	0.000000
275	6	0	10.144995	1.720975	0.000000
276	6	0	9.134220	0.710732	0.000000
277	6	0	9.134220	-0.710732	0.000000
278	6	0	10.144995	-1.720975	0.000000
279	6	0	11.565552	-1.719934	0.000000
280	6	0	12.570287	-0.700791	0.000000
281	6	0	12.570287	0.700791	0.000000
282	6	0	9.475562	2.937353	0.000000
283	6	0	7.917626	1.380550	0.000000
284	6	0	10.128645	4.206571	0.000000
285	6	0	11.588552	4.205361	0.000000
286	6	0	10.128645	-4.206571	0.000000
287	6	0	11.588552	-4.205361	0.000000
288	6	0	6.646135	-0.729642	0.000000
289	6	0	6.646135	0.729642	0.000000
290	6	0	15.036700	-0.701191	0.000000
291	6	0	15.036700	0.701191	0.000000
292	8	0	13.612169	2.747936	0.000000
293	8	0	8.104727	2.750439	0.000000
294	8	0	13.612169	-2.747936	0.000000
295	6	0	9.440472	5.424031	0.000000
296	6	0	12.273483	5.425813	0.000000
297	6	0	12.273483	-5.425813	0.000000
298	1	0	8.353681	-5.422544	0.000000
299	1	0	13.360173	-5.427733	0.000000
300	1	0	8.353681	5.422544	0.000000
301	1	0	13.360173	5.427733	0.000000
302	6	0	5.428279	1.416685	0.000000
303	6	0	5.424031	9.440472	0.000000
304	6	0	5.425813	12.273483	0.000000
305	1	0	5.427733	-13.360173	0.000000

306	1	0	5.422544	-8.353681	0.000000
307	1	0	5.428003	-2.503371	0.000000
308	1	0	5.428003	2.503371	0.000000
309	1	0	5.422544	8.353681	0.000000
310	1	0	5.427733	13.360173	0.000000
311	6	0	-0.701191	15.036700	0.000000
312	1	0	-12.112710	15.956393	0.000000
313	1	0	-9.603466	15.965532	0.000000
314	1	0	9.603466	15.965532	0.000000
315	1	0	12.112710	15.956393	0.000000
316	1	0	15.956393	-12.112710	0.000000
317	1	0	15.965532	-9.603466	0.000000
318	1	0	15.970752	-1.255078	0.000000
319	1	0	15.970752	1.255078	0.000000
320	1	0	-1.255078	15.970752	0.000000
321	6	0	15.029073	10.153400	0.000000
322	1	0	1.255078	15.970752	0.000000
323	1	0	15.956393	12.112710	0.000000
324	1	0	15.965532	9.603466	0.000000

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	4.010847	0.000000
2	6	0	4.009279	10.855673	0.000000
3	8	0	2.676790	8.178415	0.000000
4	6	0	8.366000	4.047073	0.000000
5	6	0	6.808087	2.489586	0.000000
6	6	0	4.047184	2.489608	0.000000
7	6	0	2.489608	4.047184	0.000000
8	6	0	2.489586	6.808087	0.000000
9	6	0	4.047073	8.366000	0.000000
10	6	0	7.149149	4.716947	0.000000
11	6	0	7.149298	6.138837	0.000000
12	6	0	6.138837	7.149298	0.000000
13	6	0	4.716947	7.149149	0.000000
14	6	0	3.706593	6.138676	0.000000
15	6	0	3.706481	4.716863	0.000000
16	6	0	4.716863	3.706481	0.000000
17	6	0	6.138676	3.706593	0.000000
18	6	0	8.366391	6.808315	0.000000
19	6	0	6.808315	8.366391	0.000000
20	6	0	9.637989	6.156841	0.000000
21	6	0	9.637800	4.697281	0.000000
22	6	0	1.218109	6.157311	0.000000
23	6	0	1.218070	4.697795	0.000000
24	6	0	4.697281	9.637800	0.000000
25	6	0	6.156841	9.637989	0.000000
26	6	0	4.697795	1.218070	0.000000
27	6	0	6.157311	1.218109	0.000000
28	8	0	8.178415	2.676790	0.000000
29	8	0	8.178746	8.178746	0.000000
30	8	0	2.677034	2.677034	0.000000
31	6	0	6.842462	10.856938	0.000000
32	8	0	13.532481	8.175240	0.000000
33	6	0	19.236016	4.055208	0.000000
34	6	0	17.671544	2.494419	0.000000
35	6	0	14.905693	2.487393	0.000000
36	6	0	13.346475	4.043877	0.000000
37	6	0	13.346062	6.805109	0.000000
38	6	0	14.903550	8.362473	0.000000
39	6	0	17.999238	4.725464	0.000000
40	6	0	17.998664	6.127118	0.000000
41	6	0	16.993650	7.145805	0.000000
42	6	0	15.573166	7.146165	0.000000
43	6	0	14.562891	6.135581	0.000000
44	6	0	14.563124	4.713993	0.000000
45	6	0	15.574352	3.704232	0.000000
46	6	0	16.995086	3.705838	0.000000
47	6	0	19.234714	6.798794	0.000000
48	6	0	17.668699	8.357898	0.000000
49	6	0	20.465132	6.128757	0.000000
50	6	0	20.465809	4.726421	0.000000
51	6	0	12.074555	6.154452	0.000000
52	6	0	12.074524	4.694906	0.000000
53	6	0	15.556005	9.631977	0.000000
54	6	0	17.015903	9.631303	0.000000
55	6	0	15.560017	1.218268	0.000000
56	6	0	17.020419	1.219933	0.000000
57	8	0	19.042407	2.679089	0.000000
58	8	0	19.039547	8.174606	0.000000
59	8	0	13.534162	2.673766	0.000000
60	1	0	21.398940	6.683070	0.000000
61	1	0	21.400129	4.172901	0.000000
62	6	0	14.867177	10.849214	0.000000
63	8	0	2.679089	19.042407	0.000000
64	6	0	8.362473	14.903550	0.000000
65	6	0	6.805109	13.346062	0.000000
66	6	0	4.043877	13.346475	0.000000
67	6	0	2.487393	14.905693	0.000000
68	6	0	2.494419	17.671544	0.000000
69	6	0	4.055208	19.236016	0.000000

70	6	0	7.146165	15.573166	0.000000
71	6	0	7.145805	16.993650	0.000000
72	6	0	6.127118	17.998664	0.000000
73	6	0	4.725464	17.999238	0.000000
74	6	0	3.705838	16.995086	0.000000
75	6	0	3.704232	15.574352	0.000000
76	6	0	4.713993	14.563124	0.000000
77	6	0	6.135581	14.562891	0.000000
78	6	0	8.357898	17.668699	0.000000
79	6	0	6.798794	19.234714	0.000000
80	6	0	9.631303	17.015903	0.000000
81	6	0	9.631977	15.556005	0.000000
82	6	0	1.219933	17.020419	0.000000
83	6	0	1.218268	15.560017	0.000000
84	6	0	4.726421	20.465809	0.000000
85	6	0	6.128757	20.465132	0.000000
86	6	0	4.694906	12.074524	0.000000
87	6	0	6.154452	12.074555	0.000000
88	8	0	8.175240	13.532481	0.000000
89	8	0	8.174606	19.039547	0.000000
90	8	0	2.673766	13.534162	0.000000
91	1	0	4.172901	21.400129	0.000000
92	1	0	6.683070	21.398940	0.000000
93	6	0	10.852017	17.700159	0.000000
94	8	0	13.527340	19.034148	0.000000
95	6	0	19.228018	14.904228	0.000000
96	6	0	17.663606	13.344291	0.000000
97	6	0	14.895747	13.337869	0.000000
98	6	0	13.337869	14.895747	0.000000
99	6	0	13.344291	17.663606	0.000000
100	6	0	14.904228	19.228018	0.000000
101	6	0	17.991050	15.574151	0.000000
102	6	0	17.987316	16.974143	0.000000
103	6	0	16.974143	17.987316	0.000000
104	6	0	15.574151	17.991050	0.000000
105	6	0	14.554819	16.986495	0.000000
106	6	0	14.554190	15.565340	0.000000
107	6	0	15.565340	14.554190	0.000000
108	6	0	16.986495	14.554819	0.000000
109	6	0	19.218239	17.651920	0.000000
110	6	0	17.651920	19.218239	0.000000
111	6	0	20.449666	16.982211	0.000000
112	6	0	20.454856	15.579342	0.000000
113	6	0	12.070210	17.011897	0.000000
114	6	0	12.068367	15.551427	0.000000
115	6	0	15.579342	20.454856	0.000000
116	6	0	16.982211	20.449666	0.000000
117	6	0	15.551427	12.068367	0.000000
118	6	0	17.011897	12.070210	0.000000
119	8	0	19.034148	13.527340	0.000000
120	8	0	19.027378	19.027378	0.000000
121	8	0	13.524356	13.524356	0.000000
122	1	0	21.382244	17.538534	0.000000
123	1	0	21.391278	15.029317	0.000000
124	1	0	15.029317	21.391278	0.000000
125	1	0	17.538534	21.382244	0.000000
126	6	0	10.849214	14.867177	0.000000
127	6	0	17.700159	10.852017	0.000000
128	6	0	10.856938	6.842462	0.000000
129	6	0	10.855673	4.009279	0.000000
130	1	0	2.922402	10.854350	0.000000
131	1	0	7.929342	10.858267	0.000000
132	1	0	13.780165	10.847174	0.000000
133	1	0	10.854587	18.786746	0.000000
134	1	0	10.847174	13.780165	0.000000
135	1	0	18.786746	10.854587	0.000000
136	1	0	10.858267	7.929342	0.000000
137	1	0	10.854350	2.922402	0.000000
138	6	0	-17.700159	10.852017	0.000000
139	8	0	-19.039547	8.174606	0.000000
140	6	0	-13.346475	4.043877	0.000000
141	6	0	-14.905693	2.487393	0.000000
142	6	0	-17.671544	2.494419	0.000000
143	6	0	-19.236016	4.055208	0.000000
144	6	0	-19.234714	6.798794	0.000000
145	6	0	-17.668699	8.357898	0.000000
146	6	0	-14.563124	4.713993	0.000000
147	6	0	-14.562891	6.135581	0.000000
148	6	0	-15.573166	7.146165	0.000000

149	6	0	-16.993650	7.145805	0.000000
150	6	0	-17.998664	6.127118	0.000000
151	6	0	-17.999238	4.725464	0.000000
152	6	0	-16.995086	3.705838	0.000000
153	6	0	-15.574352	3.704232	0.000000
154	6	0	-13.346062	6.805109	0.000000
155	6	0	-14.903550	8.362473	0.000000
156	6	0	-12.074555	6.154452	0.000000
157	6	0	-12.074524	4.694906	0.000000
158	6	0	-20.465132	6.128757	0.000000
159	6	0	-20.465809	4.726421	0.000000
160	6	0	-17.015903	9.631303	0.000000
161	6	0	-15.556005	9.631977	0.000000
162	6	0	-17.020419	1.219933	0.000000
163	6	0	-15.560017	1.218268	0.000000
164	8	0	-13.534162	2.673766	0.000000
165	8	0	-13.532481	8.175240	0.000000
166	8	0	-19.042407	2.679089	0.000000
167	1	0	-21.398940	6.683070	0.000000
168	1	0	-21.400129	4.172901	0.000000
169	6	0	-17.706589	0.000000	0.000000
170	6	0	-14.873656	0.000000	0.000000
171	6	0	-14.867177	10.849214	0.000000
172	8	0	-8.178746	8.178746	0.000000
173	6	0	-2.489608	4.047184	0.000000
174	6	0	-4.047184	2.489608	0.000000
175	6	0	-6.808087	2.489586	0.000000
176	6	0	-8.366000	4.047073	0.000000
177	6	0	-8.366391	6.808315	0.000000
178	6	0	-6.808315	8.366391	0.000000
179	6	0	-3.706481	4.716863	0.000000
180	6	0	-3.706593	6.138676	0.000000
181	6	0	-4.716947	7.149149	0.000000
182	6	0	-6.138837	7.149298	0.000000
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185	6	0	-6.138676	3.706593	0.000000
186	6	0	-4.716863	3.706481	0.000000
187	6	0	-2.489586	6.808087	0.000000
188	6	0	-4.047073	8.366000	0.000000
189	6	0	-1.218109	6.157311	0.000000
190	6	0	-9.637989	6.156841	0.000000
191	6	0	-9.637800	4.697281	0.000000
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193	6	0	-4.697281	9.637800	0.000000
194	6	0	-6.157311	1.218109	0.000000
195	6	0	-4.697795	1.218070	0.000000
196	8	0	-2.677034	2.677034	0.000000
197	8	0	-2.676790	8.178415	0.000000
198	8	0	-8.178415	2.676790	0.000000
199	6	0	-6.842462	10.856938	0.000000
200	8	0	-19.027378	19.027378	0.000000
201	6	0	-13.337869	14.895747	0.000000
202	6	0	-14.895747	13.337869	0.000000
203	6	0	-17.663606	13.344291	0.000000
204	6	0	-19.228018	14.904228	0.000000
205	6	0	-19.218239	17.651920	0.000000
206	6	0	-17.651920	19.218239	0.000000
207	6	0	-14.554190	15.565340	0.000000
208	6	0	-14.554819	16.986495	0.000000
209	6	0	-15.574151	17.991050	0.000000
210	6	0	-16.974143	17.987316	0.000000
211	6	0	-17.987316	16.974143	0.000000
212	6	0	-17.991050	15.574151	0.000000
213	6	0	-16.986495	14.554819	0.000000
214	6	0	-15.565340	14.554190	0.000000
215	6	0	-13.344291	17.663606	0.000000
216	6	0	-14.904228	19.228018	0.000000
217	6	0	-12.070210	17.011897	0.000000
218	6	0	-12.068367	15.551427	0.000000
219	6	0	-20.449666	16.982211	0.000000
220	6	0	-20.454856	15.579342	0.000000
221	6	0	-16.982211	20.449666	0.000000
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223	6	0	-17.011897	12.070210	0.000000
224	6	0	-15.551427	12.068367	0.000000
225	8	0	-13.524356	13.524356	0.000000
226	8	0	-13.527340	19.034148	0.000000
227	8	0	-19.034148	13.527340	0.000000

228	1	0	-21.382244	17.538534	0.000000
229	1	0	-21.391278	15.029317	0.000000
230	1	0	-17.538534	21.382244	0.000000
231	1	0	-15.029317	21.391278	0.000000
232	6	0	-10.852017	17.700159	0.000000
233	8	0	-8.174606	19.039547	0.000000
234	6	0	-2.487393	14.905693	0.000000
235	6	0	-4.043877	13.346475	0.000000
236	6	0	-6.805109	13.346062	0.000000
237	6	0	-8.362473	14.903550	0.000000
238	6	0	-8.357898	17.668699	0.000000
239	6	0	-6.798794	19.234714	0.000000
240	6	0	-3.704232	15.574352	0.000000
241	6	0	-3.705838	16.995086	0.000000
242	6	0	-4.725464	17.999238	0.000000
243	6	0	-6.127118	17.998664	0.000000
244	6	0	-7.145805	16.993650	0.000000
245	6	0	-7.146165	15.573166	0.000000
246	6	0	-6.135581	14.562891	0.000000
247	6	0	-4.713993	14.563124	0.000000
248	6	0	-2.494419	17.671544	0.000000
249	6	0	-4.055208	19.236016	0.000000
250	6	0	-1.219933	17.020419	0.000000
251	6	0	-1.218268	15.560017	0.000000
252	6	0	-9.631303	17.015903	0.000000
253	6	0	-9.631977	15.556005	0.000000
254	6	0	-6.128757	20.465132	0.000000
255	6	0	-4.726421	20.465809	0.000000
256	6	0	-6.154452	12.074555	0.000000
257	6	0	-4.694906	12.074524	0.000000
258	8	0	-2.673766	13.534162	0.000000
259	8	0	-2.679089	19.042407	0.000000
260	8	0	-8.175240	13.532481	0.000000
261	6	0	0.000000	17.706589	0.000000
262	6	0	0.000000	14.873656	0.000000
263	1	0	-6.683070	21.398940	0.000000
264	1	0	-4.172901	21.400129	0.000000
265	6	0	-10.849214	14.867177	0.000000
266	6	0	-4.009279	10.855673	0.000000
267	6	0	-10.856938	6.842462	0.000000
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269	1	0	-18.786746	10.854587	0.000000
270	1	0	-13.780165	10.847174	0.000000
271	1	0	-7.929342	10.858267	0.000000
272	1	0	-10.854587	18.786746	0.000000
273	1	0	-10.847174	13.780165	0.000000
274	1	0	-2.922402	10.854350	0.000000
275	1	0	-10.858267	7.929342	0.000000
276	1	0	-10.854350	2.922402	0.000000
277	6	0	-1.218070	4.697795	0.000000
278	6	0	0.000000	6.844311	0.000000
279	1	0	0.000000	2.924167	0.000000
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283	6	0	-6.844311	0.000000	0.000000
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288	6	0	6.798794	-19.234714	0.000000
289	6	0	4.055208	-19.236016	0.000000
290	6	0	2.494419	-17.671544	0.000000
291	6	0	2.487393	-14.905693	0.000000
292	6	0	4.043877	-13.346475	0.000000
293	6	0	7.145805	-16.993650	0.000000
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295	6	0	6.135581	-14.562891	0.000000
296	6	0	4.713993	-14.563124	0.000000
297	6	0	3.704232	-15.574352	0.000000
298	6	0	3.705838	-16.995086	0.000000
299	6	0	4.725464	-17.999238	0.000000
300	6	0	6.127118	-17.998664	0.000000
301	6	0	8.362473	-14.903550	0.000000
302	6	0	6.805109	-13.346062	0.000000
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307	6	0	4.694906	-12.074524	0.000000
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311	8	0	8.174606	-19.039547	0.000000
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314	1	0	4.172901	-21.400129	0.000000
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316	6	0	6.842462	-10.856938	0.000000
317	8	0	13.524356	-13.524356	0.000000
318	6	0	19.218239	-17.651920	0.000000
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320	6	0	14.904228	-19.228018	0.000000
321	6	0	13.344291	-17.663606	0.000000
322	6	0	13.337869	-14.895747	0.000000
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324	6	0	17.987316	-16.974143	0.000000
325	6	0	17.991050	-15.574151	0.000000
326	6	0	16.986495	-14.554819	0.000000
327	6	0	15.565340	-14.554190	0.000000
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330	6	0	15.574151	-17.991050	0.000000
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333	6	0	17.663606	-13.344291	0.000000
334	6	0	20.454856	-15.579342	0.000000
335	6	0	20.449666	-16.982211	0.000000
336	6	0	12.068367	-15.551427	0.000000
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341	6	0	16.982211	-20.449666	0.000000
342	8	0	19.027378	-19.027378	0.000000
343	8	0	19.034148	-13.527340	0.000000
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345	1	0	21.391278	-15.029317	0.000000
346	1	0	21.382244	-17.538534	0.000000
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351	6	0	8.366391	-6.808315	0.000000
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353	6	0	4.047073	-8.366000	0.000000
354	6	0	2.489586	-6.808087	0.000000
355	6	0	2.489608	-4.047184	0.000000
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357	6	0	7.149298	-6.138837	0.000000
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359	6	0	6.138676	-3.706593	0.000000
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367	6	0	9.637800	-4.697281	0.000000
368	6	0	9.637989	-6.156841	0.000000
369	6	0	1.218070	-4.697795	0.000000
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375	8	0	8.178746	-8.178746	0.000000
376	8	0	8.178415	-2.676790	0.000000
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378	6	0	10.855673	-4.009279	0.000000
379	8	0	13.534162	-2.673766	0.000000
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393	6	0	16.993650	-7.145805	0.000000
394	6	0	19.236016	-4.055208	0.000000
395	6	0	17.671544	-2.494419	0.000000
396	6	0	20.465809	-4.726421	0.000000
397	6	0	20.465132	-6.128757	0.000000
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406	8	0	13.532481	-8.175240	0.000000
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410	6	0	17.700159	-10.852017	0.000000
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413	1	0	2.922402	-10.854350	0.000000
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422	8	0	-19.034148	-13.527340	0.000000
423	6	0	-13.344291	-17.663606	0.000000
424	6	0	-14.904228	-19.228018	0.000000
425	6	0	-17.651920	-19.218239	0.000000
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432	6	0	-16.986495	-14.554819	0.000000
433	6	0	-17.991050	-15.574151	0.000000
434	6	0	-17.987316	-16.974143	0.000000
435	6	0	-16.974143	-17.987316	0.000000
436	6	0	-15.574151	-17.991050	0.000000
437	6	0	-13.337869	-14.895747	0.000000
438	6	0	-14.895747	-13.337869	0.000000
439	6	0	-12.068367	-15.551427	0.000000
440	6	0	-12.070210	-17.011897	0.000000
441	6	0	-20.454856	-15.579342	0.000000
442	6	0	-20.449666	-16.982211	0.000000
443	6	0	-17.011897	-12.070210	0.000000
444	6	0	-15.551427	-12.068367	0.000000
445	6	0	-16.982211	-20.449666	0.000000
446	6	0	-15.579342	-20.454856	0.000000
447	8	0	-13.527340	-19.034148	0.000000
448	8	0	-13.524356	-13.524356	0.000000
449	8	0	-19.027378	-19.027378	0.000000
450	1	0	-21.391278	-15.029317	0.000000
451	1	0	-21.382244	-17.538534	0.000000
452	1	0	-17.538534	-21.382244	0.000000
453	1	0	-15.029317	-21.391278	0.000000
454	6	0	-14.867177	-10.849214	0.000000
455	8	0	-8.175240	-13.532481	0.000000
456	6	0	-2.494419	-17.671544	0.000000
457	6	0	-4.055208	-19.236016	0.000000
458	6	0	-6.798794	-19.234714	0.000000
459	6	0	-8.357898	-17.668699	0.000000
460	6	0	-8.362473	-14.903550	0.000000
461	6	0	-6.805109	-13.346062	0.000000
462	6	0	-3.705838	-16.995086	0.000000
463	6	0	-3.704232	-15.574352	0.000000
464	6	0	-4.713993	-14.563124	0.000000

465	6	0	-6.135581	-14.562891	0.000000
466	6	0	-7.146165	-15.573166	0.000000
467	6	0	-7.145805	-16.993650	0.000000
468	6	0	-6.127118	-17.998664	0.000000
469	6	0	-4.725464	-17.999238	0.000000
470	6	0	-2.487393	-14.905693	0.000000
471	6	0	-4.043877	-13.346475	0.000000
472	6	0	-1.218268	-15.560017	0.000000
473	6	0	-9.631977	-15.556005	0.000000
474	6	0	-9.631303	-17.015903	0.000000
475	6	0	-6.154452	-12.074555	0.000000
476	6	0	-4.694906	-12.074524	0.000000
477	6	0	-6.128757	-20.465132	0.000000
478	6	0	-4.726421	-20.465809	0.000000
479	8	0	-2.679089	-19.042407	0.000000
480	8	0	-2.673766	-13.534162	0.000000
481	8	0	-8.174606	-19.039547	0.000000
482	1	0	-6.683070	-21.398940	0.000000
483	1	0	-4.172901	-21.400129	0.000000
484	6	0	-6.842462	-10.856938	0.000000
485	8	0	-19.042407	-2.679089	0.000000
486	6	0	-13.346062	-6.805109	0.000000
487	6	0	-14.903550	-8.362473	0.000000
488	6	0	-17.668699	-8.357898	0.000000
489	6	0	-19.234714	-6.798794	0.000000
490	6	0	-19.236016	-4.055208	0.000000
491	6	0	-17.671544	-2.494419	0.000000
492	6	0	-14.562891	-6.135581	0.000000
493	6	0	-14.563124	-4.713993	0.000000
494	6	0	-15.574352	-3.704232	0.000000
495	6	0	-16.995086	-3.705838	0.000000
496	6	0	-17.999238	-4.725464	0.000000
497	6	0	-17.998664	-6.127118	0.000000
498	6	0	-16.993650	-7.145805	0.000000
499	6	0	-15.573166	-7.146165	0.000000
500	6	0	-13.346475	-4.043877	0.000000
501	6	0	-14.905693	-2.487393	0.000000
502	6	0	-12.074524	-4.694906	0.000000
503	6	0	-12.074555	-6.154452	0.000000
504	6	0	-20.465809	-4.726421	0.000000
505	6	0	-20.465132	-6.128757	0.000000
506	6	0	-17.020419	-1.219933	0.000000
507	6	0	-15.560017	-1.218268	0.000000
508	6	0	-17.015903	-9.631303	0.000000
509	6	0	-15.556005	-9.631977	0.000000
510	8	0	-13.532481	-8.175240	0.000000
511	8	0	-13.534162	-2.673766	0.000000
512	8	0	-19.039547	-8.174606	0.000000
513	1	0	-21.400129	-4.172901	0.000000
514	1	0	-21.398940	-6.683070	0.000000
515	6	0	-10.855673	-4.009279	0.000000
516	8	0	-8.178415	-2.676790	0.000000
517	6	0	-2.489586	-6.808087	0.000000
518	6	0	-4.047073	-8.366000	0.000000
519	6	0	-6.808315	-8.366391	0.000000
520	6	0	-8.366391	-6.808315	0.000000
521	6	0	-8.366000	-4.047073	0.000000
522	6	0	-6.808087	-2.489586	0.000000
523	6	0	-3.706593	-6.138676	0.000000
524	6	0	-3.706481	-4.716863	0.000000
525	6	0	-4.716863	-3.706481	0.000000
526	6	0	-6.138676	-3.706593	0.000000
527	6	0	-7.149149	-4.716947	0.000000
528	6	0	-7.149298	-6.138837	0.000000
529	6	0	-6.138837	-7.149298	0.000000
530	6	0	-4.716947	-7.149149	0.000000
531	6	0	-2.489608	-4.047184	0.000000
532	6	0	-4.047184	-2.489608	0.000000
533	6	0	-1.218070	-4.697795	0.000000
534	6	0	-1.218109	-6.157311	0.000000
535	6	0	-9.637800	-4.697281	0.000000
536	6	0	-9.637989	-6.156841	0.000000
537	6	0	-6.157311	-1.218109	0.000000
538	6	0	-4.697795	-1.218070	0.000000
539	6	0	-6.156841	-9.637989	0.000000
540	6	0	-4.697281	-9.637800	0.000000
541	8	0	-2.676790	-8.178415	0.000000
542	8	0	-2.677034	-2.677034	0.000000
543	8	0	-8.178746	-8.178746	0.000000

544	6	0	0.000000	-4.010847	0.000000
545	6	0	0.000000	-6.844311	0.000000
546	6	0	-10.856938	-6.842462	0.000000
547	6	0	-4.009279	-10.855673	0.000000
548	6	0	-10.849214	-14.867177	0.000000
549	6	0	-10.852017	-17.700159	0.000000
550	1	0	-18.786746	-10.854587	0.000000
551	1	0	-13.780165	-10.847174	0.000000
552	1	0	-7.929342	-10.858267	0.000000
553	1	0	-10.854350	-2.922402	0.000000
554	1	0	-10.858267	-7.929342	0.000000
555	1	0	-2.922402	-10.854350	0.000000
556	1	0	-10.847174	-13.780165	0.000000
557	1	0	-10.854587	-18.786746	0.000000
558	6	0	-1.219933	-17.020419	0.000000
559	6	0	0.000000	-14.873656	0.000000
560	1	0	0.000000	-18.793364	0.000000
561	1	0	0.000000	-2.924167	0.000000
562	1	0	0.000000	-7.931207	0.000000
563	1	0	0.000000	-13.786564	0.000000
564	6	0	-4.010847	0.000000	0.000000
565	6	0	4.010847	0.000000	0.000000
566	6	0	6.844311	0.000000	0.000000
567	6	0	14.873656	0.000000	0.000000
568	6	0	17.706589	0.000000	0.000000
569	1	0	-18.793364	0.000000	0.000000
570	1	0	-13.786564	0.000000	0.000000
571	1	0	-7.931207	0.000000	0.000000
572	1	0	-2.924167	0.000000	0.000000
573	1	0	2.924167	0.000000	0.000000
574	1	0	7.931207	0.000000	0.000000
575	1	0	13.786564	0.000000	0.000000
576	1	0	18.793364	0.000000	0.000000

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-13.641931	2.503201	0.000000
2	1	0	11.416333	-7.876271	0.000000
3	1	0	-8.536143	10.313417	10.531434
4	8	0	-7.563863	11.436700	8.178446
5	1	0	-2.503201	-13.641931	0.000000
6	6	0	-1.378618	-13.668494	-2.490655
7	6	0	-4.162485	-13.229663	-6.154693
8	6	0	1.416552	13.645387	0.000000
9	8	0	2.743500	13.554673	-2.677299
10	6	0	-2.921019	13.499327	-6.810028
11	6	0	-1.367981	13.533273	-8.377822
12	6	0	1.367981	13.533273	-8.377822
13	6	0	2.933379	13.556911	-4.047519
14	6	0	1.378618	13.668494	-2.490655
15	6	0	-1.719623	13.677532	-6.139862
16	6	0	-1.723990	13.705156	-4.717845
17	6	0	-0.712329	13.757690	-3.706913
18	6	0	0.712329	13.757690	-3.706913
19	6	0	1.723990	13.705156	-4.717845
20	6	0	1.719623	13.677532	-6.139862
21	6	0	0.701070	13.682462	-7.147310
22	6	0	-0.701070	13.682462	-7.147310
23	6	0	-2.933379	13.556911	-4.047519
24	6	0	-1.378618	13.668494	-2.490655
25	6	0	-4.171484	13.256321	-4.696560
26	6	0	-4.162485	13.229663	-6.154693
27	6	0	0.729271	13.659328	-1.218036
28	6	0	-0.729271	13.659328	-1.218036
29	6	0	0.700589	13.435775	-9.604942
30	6	0	-0.700589	13.435775	-9.604942
31	8	0	-2.738509	13.435427	-8.178446
32	8	0	-2.743500	13.554673	-2.677299
33	1	0	1.256723	13.328652	-10.531434
34	1	0	-1.256723	13.328652	-10.531434
35	6	0	-1.416552	13.645387	0.000000
36	8	0	-7.644654	11.524549	-2.677299
37	6	0	-11.610938	7.479993	-6.810028
38	6	0	-10.536778	8.602160	-8.377822
39	6	0	-8.602160	10.536778	-8.377822
40	6	0	-7.479993	11.610938	-6.810028
41	6	0	-7.511971	11.660395	-4.047519
42	6	0	-8.690255	10.639915	-2.490655
43	6	0	-10.887433	8.455519	-6.139862
44	6	0	-10.910054	8.471963	-4.717845
45	6	0	-10.231848	9.224464	-3.706913
46	6	0	-9.224464	10.231848	-3.706913
47	6	0	-8.471963	10.910054	-4.717845
48	6	0	-8.455519	10.887433	-6.139862
49	6	0	-9.179230	10.170693	-7.147310
50	6	0	-10.170693	9.179230	-7.147310
51	6	0	-11.660395	7.511971	-4.047519
52	6	0	-10.639915	8.690255	-2.490655
53	6	0	-12.323319	6.423949	-4.696560
54	6	0	-12.298105	6.411463	-6.154693
55	6	0	-6.423949	12.323319	-4.696560
56	6	0	-6.411463	12.298105	-6.154693
57	6	0	-9.142931	10.174276	-1.218036
58	6	0	-10.174276	9.142931	-1.218036
59	6	0	-9.005136	9.995919	-9.604942
60	6	0	-9.995919	9.005136	-9.604942
61	8	0	-11.436700	7.563863	-8.178446
62	8	0	-11.524549	7.644654	-2.677299
63	8	0	-7.563863	11.436700	-8.178446
64	1	0	-8.536143	10.313417	-10.531434
65	1	0	-10.313417	8.536143	-10.531434
66	6	0	-8.647092	10.650399	0.000000
67	8	0	2.738509	13.435427	8.178446
68	6	0	-2.933379	13.556911	4.047519

69	6	0	-1.378618	13.668494	2.490655
70	6	0	1.378618	13.668494	2.490655
71	6	0	2.933379	13.556911	4.047519
72	6	0	2.921019	13.499327	6.810028
73	6	0	1.367981	13.533273	8.377822
74	6	0	-1.723990	13.705156	4.717845
75	6	0	-1.719623	13.677532	6.139862
76	6	0	-0.701070	13.682462	7.147310
77	6	0	0.701070	13.682462	7.147310
78	6	0	1.719623	13.677532	6.139862
79	6	0	1.723990	13.705156	4.717845
80	6	0	0.712329	13.757690	3.706913
81	6	0	-0.712329	13.757690	3.706913
82	6	0	-2.921019	13.499327	6.810028
83	6	0	-1.367981	13.533273	8.377822
84	6	0	-4.162485	13.229663	6.154693
85	6	0	-4.171484	13.256321	4.696560
86	6	0	4.162485	13.229663	6.154693
87	6	0	4.171484	13.256321	4.696560
88	6	0	0.700589	13.435775	9.604942
89	6	0	-0.700589	13.435775	9.604942
90	6	0	0.729271	13.659328	1.218036
91	6	0	-0.729271	13.659328	1.218036
92	8	0	-2.743500	13.554673	2.677299
93	8	0	-2.738509	13.435427	8.178446
94	8	0	2.743500	13.554673	2.677299
95	6	0	5.296918	12.787891	6.842300
96	6	0	5.318249	12.839390	4.009865
97	1	0	1.256723	13.328652	10.531434
98	1	0	-1.256723	13.328652	10.531434
99	6	0	-5.296918	12.787891	6.842300
100	6	0	-11.660395	7.511971	4.047519
101	6	0	-10.639915	8.690255	2.490655
102	6	0	-8.690255	10.639915	2.490655
103	6	0	-7.511971	11.660395	4.047519
104	6	0	-7.479993	11.610938	6.810028
105	6	0	-10.910054	8.471963	4.717845
106	6	0	-10.887433	8.455519	6.139862
107	6	0	-10.170693	9.179230	7.147310
108	6	0	-9.179230	10.170693	7.147310
109	6	0	-8.471963	10.910054	4.717845
110	6	0	-9.224464	10.231848	3.706913
111	6	0	-10.231848	9.224464	3.706913
112	6	0	-11.610938	7.479993	6.810028
113	6	0	-10.536778	8.602160	8.377822
114	6	0	-12.298105	6.411463	6.154693
115	6	0	-12.323319	6.423949	4.696560
116	6	0	-6.411463	12.298105	6.154693
117	6	0	-6.423949	12.323319	4.696560
118	6	0	-9.995919	9.005136	9.604942
119	6	0	-9.142931	10.174276	1.218036
120	6	0	-10.174276	9.142931	1.218036
121	8	0	-11.524549	7.644654	2.677299
122	8	0	-11.436700	7.563863	8.178446
123	8	0	-7.644654	11.524549	2.677299
124	1	0	-10.313417	8.536143	10.531434
125	6	0	-5.318249	12.839390	4.009865
126	6	0	-10.650399	8.647092	0.000000
127	6	0	-5.318249	12.839390	-4.009865
128	6	0	-5.296918	12.787891	-6.842300
129	1	0	2.503201	13.641931	0.000000
130	1	0	-2.503201	13.641931	0.000000
131	1	0	-7.876271	11.416333	0.000000
132	1	0	-5.273614	12.731631	7.927122
133	1	0	-5.311533	12.823174	2.923367
134	1	0	-11.416333	7.876271	0.000000
135	1	0	-5.311533	12.823174	-2.923367
136	1	0	-5.273614	12.731631	-7.927122
137	8	0	-13.554673	2.743500	-2.677299
138	6	0	-13.499327	-2.921019	-6.810028
139	6	0	-13.533273	-1.367981	-8.377822
140	6	0	-13.533273	1.367981	-8.377822
141	6	0	-13.499327	2.921019	-6.810028
142	6	0	-13.556911	2.933379	-4.047519
143	6	0	-13.668494	1.378618	-2.490655
144	6	0	-13.677532	-1.719623	-6.139862
145	6	0	-13.705156	-1.723990	-4.717845
146	6	0	-13.757690	-0.712329	-3.706913
147	6	0	-13.757690	0.712329	-3.706913

148	6	0	-13.705156	1.723990	-4.717845
149	6	0	-13.677532	1.719623	-6.139862
150	6	0	-13.682462	0.701070	-7.147310
151	6	0	-13.682462	-0.701070	-7.147310
152	6	0	-13.556911	-2.933379	-4.047519
153	6	0	-13.668494	-1.378618	-2.490655
154	6	0	-13.256321	-4.171484	-4.696560
155	6	0	-13.229663	-4.162485	-6.154693
156	6	0	-13.256321	4.171484	-4.696560
157	6	0	-13.229663	4.162485	-6.154693
158	6	0	-13.659328	0.729271	-1.218036
159	6	0	-13.659328	-0.729271	-1.218036
160	6	0	-13.435775	0.700589	-9.604942
161	6	0	-13.435775	-0.700589	-9.604942
162	8	0	-13.435427	-2.738509	-8.178446
163	8	0	-13.554673	-2.743500	-2.677299
164	8	0	-13.435427	2.738509	-8.178446
165	6	0	-12.839390	5.318249	-4.009865
166	1	0	-13.328652	1.256723	-10.531434
167	1	0	-13.328652	-1.256723	-10.531434
168	6	0	-13.645387	-1.416552	0.000000
169	8	0	-11.524549	-7.644654	-2.677299
170	6	0	-7.479993	-11.610938	-6.810028
171	6	0	-8.602160	-10.536778	-8.377822
172	6	0	-10.536778	-8.602160	-8.377822
173	6	0	-11.610938	-7.479993	-6.810028
174	6	0	-11.660395	-7.511971	-4.047519
175	6	0	-10.639915	-8.690255	-2.490655
176	6	0	-8.455519	-10.887433	-6.139862
177	6	0	-8.471963	-10.910054	-4.717845
178	6	0	-9.224464	-10.231848	-3.706913
179	6	0	-10.231848	-9.224464	-3.706913
180	6	0	-10.910054	-8.471963	-4.717845
181	6	0	-10.887433	-8.455519	-6.139862
182	6	0	-10.170693	-9.179230	-7.147310
183	6	0	-9.179230	-10.170693	-7.147310
184	6	0	-7.511971	-11.660395	-4.047519
185	6	0	-8.690255	-10.639915	-2.490655
186	6	0	-6.423949	-12.323319	-4.696560
187	6	0	-6.411463	-12.298105	-6.154693
188	6	0	-12.323319	-6.423949	-4.696560
189	6	0	-12.298105	-6.411463	-6.154693
190	6	0	-10.174276	-9.142931	-1.218036
191	6	0	-9.142931	-10.174276	-1.218036
192	6	0	-9.995919	-9.005136	-9.604942
193	6	0	-9.005136	-9.995919	-9.604942
194	8	0	-7.563863	-11.436700	-8.178446
195	8	0	-7.644654	-11.524549	-2.677299
196	8	0	-11.436700	-7.563863	-8.178446
197	1	0	-10.313417	-8.536143	-10.531434
198	1	0	-8.536143	-10.313417	-10.531434
199	6	0	-10.650399	-8.647092	0.000000
200	8	0	-13.435427	2.738509	8.178446
201	6	0	-13.556911	-2.933379	4.047519
202	6	0	-13.668494	-1.378618	2.490655
203	6	0	-13.668494	1.378618	2.490655
204	6	0	-13.556911	2.933379	4.047519
205	6	0	-13.499327	2.921019	6.810028
206	6	0	-13.533273	1.367981	8.377822
207	6	0	-13.705156	-1.723990	4.717845
208	6	0	-13.677532	-1.719623	6.139862
209	6	0	-13.682462	-0.701070	7.147310
210	6	0	-13.682462	0.701070	7.147310
211	6	0	-13.677532	1.719623	6.139862
212	6	0	-13.705156	1.723990	4.717845
213	6	0	-13.757690	0.712329	3.706913
214	6	0	-13.757690	-0.712329	3.706913
215	6	0	-13.499327	-2.921019	6.810028
216	6	0	-13.533273	-1.367981	8.377822
217	6	0	-13.229663	-4.162485	6.154693
218	6	0	-13.256321	-4.171484	4.696560
219	6	0	-13.229663	4.162485	6.154693
220	6	0	-13.256321	4.171484	4.696560
221	6	0	-13.435775	0.700589	9.604942
222	6	0	-13.435775	-0.700589	9.604942
223	6	0	-13.659328	0.729271	1.218036
224	6	0	-13.659328	-0.729271	1.218036
225	8	0	-13.554673	-2.743500	2.677299
226	8	0	-13.435427	-2.738509	8.178446

227	8	0	-13.554673	2.743500	2.677299
228	1	0	-13.328652	1.256723	10.531434
229	1	0	-13.328652	-1.256723	10.531434
230	6	0	-12.787891	-5.296918	6.842300
231	8	0	-11.436700	-7.563863	8.178446
232	6	0	-7.511971	-11.660395	4.047519
233	6	0	-8.690255	-10.639915	2.490655
234	6	0	-10.639915	-8.690255	2.490655
235	6	0	-11.660395	-7.511971	4.047519
236	6	0	-11.610938	-7.479993	6.810028
237	6	0	-10.536778	-8.602160	8.377822
238	6	0	-8.471963	-10.910054	4.717845
239	6	0	-8.455519	-10.887433	6.139862
240	6	0	-9.179230	-10.170693	7.147310
241	6	0	-10.170693	-9.179230	7.147310
242	6	0	-10.887433	-8.455519	6.139862
243	6	0	-10.910054	-8.471963	4.717845
244	6	0	-10.231848	-9.224464	3.706913
245	6	0	-9.224464	-10.231848	3.706913
246	6	0	-7.479993	-11.610938	6.810028
247	6	0	-8.602160	-10.536778	8.377822
248	6	0	-12.298105	-6.411463	6.154693
249	6	0	-12.323319	-6.423949	4.696560
250	6	0	-9.995919	-9.005136	9.604942
251	6	0	-9.005136	-9.995919	9.604942
252	6	0	-10.174276	-9.142931	1.218036
253	6	0	-9.142931	-10.174276	1.218036
254	8	0	-7.644654	-11.524549	2.677299
255	8	0	-7.563863	-11.436700	8.178446
256	8	0	-11.524549	-7.644654	2.677299
257	1	0	-10.313417	-8.536143	10.531434
258	1	0	-8.536143	-10.313417	10.531434
259	6	0	-12.839390	-5.318249	4.009865
260	6	0	-8.647092	-10.650399	0.000000
261	6	0	-12.839390	-5.318249	-4.009865
262	6	0	-12.787891	-5.296918	-6.842300
263	1	0	-13.641931	-2.503201	0.000000
264	1	0	-11.416333	-7.876271	0.000000
265	1	0	-12.731631	-5.273614	7.927122
266	1	0	-12.823174	-5.311533	2.923367
267	1	0	-7.876271	-11.416333	0.000000
268	1	0	-12.823174	-5.311533	-2.923367
269	1	0	-12.731631	-5.273614	-7.927122
270	6	0	-12.787891	5.296918	-6.842300
271	6	0	-12.787891	5.296918	6.842300
272	6	0	-12.839390	5.318249	4.009865
273	1	0	-12.823174	5.311533	-2.923367
274	1	0	-12.731631	5.273614	-7.927122
275	1	0	-12.731631	5.273614	7.927122
276	1	0	-12.823174	5.311533	2.923367
277	6	0	-6.423949	-12.323319	4.696560
278	6	0	-6.411463	-12.298105	6.154693
279	6	0	-5.296918	-12.787891	6.842300
280	6	0	8.647092	10.650399	0.000000
281	8	0	7.644654	11.524549	2.677299
282	6	0	11.610938	7.479993	6.810028
283	6	0	10.536778	8.602160	8.377822
284	6	0	8.602160	10.536778	8.377822
285	6	0	7.479993	11.610938	6.810028
286	6	0	7.511971	11.660395	4.047519
287	6	0	8.690255	10.639915	2.490655
288	6	0	10.887433	8.455519	6.139862
289	6	0	10.910054	8.471963	4.717845
290	6	0	10.231848	9.224464	3.706913
291	6	0	9.224464	10.231848	3.706913
292	6	0	8.471963	10.910054	4.717845
293	6	0	8.455519	10.887433	6.139862
294	6	0	9.179230	10.170693	7.147310
295	6	0	10.170693	9.179230	7.147310
296	6	0	11.660395	7.511971	4.047519
297	6	0	10.639915	8.690255	2.490655
298	6	0	12.323319	6.423949	4.696560
299	6	0	12.298105	6.411463	6.154693
300	6	0	6.423949	12.323319	4.696560
301	6	0	6.411463	12.298105	6.154693
302	6	0	9.142931	10.174276	1.218036
303	6	0	10.174276	9.142931	1.218036
304	6	0	9.005136	9.995919	9.604942
305	6	0	9.995919	9.005136	9.604942

306	8	0	11.436700	7.563863	8.178446
307	8	0	11.524549	7.644654	2.677299
308	8	0	7.563863	11.436700	8.178446
309	1	0	8.536143	10.313417	10.531434
310	1	0	10.313417	8.536143	10.531434
311	6	0	10.650399	8.647092	0.000000
312	8	0	13.554673	2.743500	2.677299
313	6	0	13.499327	-2.921019	6.810028
314	6	0	13.533273	-1.367981	8.377822
315	6	0	13.533273	1.367981	8.377822
316	6	0	13.499327	2.921019	6.810028
317	6	0	13.556911	2.933379	4.047519
318	6	0	13.668494	1.378618	2.490655
319	6	0	13.677532	-1.719623	6.139862
320	6	0	13.705156	-1.723990	4.717845
321	6	0	13.757690	-0.712329	3.706913
322	6	0	13.757690	0.712329	3.706913
323	6	0	13.705156	1.723990	4.717845
324	6	0	13.677532	1.719623	6.139862
325	6	0	13.682462	0.701070	7.147310
326	6	0	13.682462	-0.701070	7.147310
327	6	0	13.556911	-2.933379	4.047519
328	6	0	13.668494	-1.378618	2.490655
329	6	0	13.256321	-4.171484	4.696560
330	6	0	13.229663	-4.162485	6.154693
331	6	0	13.256321	4.171484	4.696560
332	6	0	13.229663	4.162485	6.154693
333	6	0	13.659328	0.729271	1.218036
334	6	0	13.659328	-0.729271	1.218036
335	6	0	13.435775	0.700589	9.604942
336	6	0	13.435775	-0.700589	9.604942
337	8	0	13.435427	-2.738509	8.178446
338	8	0	13.554673	-2.743500	2.677299
339	8	0	13.435427	2.738509	8.178446
340	1	0	13.328652	1.256723	10.531434
341	1	0	13.328652	-1.256723	10.531434
342	6	0	13.645387	1.416552	0.000000
343	8	0	7.563863	11.436700	-8.178446
344	6	0	11.660395	7.511971	-4.047519
345	6	0	10.639915	8.690255	-2.490655
346	6	0	8.690255	10.639915	-2.490655
347	6	0	7.511971	11.660395	-4.047519
348	6	0	7.479993	11.610938	-6.810028
349	6	0	8.602160	10.536778	-8.377822
350	6	0	10.910054	8.471963	-4.717845
351	6	0	10.887433	8.455519	-6.139862
352	6	0	10.170693	9.179230	-7.147310
353	6	0	9.179230	10.170693	-7.147310
354	6	0	8.455519	10.887433	-6.139862
355	6	0	8.471963	10.910054	-4.717845
356	6	0	9.224464	10.231848	-3.706913
357	6	0	10.231848	9.224464	-3.706913
358	6	0	11.610938	7.479993	-6.810028
359	6	0	10.536778	8.602160	-8.377822
360	6	0	12.298105	6.411463	-6.154693
361	6	0	12.323319	6.423949	-4.696560
362	6	0	6.411463	12.298105	-6.154693
363	6	0	6.423949	12.323319	-4.696560
364	6	0	9.005136	9.995919	-9.604942
365	6	0	9.995919	9.005136	-9.604942
366	6	0	9.142931	10.174276	-1.218036
367	6	0	10.174276	9.142931	-1.218036
368	8	0	11.524549	7.644654	-2.677299
369	8	0	11.436700	7.563863	-8.178446
370	8	0	7.644654	11.524549	-2.677299
371	6	0	5.318249	12.839390	-4.009865
372	1	0	8.536143	10.313417	-10.531434
373	1	0	10.313417	8.536143	-10.531434
374	6	0	12.787891	5.296918	-6.842300
375	8	0	13.435427	2.738509	-8.178446
376	6	0	13.556911	-2.933379	-4.047519
377	6	0	13.668494	-1.378618	-2.490655
378	6	0	13.668494	1.378618	-2.490655
379	6	0	13.556911	2.933379	-4.047519
380	6	0	13.499327	2.921019	-6.810028
381	6	0	13.533273	1.367981	-8.377822
382	6	0	13.705156	-1.723990	-4.717845
383	6	0	13.677532	-1.719623	-6.139862
384	6	0	13.682462	-0.701070	-7.147310

385	6	0	13.682462	0.701070	-7.147310
386	6	0	13.677532	1.719623	-6.139862
387	6	0	13.705156	1.723990	-4.717845
388	6	0	13.757690	0.712329	-3.706913
389	6	0	13.757690	-0.712329	-3.706913
390	6	0	13.499327	-2.921019	-6.810028
391	6	0	13.533273	-1.367981	-8.377822
392	6	0	13.229663	-4.162485	-6.154693
393	6	0	13.256321	-4.171484	-4.696560
394	6	0	13.229663	4.162485	-6.154693
395	6	0	13.256321	4.171484	-4.696560
396	6	0	13.435775	0.700589	-9.604942
397	6	0	13.435775	-0.700589	-9.604942
398	6	0	13.659328	0.729271	-1.218036
399	6	0	13.659328	-0.729271	-1.218036
400	8	0	13.554673	-2.743500	-2.677299
401	8	0	13.435427	-2.738509	-8.178446
402	8	0	13.554673	2.743500	-2.677299
403	1	0	13.328652	1.256723	-10.531434
404	1	0	13.328652	-1.256723	-10.531434
405	6	0	12.839390	5.318249	-4.009865
406	6	0	13.645387	-1.416552	0.000000
407	6	0	12.839390	5.318249	4.009865
408	6	0	12.787891	5.296918	6.842300
409	1	0	7.876271	11.416333	0.000000
410	1	0	11.416333	7.876271	0.000000
411	1	0	13.641931	2.503201	0.000000
412	1	0	12.731631	5.273614	-7.927122
413	1	0	12.823174	5.311533	-2.923367
414	1	0	13.641931	-2.503201	0.000000
415	1	0	12.823174	5.311533	2.923367
416	1	0	12.731631	5.273614	7.927122
417	6	0	10.650399	-8.647092	0.000000
418	8	0	11.524549	-7.644654	2.677299
419	6	0	7.479993	-11.610938	6.810028
420	6	0	8.602160	-10.536778	8.377822
421	6	0	10.536778	-8.602160	8.377822
422	6	0	11.610938	-7.479993	6.810028
423	6	0	11.660395	-7.511971	4.047519
424	6	0	10.639915	-8.690255	2.490655
425	6	0	8.455519	-10.887433	6.139862
426	6	0	8.471963	-10.910054	4.717845
427	6	0	9.224464	-10.231848	3.706913
428	6	0	10.231848	-9.224464	3.706913
429	6	0	10.910054	-8.471963	4.717845
430	6	0	10.887433	-8.455519	6.139862
431	6	0	10.170693	-9.179230	7.147310
432	6	0	9.179230	-10.170693	7.147310
433	6	0	7.511971	-11.660395	4.047519
434	6	0	8.690255	-10.639915	2.490655
435	6	0	6.423949	-12.323319	4.696560
436	6	0	6.411463	-12.298105	6.154693
437	6	0	12.323319	-6.423949	4.696560
438	6	0	12.298105	-6.411463	6.154693
439	6	0	10.174276	-9.142931	1.218036
440	6	0	9.142931	-10.174276	1.218036
441	6	0	9.995919	-9.005136	9.604942
442	6	0	9.005136	-9.995919	9.604942
443	8	0	7.563863	-11.436700	8.178446
444	8	0	7.644654	-11.524549	2.677299
445	8	0	11.436700	-7.563863	8.178446
446	6	0	12.839390	-5.318249	4.009865
447	1	0	10.313417	-8.536143	10.531434
448	1	0	8.536143	-10.313417	10.531434
449	6	0	8.647092	-10.650399	0.000000
450	8	0	2.743500	-13.554673	2.677299
451	6	0	-2.921019	-13.499327	6.810028
452	6	0	-1.367981	-13.533273	8.377822
453	6	0	1.367981	-13.533273	8.377822
454	6	0	2.921019	-13.499327	6.810028
455	6	0	2.933379	-13.556911	4.047519
456	6	0	1.378618	-13.668494	2.490655
457	6	0	-1.719623	-13.677532	6.139862
458	6	0	-1.723990	-13.705156	4.717845
459	6	0	-0.712329	-13.757690	3.706913
460	6	0	0.712329	-13.757690	3.706913
461	6	0	1.723990	-13.705156	4.717845
462	6	0	1.719623	-13.677532	6.139862
463	6	0	0.701070	-13.682462	7.147310

464	6	0	-0.701070	-13.682462	7.147310
465	6	0	-2.933379	-13.556911	4.047519
466	6	0	-1.378618	-13.668494	2.490655
467	6	0	-4.171484	-13.256321	4.696560
468	6	0	-4.162485	-13.229663	6.154693
469	6	0	4.171484	-13.256321	4.696560
470	6	0	4.162485	-13.229663	6.154693
471	6	0	-0.729271	-13.659328	1.218036
472	6	0	0.700589	-13.435775	9.604942
473	6	0	-0.700589	-13.435775	9.604942
474	8	0	-2.738509	-13.435427	8.178446
475	8	0	-2.743500	-13.554673	2.677299
476	8	0	2.738509	-13.435427	8.178446
477	1	0	1.256723	-13.328652	10.531434
478	1	0	-1.256723	-13.328652	10.531434
479	8	0	11.436700	-7.563863	-8.178446
480	6	0	7.511971	-11.660395	-4.047519
481	6	0	8.690255	-10.639915	-2.490655
482	6	0	10.639915	-8.690255	-2.490655
483	6	0	11.660395	-7.511971	-4.047519
484	6	0	11.610938	-7.479993	-6.810028
485	6	0	10.536778	-8.602160	-8.377822
486	6	0	8.471963	-10.910054	-4.717845
487	6	0	8.455519	-10.887433	-6.139862
488	6	0	9.179230	-10.170693	-7.147310
489	6	0	10.170693	-9.179230	-7.147310
490	6	0	10.887433	-8.455519	-6.139862
491	6	0	10.910054	-8.471963	-4.717845
492	6	0	10.231848	-9.224464	-3.706913
493	6	0	9.224464	-10.231848	-3.706913
494	6	0	7.479993	-11.610938	-6.810028
495	6	0	8.602160	-10.536778	-8.377822
496	6	0	6.411463	-12.298105	-6.154693
497	6	0	6.423949	-12.323319	-4.696560
498	6	0	12.298105	-6.411463	-6.154693
499	6	0	12.323319	-6.423949	-4.696560
500	6	0	9.995919	-9.005136	-9.604942
501	6	0	9.005136	-9.995919	-9.604942
502	6	0	10.174276	-9.142931	-1.218036
503	6	0	9.142931	-10.174276	-1.218036
504	8	0	7.644654	-11.524549	-2.677299
505	8	0	7.563863	-11.436700	-8.178446
506	8	0	11.524549	-7.644654	-2.677299
507	1	0	10.313417	-8.536143	-10.531434
508	1	0	8.536143	-10.313417	-10.531434
509	6	0	5.296918	-12.787891	-6.842300
510	8	0	2.738509	-13.435427	-8.178446
511	6	0	1.378618	-13.668494	-2.490655
512	6	0	2.933379	-13.556911	-4.047519
513	6	0	2.921019	-13.499327	-6.810028
514	6	0	1.367981	-13.533273	-8.377822
515	6	0	-1.723990	-13.705156	-4.717845
516	6	0	-1.719623	-13.677532	-6.139862
517	6	0	-0.701070	-13.682462	-7.147310
518	6	0	0.701070	-13.682462	-7.147310
519	6	0	1.719623	-13.677532	-6.139862
520	6	0	1.723990	-13.705156	-4.717845
521	6	0	0.712329	-13.757690	-3.706913
522	6	0	-0.712329	-13.757690	-3.706913
523	6	0	-2.921019	-13.499327	-6.810028
524	6	0	-1.367981	-13.533273	-8.377822
525	6	0	4.162485	-13.229663	-6.154693
526	6	0	4.171484	-13.256321	-4.696560
527	6	0	0.700589	-13.435775	-9.604942
528	6	0	-0.700589	-13.435775	-9.604942
529	6	0	0.729271	-13.659328	-1.218036
530	8	0	-2.743500	-13.554673	-2.677299
531	8	0	-2.738509	-13.435427	-8.178446
532	8	0	2.743500	-13.554673	-2.677299
533	1	0	1.256723	-13.328652	-10.531434
534	1	0	-1.256723	-13.328652	-10.531434
535	6	0	5.318249	-12.839390	-4.009865
536	6	0	5.318249	-12.839390	4.009865
537	6	0	5.296918	-12.787891	6.842300
538	1	0	7.876271	-11.416333	0.000000
539	1	0	5.273614	-12.731631	-7.927122
540	1	0	5.311533	-12.823174	-2.923367
541	1	0	5.311533	-12.823174	2.923367
542	1	0	5.273614	-12.731631	7.927122

543	6	0	12.787891	-5.296918	6.842300
544	6	0	12.787891	-5.296918	-6.842300
545	6	0	12.839390	-5.318249	-4.009865
546	1	0	12.823174	-5.311533	2.923367
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550	6	0	-5.318249	-12.839390	4.009865
551	6	0	-5.296918	-12.787891	-6.842300
552	6	0	-4.171484	-13.256321	-4.696560
553	6	0	-2.933379	-13.556911	-4.047519
554	6	0	-5.318249	-12.839390	-4.009865
555	6	0	2.921019	13.499327	-6.810028
556	8	0	2.738509	13.435427	-8.178446
557	6	0	4.162485	13.229663	-6.154693
558	6	0	4.171484	13.256321	-4.696560
559	6	0	5.296918	12.787891	-6.842300
560	1	0	5.273614	12.731631	7.927122
561	1	0	5.311533	12.823174	2.923367
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564	1	0	-5.311533	-12.823174	2.923367
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566	1	0	-5.311533	-12.823174	-2.923367
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568	6	0	0.729271	-13.659328	1.218036
569	6	0	1.416552	-13.645387	0.000000
570	6	0	-1.416552	-13.645387	0.000000
571	6	0	-0.729271	-13.659328	-1.218036
572	1	0	2.503201	-13.641931	0.000000
573	6	0	-8.455519	10.887433	6.139862
574	6	0	-8.602160	10.536778	8.377822
575	6	0	-9.005136	9.995919	9.604942
576	6	0	-13.645387	1.416552	0.000000
