Supporting Information for

Theoretical analysis of [5.5.6]cyclacenes: Electronic properties, strain energies and substituent effects

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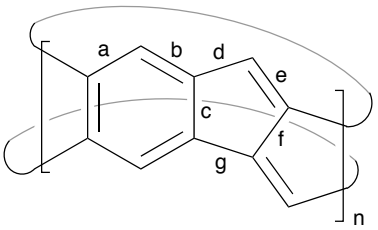
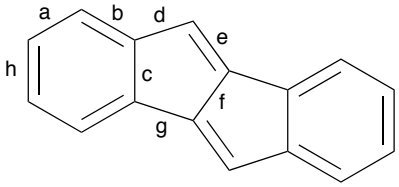
1 Structures

Table S 1. Bond lengths in [5.5.6]$_n$cyclacenes 6$_n$ and in dibenzo[*a*,*e*]pentalene (8, DBP) (TPSS-D3/def2-TZVP).





n	3	4	5	6	7	8	DBP
a	1.402	1.397	1.396	1.394	1.395	1.394	1.406
b	1.405	1.400	1.401	1.400	1.400	1.399	1.386
c	1.430	1.479	1.432	1.466	1.433	1.458	1.431
d	1.470	1.424	1.466	1.433	1.465	1.440	1.477
e	1.369	1.398	1.369	1.390	1.369	1.385	1.363
f	1.475	1.477	1.468	1.469	1.467	1.467	1.469
g	1.475	1.427	1.463	1.433	1.460	1.438	1.461
h	-	-	-	-	-	-	1.393

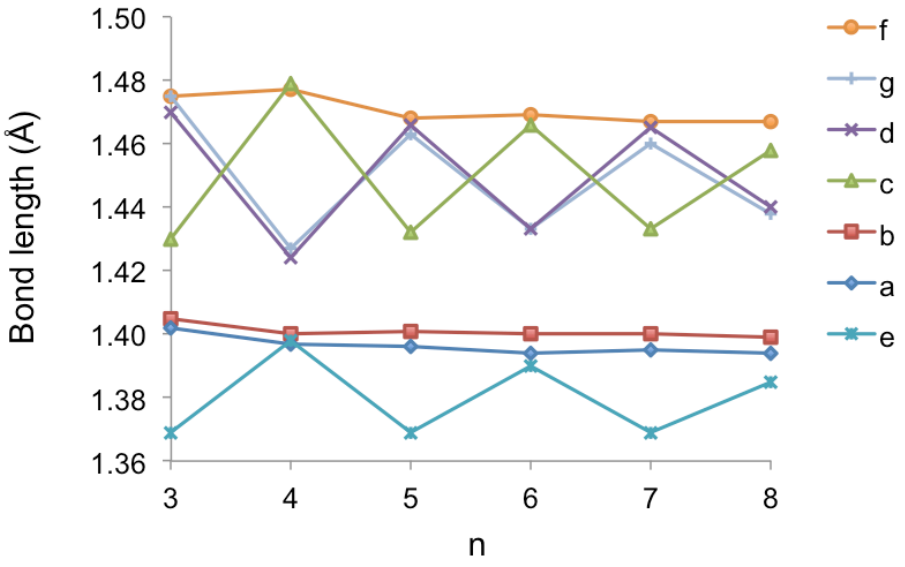


Figure S 1. Bond lengths in [5.5.6]$_n$cyclacenes **6$_n$**.

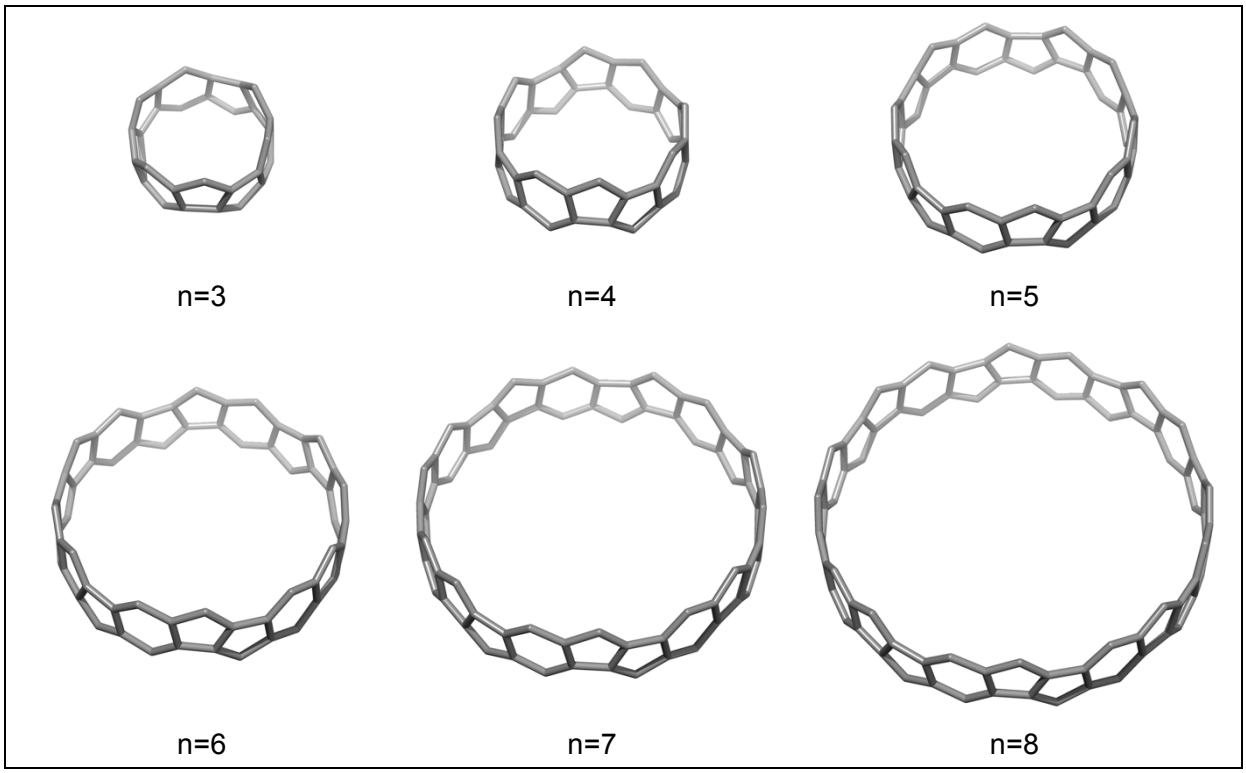


Figure S 2. Calculated structures of $[5.5.6]_n$cyclacenes $\mathbf{6_n}$ (TPSS-D3/def2-TZVP, D_n symmetries, hydrogen atoms are omitted for clarity).

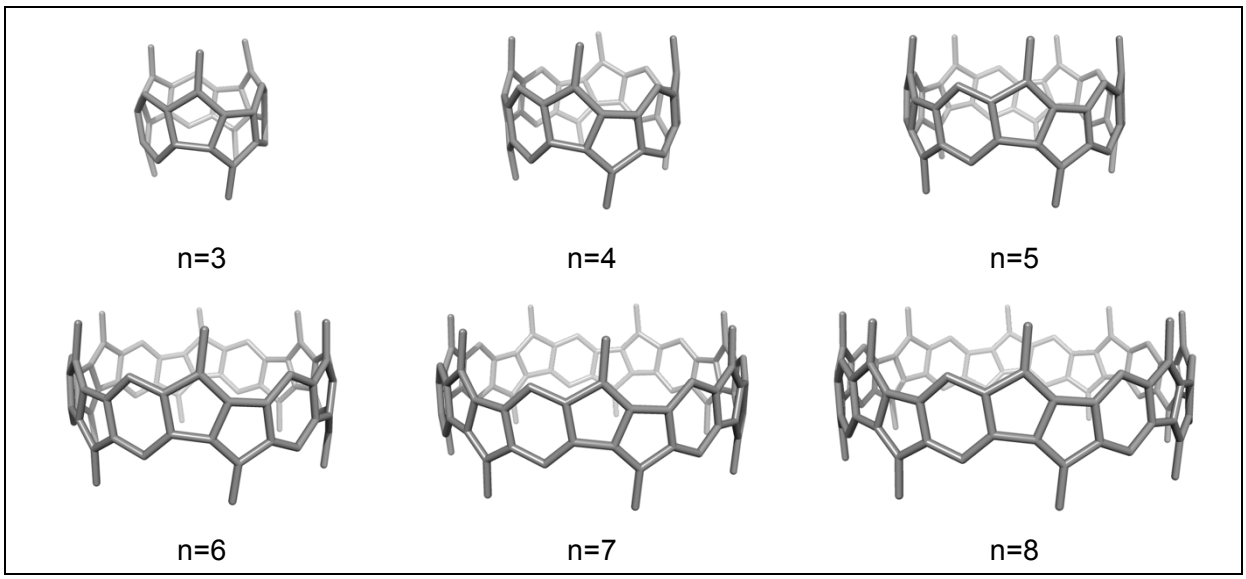


Figure S 3. Calculated structures of methyl-substituted $[5.5.6]_n$cyclacenes $\mathbf{10_n}$ (TPSS-D3/def2-TZVP, D_n symmetries, hydrogen atoms are omitted for clarity).

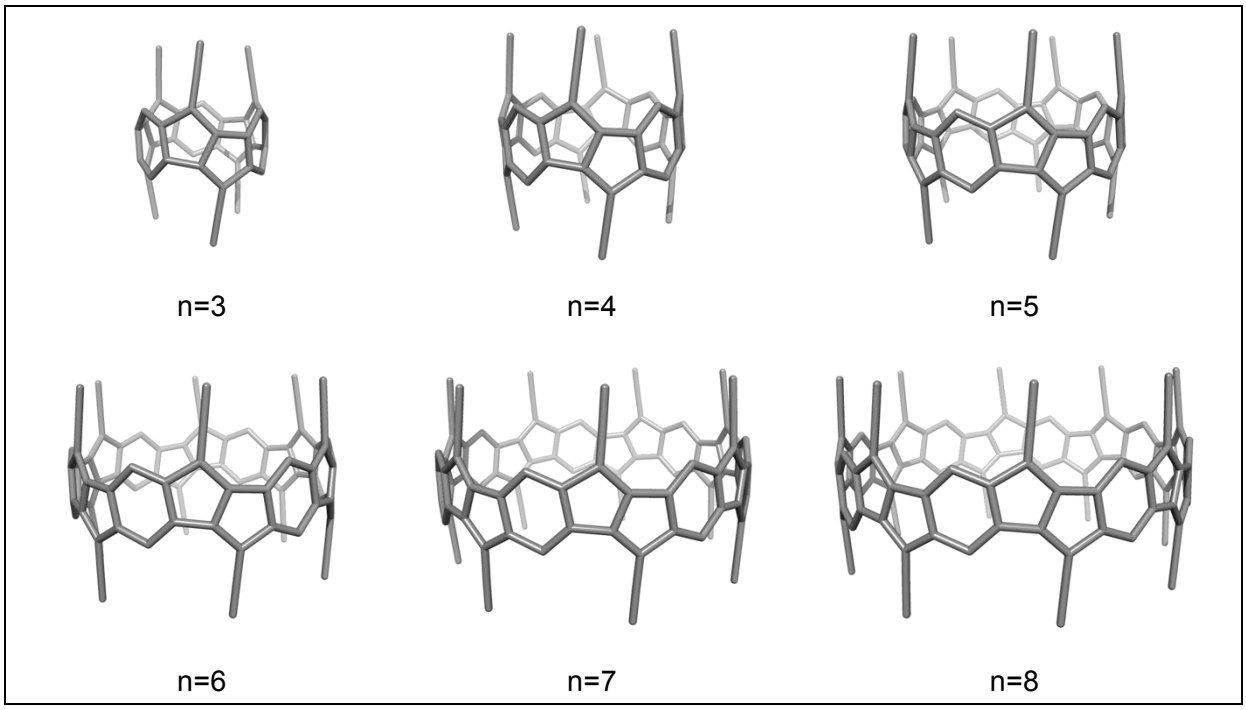


Figure S 4. Calculated structures of alkynyl-substituted $[5.5.6]_n$cyclacenes **11$_n$** (TPSS-D3/def2-TZVP, D_n symmetries, hydrogen atoms are omitted for clarity).

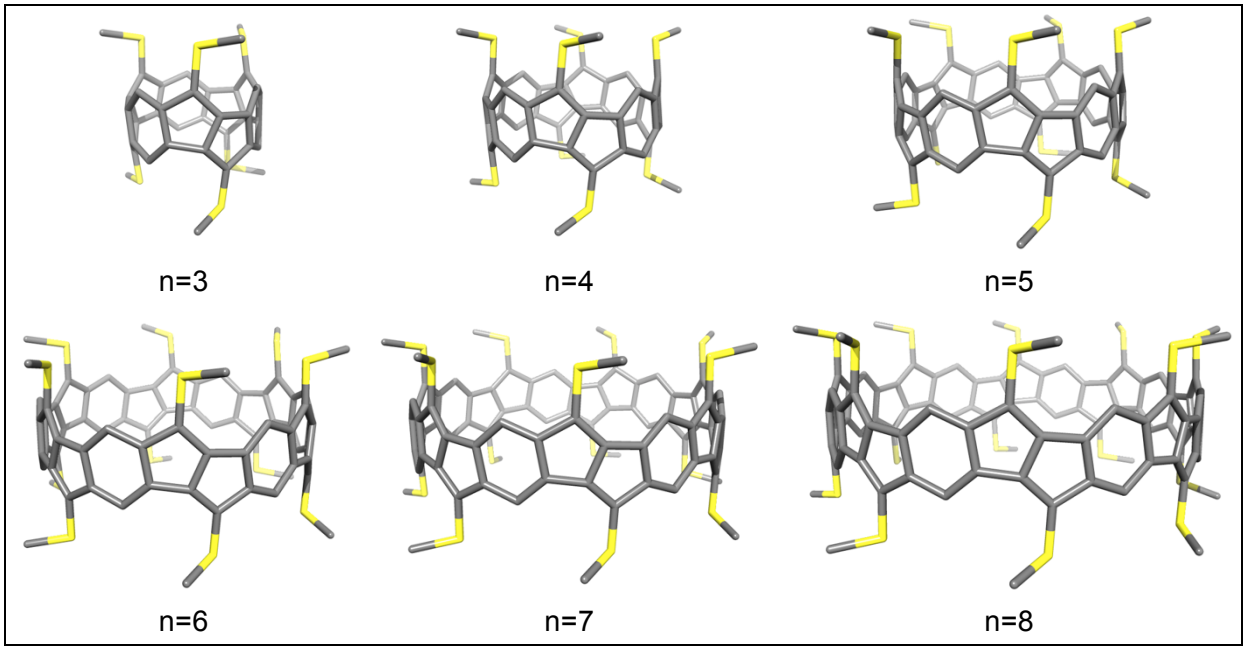


Figure S 5. Calculated structures of thiomethyl-substituted $[5.5.6]_n$cyclacenes **12$_n$** (TPSS-D3/def2-TZVP, D_n symmetries, hydrogen atoms are omitted for clarity).

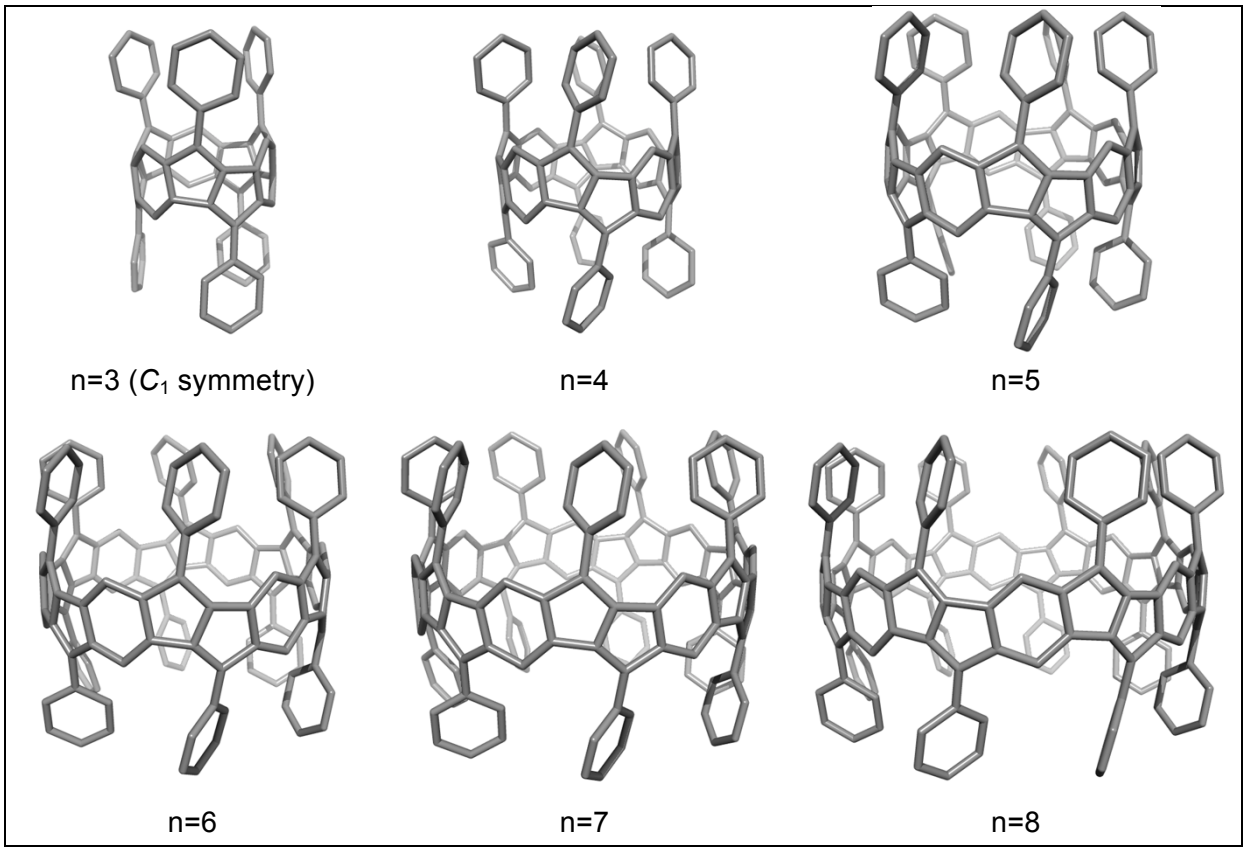
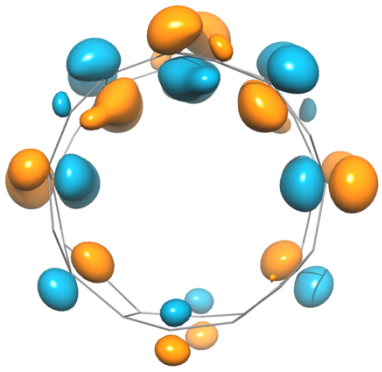
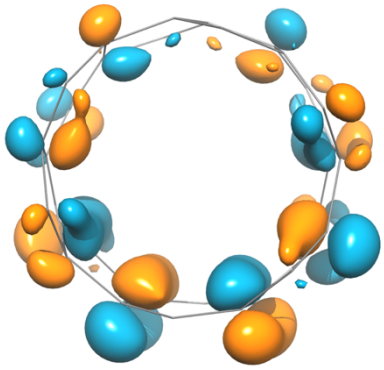


Figure S 6. Calculated structures of phenyl-substituted $[5.5.6]_n$cyclacenes **13_n** (TPSS-D3/def2-TZVP, D_n symmetries, hydrogen atoms are omitted for clarity).

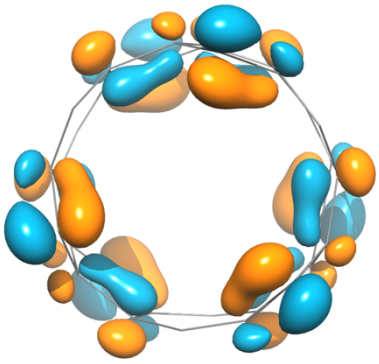
2 Frontier molecular orbitals of cyclacenes 6_n



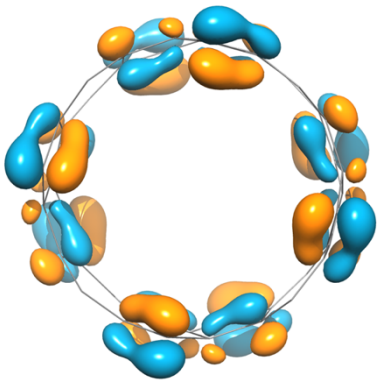
$\mathbf{6}_3$ HOMO



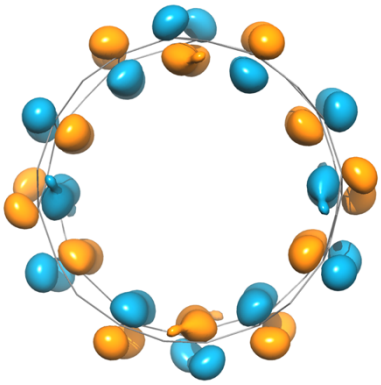
$\mathbf{6}_3$ HOMO



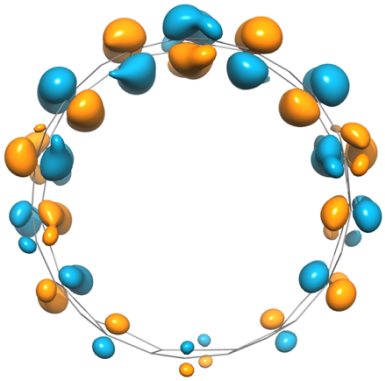
$\mathbf{6}_3$ LUMO



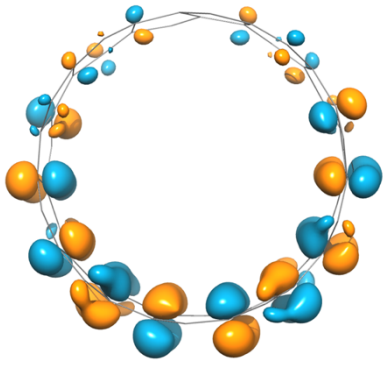
$\mathbf{6}_4$ HOMO



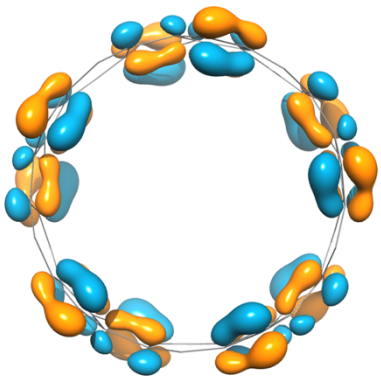
$\mathbf{6}_4$ LUMO



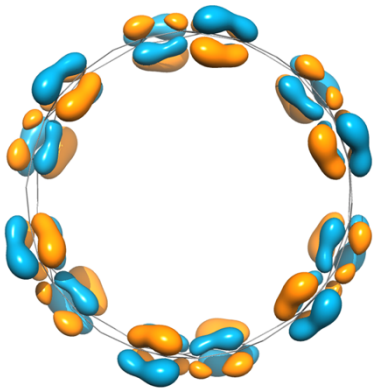
$\mathbf{6}_5$ HOMO



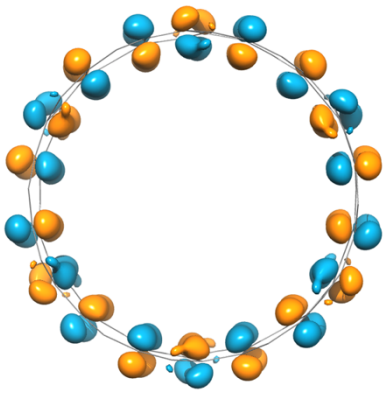
$\mathbf{6}_5$ HOMO



$\mathbf{6}_5$ LUMO



$\mathbf{6}_6$ HOMO



$\mathbf{6}_6$ LUMO

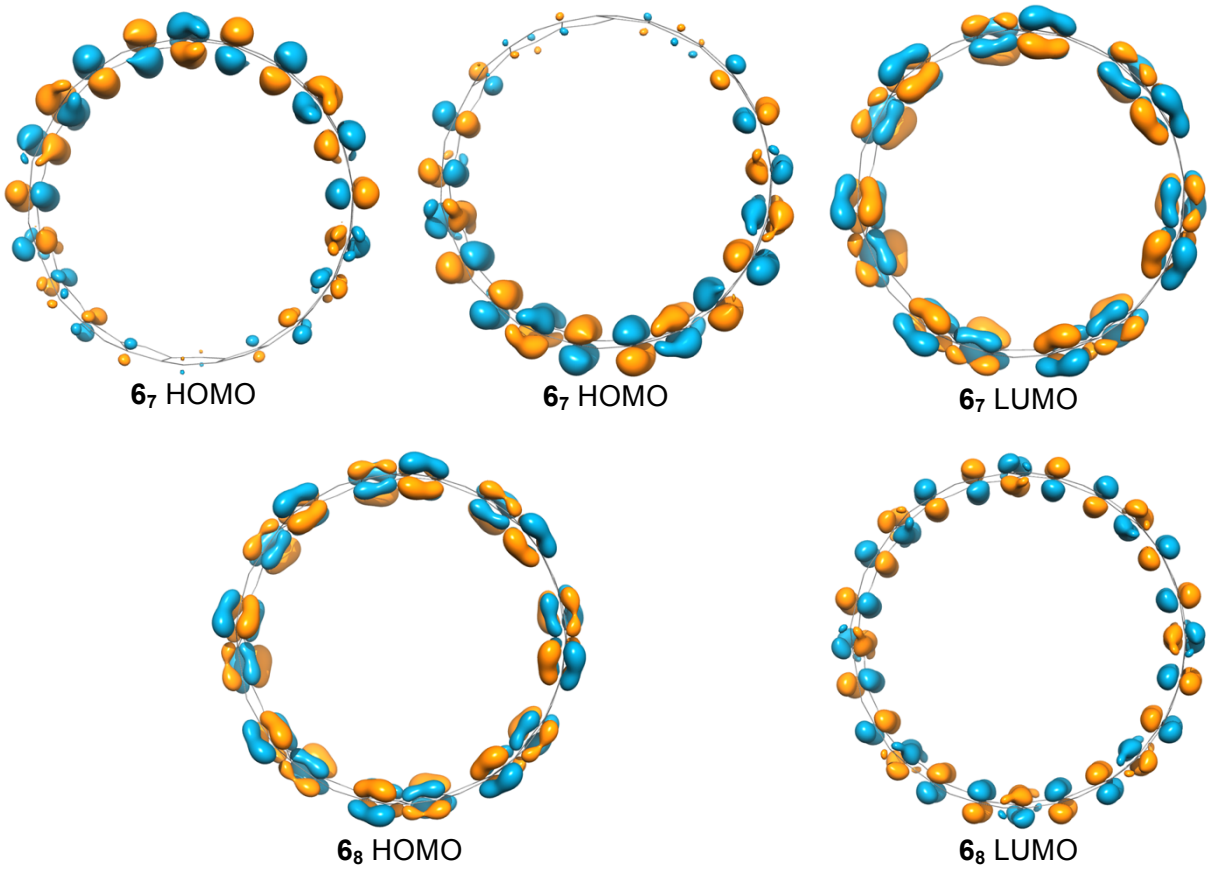


Figure S 7. Frontier molecular orbitals of $[5.5.6]_n$cyclacenes $\mathbf{6}_n$ (BP86-D3/def2-QZVP).

Table S 2. Natural occupation numbers of the four highest occupied and four lowest unoccupied orbitals of $[5.5.6]_n$cyclacenes 6_n calculated using CASSCF(8,8)/def2-SVP based on TPSS-D3/def2-TZVP-optimized geometries.

n	3	4	5
LUMO+3	0.07	0.03	0.07
LUMO+2	0.08	0.10	0.07
LUMO+1	0.07	0.10	0.07
LUMO	0.10	0.20	0.08
HOMO	1.91	1.83	1.92
HOMO-1	1.92	1.94	1.93
HOMO-2	1.92	1.90	1.93
HOMO-3	1.93	1.90	1.93

3 Energies

Open-shell singlet energies were obtained through optimization of the first singlet excited states using TDDFT.

3.1 Cyclacenes 6_n

Table S 3. Electronic energies of closed-shell singlets (CSS), open-shell singlets (OSS, from TDDFT), and triplets of [5.5.6]cyclacenes 6_n (in hartrees) calculated using BP86-D3/def2-TZVP.

n	3	4	5	6	7	8
CSS	-1150.70516	-1534.42933	-1918.10211	-2301.78005	-2685.44016	-3069.10212
OSS	-1150.68463	-1534.39844	-1918.09051	-2301.75964	-2685.43171	-3069.08762
T	-1150.68693	-1534.42054	-1918.09420	-2301.77610	-2685.43466	-3069.10083

Table S 4. Electronic energies of closed-shell singlets of [5.5.6]cyclacenes 6_n, benzene, dibenzo[*a*,*e*]pentalene, biphenyl, terphenyl, and [6]cycloparaphenylene (in hartrees) calculated using TPSS-D3/def2-TZVP (optimized in C_1 symmetry).

3	4	5	6	7	8
-1150.83842	-1534.59734	-1918.33288	-2302.05290	-2685.76624	-3069.47476
Benzene	Dibenzo[*a*,*e*]pentalene		Biphenyl	Terphenyl	[6]CPP
-232.38800	-616.08116		-463.58587	-694.78421	-1387.05353

Table S 5. Electronic Energies of closed-shell singlets (CSS) and open-shell singlets (OSS) of [5.5.6]cyclacenes 6_n (in hartrees) calculated using CASPT2/def2-SVP//TPSS-D3/def2-TZVP.

n	3	4	5
CSS	-1145.70777	-1527.80522	-1909.77651
OSS	-1145.69928	-1527.78228	-

Table S 6. Electronic Energies of closed-shell singlets of [5.5.6]cyclacenes 6_n (in hartrees) calculated using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
BHLYP	-1149.92254	-1533.35710	-1916.83981	-2300.18735	-2683.68847	-3066.99483
PW6B95	-1152.16501	-1536.36169	-1920.55771	-2304.68648	-2688.88612	-3072.98482
PBE0	-1149.28375	-1532.52331	-1915.75465	-2298.92800	-2682.16123	-3065.30639
B3LYP	-1149.98158	-1533.45519	-1916.91372	-2300.32542	-2683.78248	-3067.16859
B2PLYP	-1149.94614	-1533.42964	-1916.85144	-2300.29034	-2683.69453	-3067.12093
TPSS	-1150.89547	-1534.68586	-1918.42707	-2302.16855	-2685.89748	-3069.62186
BP86	-1150.77619	-1534.52381	-1918.21963	-2301.92075	-2685.60383	-3069.28894

Table S 7. Electronic energies of triplets of [5.5.6]cyclacenes 6_n (in hartrees) calculated using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
BHLYP	-1149.87074	-1533.37353	-1916.77668	-2300.22519	-2683.60287	-3067.04729
PW6B95	-1152.12463	-1536.36432	-1920.51957	-2304.70318	-2688.83746	-3073.01081
PBE0	-1149.24699	-1532.52559	-1915.72166	-2298.94293	-2682.11903	-3065.32970
B3LYP	-1149.94595	-1533.45501	-1916.88494	-2300.33624	-2683.74697	-3067.18670
B2PLYP	-1149.91508	-1533.40935	-1916.83719	-2300.26801	-2683.68165	-3067.09477
TPSS	-1150.86939	-1534.67800	-1918.41712	-2302.16604	-2685.88921	-3069.62233
BP86	-1150.75134	-1534.51495	-1918.21183	-2301.91673	-2685.59843	-3069.28760

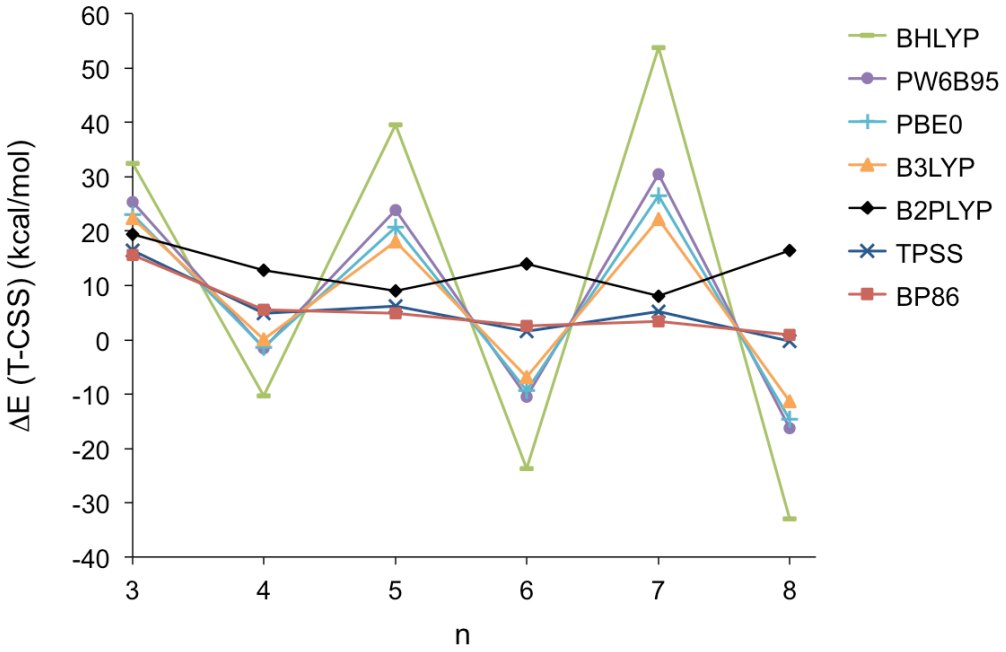


Figure S 8. Energy differences between triplet (T) and closed-shell singlet (CSS) ground states of $[5.5.6]_n$cyclacenes (**6_n**) calculated using different density functionals (*functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP).

Table S 8. Energy differences (kcal/mol) between triplets and closed-shell singlets (in kcal/mol) of $[5.5.6]_n$cyclacenes 6_n using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
BHLYP	32.5	-10.3	39.6	-23.7	53.7	-32.9
PW6B95	25.3	-1.6	23.9	-10.5	30.5	-16.3
PBE0	23.1	-1.4	20.7	-9.4	26.5	-14.6
B3LYP	22.4	0.1	18.1	-6.8	22.3	-11.4
B2PLYP	19.5	12.7	8.9	14.0	8.1	16.4
TPSS	16.4	4.9	6.2	1.6	5.2	-0.3
BP86	15.6	5.6	4.9	2.5	3.4	0.8

3.2 Methyl-substituted cyclacenes 10_n

Table S 9. Electronic energies of closed-shell singlets of methyl-substituted $[5.5.6]_n$cyclacenes 10_n (in hartrees) calculated using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	-1388.51335	-1851.47898	-2314.46034	-2777.35852	-3240.34773	-3703.28240
B3LYP	-1385.88283	-1847.97660	-2310.07246	-2772.10292	-3234.20215	-3696.25902
BP86	-1386.85020	-1849.27354	-2311.66343	-2774.04091	-3236.42170	-3698.79337

Table S 10. Electronic energies of triplets of methyl-substituted $[5.5.6]_n$cyclacenes 10_n (in hartrees) calculated using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	-1388.47575	-1851.48442	-2314.42033	-2777.37799	-3240.30295	-3703.24406
B3LYP	-1385.85165	-1847.97951	-2310.04025	-2772.11820	-3234.16709	-3696.22974
BP86	-1386.83430	-1849.26799	-2311.65081	-2774.04062	-3236.40951	-3698.78565

Table S 11. Energy differences (kcal/mol) between triplets and closed-shell singlets (in kcal/mol) of methyl-substituted $[5.5.6]_n$cyclacenes 10_n using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	23.6	-3.4	25.1	-12.2	28.1	24.1
B3LYP	19.6	-1.8	20.2	-9.6	22.0	18.4
BP86	10.0	3.5	7.9	0.2	7.6	4.8

Table S 12. Electronic energies of closed-shell singlets (CSS) and open-shell singlets (OSS, from TDDFT) of methyl-substituted $[5.5.6]_n$cyclacenes 10_n (in hartrees) and energy differences (in kcal/mol) calculated using BP86-D3/def2-TZVP.

n	3	4	5	6	7	8
CSS	-1386.76008	-1849.15354	-2311.51373	-2773.86171	-3236.21289	-3698.55503
OSS	-1386.73753	-1849.13716	-2311.49683	-2773.84424	-3236.19750	-3698.54416
OSS-CSS	9.5	10.3	6.6	9.8	7.0	5.4

3.3 Alkynyl-substituted cyclacenes 11_n

Table S 13. Electronic energies of closed-shell singlets of alkynyl-substituted $[5.5.6]_n$cyclacenes 11_n (in hartrees) calculated using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	-1609.90453	-2146.68058	-2683.44663	-3220.15716	-3756.92677	-4293.60919
B3LYP	-1606.87085	-2142.63995	-2678.38599	-3214.09464	-3749.83910	-4285.52406
BP86	-1607.95196	-2144.08526	-2680.16568	-3216.25413	-3752.32296	-4288.39669

Table S 14. Electronic energies of triplets of alkynyl-substituted $[5.5.6]_n$cyclacenes 11_n (in hartrees) calculated using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	-1609.87215	-2146.68196	-2683.41413	-3220.17175	-3756.88507	-4293.63200
B3LYP	-1606.84249	-2142.63892	-2678.36182	-3214.10387	-3749.80928	-4285.53969
BP86	-1607.93214	-2144.07706	-2680.15917	-3216.25036	-3752.31916	-4288.39511

Table S 15. Energy differences (kcal/mol) between triplets and closed-shell singlets (in kcal/mol) of alkynyl-substituted $[5.5.6]_n$cyclacenes 11_n using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	20.3	-0.9	20.4	-9.2	26.2	-14.3
B3LYP	17.8	0.6	15.2	-5.8	18.7	-9.8
BP86	12.4	5.1	4.1	2.4	2.4	1.0

Table S 16. Electronic energies of closed-shell singlets (CSS) and open-shell singlets (OSS, from TDDFT) of alkynyl-substituted $[5.5.6]_n$cyclacenes 11_n (in hartrees) and energy differences (in kcal/mol) calculated using BP86-D3/def2-TZVP.

n	3	4	5	6	7	8
CSS	-1607.85419	-2143.95488	-2680.00322	-3216.05956	-3752.09639	-4288.13803
OSS	-1607.83932	-2143.93682	-2679.99463	-3216.04237	-3752.09049	-4288.12577
OSS-CSS	9.3	11.3	5.4	10.8	3.7	7.7

3.4 Thiomethyl-substituted cyclacenes 12_n

Table S 17. Electronic energies of closed-shell singlets of thiomethyl-substituted $[5.5.6]_n$cyclacenes 12_n (in hartrees) calculated using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	-3779.61797	-5039.62652	-6299.61049	-7559.57999	-8819.54215	-10079.49886
B3LYP	-3774.78544	-5033.18167	-6291.55382	-7549.91155	-8808.26250	-10066.60892
BP86	-3776.34951	-5035.25183	-6294.13522	-7553.00431	-8811.86788	-10070.72694

Table S 18. Electronic energies of triplets of thiomethyl-substituted $[5.5.6]_n$cyclacenes 12_n (in hartrees) calculated using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	-3779.58790	-5039.61299	-6299.56887	-7559.55666	-8819.49347	-10079.44760
B3LYP	-3774.75762	-5033.17144	-6291.51634	-7549.89352	-8808.21933	-10066.56358
BP86	-3776.32914	-5035.25034	-6294.11194	-7553.00035	-8811.84318	-10070.70168

Table S 19. Energy differences (kcal/mol) between triplets and closed-shell singlets (in kcal/mol) of thiomethyl-substituted $[5.5.6]_n$cyclacenes 12_n using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	18.9	8.5	26.1	14.6	30.5	32.2
B3LYP	17.5	6.4	23.5	11.3	27.1	28.5
BP86	12.8	0.9	14.6	2.5	15.5	15.9

Table S 20. Electronic energies of closed-shell singlets (CSS) and open-shell singlets (OSS, from TDDFT) of thiomethyl-substituted $[5.5.6]_n$cyclacenes 12_n (in hartrees) and energy differences (in kcal/mol) calculated using BP86-D3/def2-TZVP.

n	3	4	5	6	7	8
CSS	-3776.35020	-5035.25266	-6294.13621	-7553.00553	-8811.86926	-10070.72850
OSS	-3776.32218	-5035.24330	-6294.11956	-7552.99818	-8811.85639	-10070.72084
OSS-CSS	16.9	5.9	10.4	4.6	8.1	4.8

3.5 Phenyl-substituted cyclacenes 13_n

Table S 21. Electronic energies of closed-shell singlets of phenyl-substituted $[5.5.6]_n$cyclacenes 13_n (in hartrees) calculated using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	-2540.86299	-3387.96172	-4235.06351	-5082.08604	-5929.18350	-6776.23259
B3LYP	-2536.06183	-3381.56867	-4227.06026	-5072.48872	-5917.97093	-6763.41734
BP86	-2537.78213	-3383.86470	-4229.89995	-5075.91968	-5921.93597	-6767.94547

Table S 22. Electronic energies of triplets of phenyl-substituted $[5.5.6]_n$cyclacenes 13_n (in hartrees) calculated using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	-2540.84484	-3387.96648	-4235.02892	-5082.10510	-5929.14596	-6776.20152
B3LYP	-2536.04641	-3381.57111	-4227.03294	-5072.50280	-5917.94181	-6763.39432
BP86	-2537.77177	-3383.85951	-4229.89041	-5075.92025	-5921.92767	-6767.94193

Table S 23. Energy differences (kcal/mol) between triplets and closed-shell singlets (in kcal/mol) of phenyl-substituted $[5.5.6]_n$cyclacenes 13_n using *functional*-D3/def2-QZVP//TPSS-D3/def2-TZVP.

n	3	4	5	6	7	8
PW6B95	11.4	-3.0	21.7	-12.0	23.6	19.5
B3LYP	9.7	-1.5	17.1	-8.8	18.3	14.4
BP86	6.5	3.3	6.0	-0.4	5.2	2.2

Table S 24. Electronic energies of closed-shell singlets (CSS) and open-shell singlets (OSS, from TDDFT) of phenyl-substituted $[5.5.6]_n$cyclacenes 13_n (in hartrees) and energy differences (in kcal/mol) calculated using BP86-D3/def2-TZVP.

n	3	4	5	6	7	8
CSS	-2537.79130	-3383.86698	-4229.90271	-5075.92273	-5921.93876	-6767.94817
OSS	-	-3383.85232	-4229.88976	-5075.90897	-5921.92782	-6767.94204
OSS-CSS	-	8.1	5.3	7.5	4.7	2.6

4 Coordinates

4.1 Calculated coordinates of dibenzopentalene (8) and benzene (9)

Table S 25. Coordinates of the calculated structure of dibenzopentalene (8) (TPSS-D3/def2-TZVP).

	x	y	z
C	-2.053434	-2.375364	0
C	-1.888755	-3.771406	0
C	-0.926582	-1.567651	0
C	0.380132	-2.151211	0
C	0.532065	-3.531901	0
C	-0.61675	-4.340459	0
C	1.382767	-1.072755	0
C	-0.724738	-0.120659	0
C	0.724758	0.120698	0
C	-1.382752	1.0728	0
C	0.926603	1.567681	0
C	-0.380171	2.151227	0
C	2.053411	2.375404	0
C	-0.53205	3.531891	0
C	1.888747	3.771466	0
C	0.616761	4.340496	0
H	3.050428	1.943168	0
H	2.764849	4.413548	0
H	0.511568	5.421606	0
H	-1.520347	3.984371	0
H	-2.454923	1.238345	0
H	2.454901	-1.238567	0
H	-3.05047	-1.94318	0
H	-2.764787	-4.41359	0
H	-0.511582	-5.421567	0
H	1.52035	-3.984394	0

Table S 26. Coordinates of the calculated structure of benzene (9) (TPSS-D3/def2-TZVP).

	x	y	z
C	-1.208825	0.697902	0
C	-1.208825	-0.697902	0
C	0	1.395785	0
C	1.208825	0.697902	0
C	1.208825	-0.697902	0
C	0	-1.395785	0
H	2.149818	1.241208	0
H	0	2.482355	0
H	-2.149818	1.241208	0
H	-2.149818	-1.241208	0
H	0	-2.482355	0
H	2.149818	-1.241208	0

4.2 Calculated coordinates of biphenyl, terphenyl, and [6]cycloparaphenylene

Table S 27. Coordinates of the calculated structure of biphenyl (TPSS-D3/def2-TZVP).

	x	y	z
C	1.4614295	1.145984	-0.372233
C	0.7400479	0.0000604	-0.0000961
C	1.4612834	-1.1459137	0.3721561
C	2.8542166	-1.1462188	0.3729175
C	3.5576397	-0.0000573	0.0001038
H	3.3922439	2.0409792	-0.6738082
H	0.922599	2.0347461	-0.6888266
H	0.922345	-2.0346071	0.6887589
H	3.3919685	-2.0411239	0.6738778
H	4.6438419	-0.000082	0.0002195
C	-0.7400479	0.0000948	-0.0002235
C	-1.4613414	-1.1458709	-0.3723901
C	-1.4613715	1.1460296	0.3719904
C	-2.8542747	-1.1462197	-0.3727977
H	-0.9224548	-2.0345199	-0.6892056

C	-2.8543034	1.1461554	0.3729567
H	-0.9224892	2.0348361	0.688371
C	-3.5576396	-0.0000921	0.0002306
H	-3.3920755	-2.0411336	-0.6736443
H	-3.3921368	2.0409726	0.6740323
H	-4.6438419	-0.0001726	0.0004561

Table S 28. Coordinates of the calculated structure of terphenyl (TPSS-D3/def2-TZVP).

	x	y	z
C	5.0151187	-1.184814	0.2211865
C	3.6223815	-1.1845754	0.2208481
C	2.9002884	-0.0000358	0.0000462
C	3.6222845	1.1845415	-0.2208711
C	5.0150213	1.1848675	-0.2213557
C	5.7185747	0.0000409	-0.0001636
H	5.5529552	-2.1110709	0.4038843
H	3.0841632	-2.1069842	0.4206424
H	3.0839882	2.1068999	-0.4206876
H	5.5527811	2.1111822	-0.4039865
H	6.8047508	0.000057	-0.000317
C	1.4221026	-0.0000741	0.0001709
C	0.6948344	1.0973088	0.4892171
C	0.6948101	-1.0974497	-0.4888556
C	-0.6948215	1.0973957	0.4890493
H	1.2278092	1.9460654	0.9087005
C	-0.6948458	-1.0973893	-0.4889496
H	1.2277759	-1.9463732	-0.9080128
C	-1.4221067	0.0000195	0.0000311
H	-1.2277868	1.9463716	0.9080928
H	-1.2278197	-1.9462244	-0.9082674
C	-2.9002884	0.000029	0.0000487
C	-3.6223206	1.1845674	-0.2209205
C	-3.6223331	-1.1845066	0.2209927
C	-5.0150573	1.1848324	-0.2214854
H	-3.0840577	2.1069647	-0.4206321
C	-5.0150697	-1.1848071	0.2212897
H	-3.0840868	-2.106853	0.4209833
C	-5.7185707	0.0000133	-0.0001143
H	-5.5528509	2.11107	-0.404413
H	-5.552875	-2.111091	0.4039479
H	-6.804749	0.0000219	-0.0000995

Table S 29. Coordinates of the calculated structure of [6]CPP (TPSS-D3/def2-TZVP).

	x	y	z
C	4.2291503	1.4118832	1.0472527
C	3.0314025	2.3536372	-1.2635578
H	3.6233798	0.5150678	-2.1619621
C	3.5890469	2.6461127	1.046138
H	4.6995792	1.065698	1.9638365
C	2.8376849	3.0713558	-0.0686943
H	2.5095675	2.6630279	-2.1639521
H	3.5763528	3.231385	1.9618828
C	4.0853751	-1.7877089	-1.0480479
C	3.5558268	-1.448279	1.2618323
C	3.337216	-2.9595931	-1.0467431
H	4.5846686	-1.4850682	-1.9647631
C	2.8087799	-2.6184075	1.263133
H	3.5636148	-0.8404537	2.1614629
C	2.5508929	-3.3156477	0.0682434
H	3.271844	-3.5413513	-1.9625155
H	2.261613	-2.8797887	2.1637272
C	1.2411752	-3.9955606	-0.0613302
C	0.4965076	-4.4314844	1.0538811
C	0.5234734	-3.8072252	-1.2570941
C	-0.8923923	-4.3684126	1.054093
H	1.0091036	-4.7112511	1.9705312
C	-0.8633609	-3.7442508	-1.2568977
H	1.0528586	-3.511884	-2.157833
C	-1.5948225	-3.8668331	-0.0609412
H	-1.4279627	-4.6005817	1.9709146
H	-1.3640748	-3.4020815	-2.1574548
C	-2.8376883	-3.0713515	0.0688739
C	-3.5891567	-2.6462285	-1.0459315
C	-3.031289	-2.3535036	1.2636805
C	-4.2292309	-1.4119832	-1.0471312
H	-3.5765818	-3.2316212	-1.9616014
C	-3.6703436	-1.1210874	1.2624657
H	-2.509348	-2.6627891	2.1640495
C	-4.1445889	-0.5511271	0.066387

H	-4.6997024	-1.0658759	-1.9637229
H	-3.6232296	-0.5148511	2.16195
C	-4.078625	0.9228388	-0.0657097
C	-4.0855051	1.7878169	1.0478511
C	-3.5556757	1.4481494	-1.2619318
C	-3.3373568	2.9597086	1.0465113
H	-4.5849035	1.4852662	1.9645392
C	-2.8086249	2.6182755	-1.2632628
H	-3.5633592	0.8402243	-2.1614959
C	-2.5508923	3.3156435	-0.0684125
H	-3.2721144	3.5415767	1.9622238
H	-2.2613317	2.8795597	-2.1638088
C	-1.2411834	3.9955567	0.0612571
C	-0.4964337	4.4315005	-1.0538914
C	-0.5235716	3.8072007	1.2570721
C	0.8924682	4.3684695	-1.0539826
H	-1.0089594	4.7112402	-1.9705895
C	0.8632614	3.7441954	1.2569748
H	-1.0530321	3.5118702	2.1577709
C	1.5948141	3.8668353	0.0610796
H	1.4281145	4.6007289	-1.9707368
H	1.3638986	3.4019547	2.157547
C	4.078633	-0.9228439	0.0656036
C	4.1445966	0.5511337	-0.0663566

4.3 Calculated coordinates of cyclacenes 6_n

Below can be found coordinates for the calculated structures of $[5.5.6]_n$cyclacenes **6_n** as singlets and triplets at the TPSS-D3/def2-TZVP level of theory and of the open-shell singlets calculated using TDDFT at the BP86-D3/def2-TZVP level of theory, optimized in point group D_n.

Table S 30. Coordinates of the calculated structure of 6_3 (n=3) (TPSS-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.932415	2.04453	-1.610078
C	-2.757746	1.049521	-0.909338
C	-2.710881	1.312623	0.495595
C	-1.761305	2.428403	0.668451
C	-1.222406	2.739537	-0.668451
C	-2.885226	-0.258996	-1.404528
C	-2.710881	-1.312623	-0.495595
C	-2.757746	-1.049521	0.909338
C	-2.885226	0.258996	1.404528
C	-1.761305	-2.428403	-0.668451
C	-1.222406	-2.739537	0.668451
C	-1.932415	-2.04453	1.610078
C	0.218676	-3.004004	0.495595
C	0.469962	-2.913039	-0.909338
C	-0.804408	-2.695786	-1.610078
C	1.66691	-2.369181	-1.404528
C	2.492206	-1.69138	-0.495595
C	2.287785	-1.863518	0.909338
C	1.218316	-2.628177	1.404528
C	2.983711	-0.311134	-0.668451
C	2.983711	0.311134	0.668451
C	2.736823	-0.651255	1.610078
C	2.492206	1.69138	0.495595
C	2.287785	1.863518	-0.909338
C	2.736823	0.651255	-1.610078
C	1.218316	2.628177	-1.404528
C	0.218676	3.004004	-0.495595
C	0.469962	2.913039	0.909338
C	1.66691	2.369181	1.404528
C	-0.804408	2.695786	1.610078
H	0.997219	2.59431	-2.468826
H	1.748129	2.160772	2.468826
H	2.584958	0.496469	-2.673196
H	2.584958	-0.496469	2.673196
H	1.748129	-2.160772	-2.468826
H	0.997219	-2.59431	2.468826
H	-0.862524	-2.486874	-2.673196
H	-1.722434	-1.990405	2.673196
H	-2.745348	-0.433538	-2.468826
H	-2.745348	0.433538	2.468826
H	-1.722434	1.990405	-2.673196
H	-0.862524	2.486874	2.673196

Table S 31. Coordinates of the calculated structure of the triplet of 6_3 (n=3) (TPSS-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.942043	2.034174	-1.626686
C	-2.729946	1.043872	-0.930119
C	-2.677356	1.311167	0.500913
C	-1.756419	2.421778	0.670687
C	-1.219112	2.731992	-0.670687
C	-2.867691	-0.265985	-1.415799
C	-2.677356	-1.311167	-0.500913
C	-2.729946	-1.043872	0.930119
C	-2.867691	0.265985	1.415799
C	-1.756419	-2.421778	-0.670687
C	-1.219112	-2.731992	0.670687
C	-1.942043	-2.034174	1.626686
C	0.203175	-2.974242	0.500913
C	0.460953	-2.886139	-0.930119
C	-0.790625	-2.698946	-1.626686
C	1.664195	-2.350501	-1.415799
C	2.474182	-1.663075	-0.500913
C	2.268993	-1.842267	0.930119
C	1.203496	-2.616486	1.415799
C	2.975531	-0.310215	-0.670687
C	2.975531	0.310215	0.670687
C	2.732668	-0.664772	1.626686
C	2.474182	1.663075	0.500913
C	2.268993	1.842267	-0.930119
C	2.732668	0.664772	-1.626686
C	1.203496	2.616486	-1.415799
C	0.203175	2.974242	-0.500913
C	0.460953	2.886139	0.930119
C	1.664195	2.350501	1.415799
C	-0.790625	2.698946	1.626686
H	0.982416	2.59802	-2.480207
H	1.758743	2.149807	2.480207
H	2.596799	0.508889	-2.690851
H	2.596799	-0.508889	2.690851
H	1.758743	-2.149807	-2.480207
H	0.982416	-2.59802	2.480207
H	-0.857688	-2.503339	-2.690851
H	-1.739111	-1.994449	2.690851
H	-2.741159	-0.448212	-2.480207
H	-2.741159	0.448212	2.480207
H	-1.739111	1.994449	-2.690851
H	-0.857688	2.503339	2.690851

Table S 32. Coordinates of the calculated structure of the open-shell singlet of 6_3 (n=3) (TDDFT, BP86-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.9422232	2.0336086	-1.631175
C	-2.7270135	1.0428651	-0.934948
C	-2.6746447	1.3136186	0.5002394
C	-1.7618009	2.4286433	0.6712339
C	-1.2223664	2.740086	-0.6712339
C	-2.867071	-0.269503	-1.4175548
C	-2.6746447	-1.3136186	-0.5002394
C	-2.7270135	-1.0428651	0.934948
C	-2.867071	0.269503	1.4175548
C	-1.7618009	-2.4286433	-0.6712339
C	-1.2223664	-2.740086	0.6712339
C	-1.9422232	-2.0336086	1.631175
C	0.1996952	-2.9731195	0.5002394
C	0.460359	-2.8830955	-0.934948
C	-0.7900451	-2.6988189	-1.631175
C	1.666932	-2.3482048	-1.4175548
C	2.4749494	-1.6595009	-0.5002394
C	2.2666544	-1.8402304	0.934948
C	1.200139	-2.6177078	1.4175548
C	2.9841673	-0.3114426	-0.6712339
C	2.9841673	0.3114426	0.6712339
C	2.7322683	-0.6652103	1.631175
C	2.4749494	1.6595009	0.5002394
C	2.2666544	1.8402304	-0.934948
C	2.7322683	0.6652103	-1.631175
C	1.200139	2.6177078	-1.4175548
C	0.1996952	2.9731195	-0.5002394
C	0.460359	2.8830955	0.934948
C	1.666932	2.3482048	1.4175548
C	-0.7900451	2.6988189	1.631175
H	0.9758322	2.6005661	-2.4857986
H	1.7642402	2.1453785	2.4857986
H	2.5917849	0.5052445	-2.6983853

H	2.5917849	-0.5052445	2.6983853
H	1.7642402	-2.1453785	-2.4857986
H	0.9758322	-2.6005661	2.4857986
H	-0.8583379	-2.4971738	-2.6983853
H	-1.733447	-1.9919293	2.6983853
H	-2.7400724	-0.4551876	-2.4857986
H	-2.7400724	0.4551876	2.4857986
H	-1.733447	1.9919293	-2.6983853
H	-0.8583379	2.4971738	2.6983853

Table S 33. Coordinates of the calculated structure of 6_4 (n=4) (TPSS-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.710793	-1.045151	-0.942943
C	3.672194	-1.310545	0.511263
C	3.809126	0.264746	-1.426758
C	3.672194	1.310545	-0.511263
C	3.710793	1.045151	0.942943
C	3.809126	-0.264746	1.426758
C	3.120495	-2.141914	-1.632186
C	2.982268	-2.548813	0.671689
C	2.548813	-2.982268	-0.671689
C	2.141914	-3.120495	1.632186
C	1.310545	-3.672194	-0.511263
C	1.045151	-3.710793	0.942943
C	0.264746	-3.809126	-1.426758
C	-0.264746	-3.809126	1.426758
C	-1.045151	-3.710793	-0.942943
C	-1.310545	-3.672194	0.511263
C	-2.548813	-2.982268	0.671689
C	-2.141914	-3.120495	-1.632186
C	-2.982268	-2.548813	-0.671689
C	-3.120495	-2.141914	1.632186
C	-3.672194	-1.310545	-0.511263
C	-3.710793	-1.045151	0.942943
C	-3.809126	-0.264746	-1.426758
C	-3.809126	0.264746	1.426758
C	-3.672194	1.310545	0.511263
C	-3.710793	1.045151	-0.942943
C	-3.120495	2.141914	-1.632186
C	-2.982268	2.548813	0.671689
C	-2.548813	2.982268	-0.671689
C	-2.141914	3.120495	1.632186
C	-1.045151	3.710793	0.942943
C	-1.310545	3.672194	-0.511263
C	0.264746	3.809126	1.426758
C	-0.264746	3.809126	-1.426758
C	1.045151	3.710793	-0.942943
C	1.310545	3.672194	0.511263
C	2.141914	3.120495	-1.632186
C	2.548813	2.982268	0.671689
C	2.982268	2.548813	-0.671689
C	3.120495	2.141914	1.632186
H	-3.709004	0.453336	2.492921
H	-3.709004	-0.453336	-2.492921
H	-2.951115	-2.169123	2.702308
H	-2.169123	-2.951115	-2.702308
H	-0.453336	-3.709004	2.492921
H	0.453336	-3.709004	-2.492921
H	2.169123	-2.951115	2.702308
H	2.951115	-2.169123	-2.702308
H	3.709004	-0.453336	2.492921
H	3.709004	0.453336	-2.492921
H	2.951115	2.169123	2.702308
H	2.169123	2.951115	-2.702308
H	0.453336	3.709004	2.492921
H	-0.453336	3.709004	-2.492921
H	-2.169123	2.951115	2.702308
H	-2.951115	2.169123	-2.702308

Table S 34. Coordinates of the calculated structure of the triplet of 6_4 (n=4) (TPSS-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.737442	-1.049552	-0.924793
C	3.704715	-1.310522	0.505253
C	3.828114	0.259226	-1.41711
C	3.704715	1.310522	-0.505253
C	3.737442	1.049552	0.924793

C	3.828114	-0.259226	1.41711
C	3.118611	-2.155615	-1.619132
C	2.992284	-2.559889	0.669468
C	2.559889	-2.992284	-0.669468
C	2.155615	-3.118611	1.619132
C	1.310522	-3.704715	-0.505253
C	1.049552	-3.737442	0.924793
C	0.259226	-3.828114	-1.41711
C	-0.259226	-3.828114	1.41711
C	-1.049552	-3.737442	-0.924793
C	-1.310522	-3.704715	0.505253
C	-2.559889	-2.992284	0.669468
C	-2.155615	-3.118611	-1.619132
C	-2.992284	-2.559889	-0.669468
C	-3.118611	-2.155615	1.619132
C	-3.704715	-1.310522	-0.505253
C	-3.737442	-1.049552	0.924793
C	-3.828114	-0.259226	-1.41711
C	-3.828114	0.259226	1.41711
C	-3.704715	1.310522	0.505253
C	-3.737442	1.049552	-0.924793
C	-3.118611	2.155615	-1.619132
C	-2.992284	2.559889	0.669468
C	-2.559889	2.992284	-0.669468
C	-2.155615	3.118611	1.619132
C	-1.049552	3.737442	0.924793
C	-1.310522	3.704715	-0.505253
C	0.259226	3.828114	1.41711
C	-0.259226	3.828114	-1.41711
C	1.049552	3.737442	-0.924793
C	1.310522	3.704715	0.505253
C	2.155615	3.118611	-1.619132
C	2.559889	2.992284	0.669468
C	2.992284	2.559889	-0.669468
C	3.118611	2.155615	1.619132
H	-3.719858	0.441785	2.483581
H	-3.719858	-0.441785	-2.483581
H	-2.942199	-2.17327	2.688958
H	-2.17327	-2.942199	-2.688958
H	-0.441785	-3.719858	2.483581
H	0.441785	-3.719858	-2.483581
H	2.17327	-2.942199	2.688958
H	2.942199	-2.17327	-2.688958
H	3.719858	-0.441785	2.483581
H	3.719858	0.441785	-2.483581
H	2.942199	2.17327	2.688958
H	2.17327	2.942199	-2.688958
H	0.441785	3.719858	2.483581
H	-0.441785	3.719858	-2.483581
H	-2.17327	2.942199	2.688958
H	-2.942199	2.17327	-2.688958

Table S 35. Coordinates of the calculated structure of the open-shell singlet of 6_4 (n=4) (TDDFT, BP86-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.698064	-1.0445407	-0.9594924
C	3.660577	-1.3110701	0.5103479
C	3.8016701	0.2683811	-1.434054
C	3.660577	1.3110701	-0.5103479
C	3.698064	1.0445407	0.9594924
C	3.8016701	-0.2683811	1.434054
C	3.1260509	-2.1468951	-1.6491165
C	2.9855635	-2.5505081	0.6753781
C	2.5505081	-2.9855635	-0.6753781
C	2.1468951	-3.1260509	1.6491165
C	1.3110701	-3.660577	-0.5103479
C	1.0445407	-3.698064	0.9594924
C	0.2683811	-3.8016701	-1.434054
C	-0.2683811	-3.8016701	1.434054
C	-1.0445407	-3.698064	-0.9594924
C	-1.3110701	-3.660577	0.5103479
C	-2.5505081	-2.9855635	0.6753781
C	-2.1468951	-3.1260509	-1.6491165
C	-2.9855635	-2.5505081	-0.6753781
C	-3.1260509	-2.1468951	1.6491165
C	-3.660577	-1.3110701	-0.5103479
C	-3.698064	-1.0445407	0.9594924
C	-3.8016701	-0.2683811	-1.434054
C	-3.8016701	0.2683811	1.434054
C	-3.660577	1.3110701	0.5103479
C	-3.698064	1.0445407	-0.9594924
C	-3.1260509	2.1468951	-1.6491165
C	-2.9855635	2.5505081	0.6753781
C	-2.5505081	2.9855635	-0.6753781

C	-2.1468951	3.1260509	1.6491165
C	-1.0445407	3.698064	0.9594924
C	-1.3110701	3.660577	-0.5103479
C	0.2683811	3.8016701	1.434054
C	-0.2683811	3.8016701	-1.434054
C	1.0445407	3.698064	-0.9594924
C	1.3110701	3.660577	0.5103479
C	2.1468951	3.1260509	-1.6491165
C	2.5505081	2.9855635	0.6753781
C	2.9855635	2.5505081	-0.6753781
C	3.1260509	2.1468951	1.6491165
H	-3.7079734	0.4673615	2.5031581
H	-3.7079734	-0.4673615	-2.5031581
H	-2.9481592	-2.1766115	2.721243
H	-2.1766115	-2.9481592	-2.721243
H	-0.4673615	-3.7079734	2.5031581
H	0.4673615	-3.7079734	-2.5031581
H	2.1766115	-2.9481592	2.721243
H	2.9481592	-2.1766115	-2.721243
H	3.7079734	-0.4673615	2.5031581
H	3.7079734	0.4673615	-2.5031581
H	2.9481592	2.1766115	2.721243
H	2.1766115	2.9481592	-2.721243
H	0.4673615	3.7079734	2.5031581
H	-0.4673615	3.7079734	-2.5031581
H	-2.1766115	2.9481592	2.721243
H	-2.9481592	2.1766115	-2.721243

Table S 36. Coordinates of the calculated structure of 6_5 (n=5) (TPSS-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	-4.229459	-2.232017	1.606284
C	-4.754748	-1.055737	0.907386
C	-4.735855	-1.307479	-0.502677
C	-4.142158	-2.634503	-0.668492
C	-3.785559	-3.125321	0.668492
C	-4.819499	0.250486	1.410885
C	-4.735855	1.307479	0.502677
C	-4.754748	1.055737	-0.907386
C	-4.819499	-0.250486	-1.410885
C	-4.142158	2.634503	0.668492
C	-3.785559	3.125321	-0.668492
C	-4.229459	2.232017	-1.606284
C	-2.706946	4.100033	-0.502677
C	-2.473363	4.195793	0.907386
C	-3.429749	3.332723	1.606284
C	-1.25108	4.661021	1.410885
C	-0.219974	4.908099	0.502677
C	-0.465233	4.848274	-0.907386
C	-1.727534	4.506212	-1.410885
C	1.225564	4.753533	0.668492
C	1.802554	4.566058	-0.668492
C	0.8158	4.712185	-1.606284
C	3.06287	3.841438	-0.502677
C	3.226125	3.648879	0.907386
C	2.109757	4.291753	1.606284
C	4.046289	2.630183	1.410885
C	4.599904	1.725893	0.502677
C	4.467218	1.940662	-0.907386
C	3.751825	3.035478	-1.410885
C	4.733651	0.680273	-1.606284
C	4.899599	-0.303342	-0.668492
C	4.899599	0.303342	0.668492
C	4.599904	-1.725893	-0.502677
C	4.467218	-1.940662	0.907386
C	4.733651	-0.680273	1.606284
C	4.046289	-2.630183	-1.410885
C	3.226125	-3.648879	-0.907386
C	3.06287	-3.841438	0.502677
C	3.751825	-3.035478	1.410885
C	-3.429749	-3.332723	-1.606284
H	4.073663	2.429836	2.479306
H	3.569742	3.123423	-2.479306
H	1.957949	4.232077	2.679014
H	0.903538	4.574675	-2.679014
H	-1.05208	4.625144	2.479306
H	-1.867441	4.360218	-2.479306
H	-3.419905	3.169904	2.679014
H	-4.071566	2.272968	-2.679014
H	-4.723884	0.428661	2.479306
H	-4.723884	-0.428661	-2.479306
H	-4.071566	-2.272968	2.679014
H	-3.419905	-3.169904	-2.679014
H	3.569742	-3.123423	2.479306

H	4.073663	-2.429836	-2.479306
H	4.629984	-0.554336	2.679014
H	4.629984	0.554336	-2.679014
C	-2.706946	-4.100033	0.502677
C	-2.473363	-4.195793	-0.907386
C	-1.727534	-4.506212	1.410885
C	-1.25108	-4.661021	-1.410885
C	-0.219974	-4.908099	-0.502677
C	-0.465233	-4.848274	0.907386
C	0.8158	-4.712185	1.606284
C	1.225564	-4.753533	-0.668492
C	1.802554	-4.566058	0.668492
C	2.109757	-4.291753	-1.606284
H	0.903538	-4.574675	2.679014
H	1.957949	-4.232077	-2.679014
H	-1.867441	-4.360218	2.479306
H	-1.05208	-4.625144	-2.479306

Table S 37. Coordinates of the calculated structure of the triplet of 6_5 (n=5) (TPSS-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	4.219867	-2.201943	-1.624376
C	4.711405	-1.049706	-0.934313
C	4.685688	-1.309928	0.511367
C	4.118441	-2.61836	0.669963
C	3.762876	-3.107752	-0.669963
C	4.782684	0.261052	-1.424172
C	4.685688	1.309928	-0.511367
C	4.711405	1.049706	0.934313
C	4.782684	-0.261052	1.424172
C	4.118441	2.61836	-0.669963
C	3.762876	3.107752	0.669963
C	4.219867	2.201943	1.624376
C	2.693773	4.051564	0.511367
C	2.454234	4.156436	-0.934313
C	3.398183	3.332894	-1.624376
C	1.229655	4.629272	-1.424172
C	0.202142	4.861144	-0.511367
C	0.457575	4.805189	0.934313
C	1.726206	4.467933	1.424172
C	-1.21754	4.725987	-0.669963
C	-1.792855	4.539056	0.669963
C	-0.790162	4.69377	1.624376
C	-3.020845	3.813932	0.511367
C	-3.194605	3.618524	-0.934313
C	-2.119674	4.261785	-1.624376
C	-4.022715	2.599995	-1.424172
C	-4.560758	1.694424	-0.511367
C	-4.428608	1.920065	0.934313
C	-3.71583	3.022387	1.424172
C	-4.708214	0.698966	1.624376
C	-4.870922	-0.302461	0.669963
C	-4.870922	0.302461	-0.669963
C	-4.560758	-1.694424	0.511367
C	-4.428608	-1.920065	-0.934313
C	-4.708214	-0.698966	-1.624376
C	-4.022715	-2.599995	1.424172
C	-3.194605	-3.618524	0.934313
C	-3.020845	-3.813932	-0.511367
C	-3.71583	-3.022387	-1.424172
C	3.398183	-3.332894	1.624376
H	-4.062982	2.398456	-2.49196
H	-3.536597	3.122962	2.49196
H	-1.969807	4.217548	-2.697152
H	-0.885405	4.569892	2.697152
H	1.025537	4.605289	-2.49196
H	1.877244	4.328552	2.49196
H	3.402422	3.176692	-2.697152
H	4.07262	2.254244	2.697152
H	4.696798	0.447769	-2.49196
H	4.696798	-0.447769	2.49196
H	4.07262	-2.254244	-2.697152
H	3.402422	-3.176692	2.697152
H	-3.536597	-3.122962	-2.49196
H	-4.062982	-2.398456	2.49196
H	-4.61983	-0.570104	-2.697152
H	-4.61983	0.570104	2.697152
C	2.693773	-4.051564	-0.511367
C	2.454234	-4.156436	0.934313
C	1.726206	-4.467933	-1.424172
C	1.229655	-4.629272	1.424172
C	0.202142	-4.861144	0.511367
C	0.457575	-4.805189	-0.934313
C	-0.790162	-4.69377	-1.624376

C	-1.21754	-4.725987	0.669963
C	-1.792855	-4.539056	-0.669963
C	-2.119674	-4.261785	1.624376
H	-0.885405	-4.569892	-2.697152
H	-1.969807	-4.217548	2.697152
H	1.877244	-4.328552	-2.49196
H	1.025537	-4.605289	2.49196

Table S 38. Coordinates of the calculated structure of the open-shell singlet of 6_5 (n=5) (TDDFT, BP86-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	-4.22752	-2.2250661	1.6192447
C	-4.7367304	-1.0528657	0.9223667
C	-4.7170916	-1.3101361	-0.5045618
C	-4.1398858	-2.630968	-0.6702435
C	-3.7814944	-3.1242515	0.6702435
C	-4.808337	0.2551301	1.4184441
C	-4.7170916	1.3101361	0.5045618
C	-4.7367304	1.0528657	-0.9223667
C	-4.808337	-0.2551301	-1.4184441
C	-4.1398858	2.630968	0.6702435
C	-3.7814944	3.1242515	-0.6702435
C	-4.22752	2.2250661	-1.6192447
C	-2.703675	4.0813663	-0.5045618
C	-2.465065	4.1795449	0.9223667
C	-3.4225391	3.3330272	1.6192447
C	-1.2432147	4.6518397	1.4184441
C	-0.2116479	4.891075	0.5045618
C	-0.4623954	4.8302517	-0.9223667
C	-1.728501	4.4941607	-1.4184441
C	1.2229042	4.7502792	0.6702435
C	1.8027938	4.5618617	-0.6702435
C	0.8097881	4.7081937	-1.6192447
C	3.0461285	3.8325593	-0.5045618
C	3.2132365	3.6359666	0.9223667
C	2.1122745	4.2849902	1.6192447
C	4.039988	2.619865	1.4184441
C	4.586286	1.7127145	0.5045618
C	4.4509544	1.932394	-0.9223667
C	3.7400646	3.0326741	-1.4184441
C	4.7279965	0.6847576	-1.6192447
C	4.8956822	-0.304866	-0.6702435
C	4.8956822	0.304866	0.6702435
C	4.586286	-1.7127145	-0.5045618
C	4.4509544	-1.932394	0.9223667
C	4.7279965	-0.6847576	1.6192447
C	4.039988	-2.619865	-1.4184441
C	3.2132365	-3.6359666	-0.9223667
C	3.0461285	-3.8325593	0.5045618
C	3.7400646	-3.0326741	1.4184441
C	-3.4225391	-3.3330272	-1.6192447
H	4.0740588	2.4156635	2.49018
H	3.556386	3.1281791	-2.49018
H	1.9571735	4.2285399	2.6952962
H	0.9020867	4.5713583	-2.6952962
H	-1.0384791	4.6211413	2.49018
H	-1.8760914	4.3489845	-2.49018
H	-3.4167805	3.1680733	2.6952962
H	-4.06886	2.2705629	-2.6952962
H	-4.7158742	0.4403588	2.49018
H	-4.7158742	-0.4403588	-2.49018
H	-4.06886	-2.2705629	2.6952962
H	-3.4167805	-3.1680733	-2.6952962
H	3.556386	-3.1281791	2.49018
H	4.0740588	-2.4156635	-2.49018
H	4.6263803	-0.554692	2.6952962
H	4.6263803	0.554692	-2.6952962
C	-2.703675	-4.0813663	0.5045618
C	-2.465065	-4.1795449	-0.9223667
C	-1.728501	-4.4941607	1.4184441
C	-1.2432147	-4.6518397	-1.4184441
C	-0.2116479	-4.891075	-0.5045618
C	-0.4623954	-4.8302517	0.9223667
C	0.8097881	-4.7081937	1.6192447
C	1.2229042	-4.7502792	-0.6702435
C	1.8027938	-4.5618617	0.6702435
C	2.1122745	-4.2849902	-1.6192447
H	0.9020867	-4.5713583	2.6952962
H	1.9571735	-4.2285399	-2.6952962
H	-1.8760914	-4.3489845	2.49018
H	-1.0384791	-4.6211413	-2.49018

Table S 39. Coordinates of the calculated structure of 6_6 (n=6) (TPSS-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.277969	-2.235904	1.620761
C	-5.692969	-1.050926	0.93047
C	-5.673192	-1.309192	-0.512528
C	-5.197193	-2.65157	-0.66965
C	-4.894924	-3.175116	0.66965
C	-5.751909	0.257312	1.424088
C	-5.673192	1.309192	0.512528
C	-5.692969	1.050926	-0.93047
C	-5.751909	-0.257312	-1.424088
C	-5.197193	2.65157	0.66965
C	-4.894924	3.175116	-0.66965
C	-5.277969	2.235904	-1.620761
C	-3.970389	4.258532	-0.512528
C	-3.756613	4.404793	0.93047
C	-4.575334	3.452903	1.620761
C	-2.653116	5.109956	1.424088
C	-1.702802	5.567724	0.512528
C	-1.936356	5.455718	-0.93047
C	-3.098794	4.852643	-1.424088
C	-0.30227	5.826686	0.66965
C	0.30227	5.826686	-0.66965
C	-0.702635	5.688807	-1.620761
C	1.702802	5.567724	-0.512528
C	1.936356	5.455718	0.93047
C	0.702635	5.688807	1.620761
C	3.098794	4.852643	1.424088
C	3.970389	4.258532	0.512528
C	3.756613	4.404793	-0.93047
C	2.653116	5.109956	-1.424088
C	4.575334	3.452903	-1.620761
C	5.197193	2.65157	-0.66965
C	4.894924	3.175116	0.66965
C	5.673192	1.309192	-0.512528
C	5.692969	1.050926	0.93047
C	5.277969	2.235904	1.620761
C	5.751909	0.257312	-1.424088
C	5.692969	-1.050926	-0.93047
C	5.673192	-1.309192	0.512528
C	5.751909	-0.257312	1.424088
C	-4.575334	-3.452903	-1.620761
H	3.222407	4.69575	2.49296
H	2.455435	5.138561	-2.49296
H	0.580025	5.613438	2.695437
H	-0.580025	5.613438	-2.695437
H	-2.455435	5.138561	2.49296
H	-3.222407	4.69575	-2.49296
H	-4.571367	3.309035	2.695437
H	-5.151392	2.304403	-2.695437
H	-5.677842	0.442812	2.49296
H	-5.677842	-0.442812	-2.49296
H	-5.151392	-2.304403	2.695437
H	-4.571367	-3.309035	-2.695437
H	5.677842	-0.442812	2.49296
H	5.677842	0.442812	-2.49296
H	5.151392	2.304403	2.695437
H	4.571367	3.309035	-2.695437
C	-3.970389	-4.258532	0.512528
C	-3.756613	-4.404793	-0.93047
C	-3.098794	-4.852643	1.424088
C	-2.653116	-5.109956	-1.424088
C	-1.702802	-5.567724	-0.512528
C	-1.936356	-5.455718	0.93047
C	-0.702635	-5.688807	1.620761
C	-0.30227	-5.826686	-0.66965
C	0.30227	-5.826686	0.66965
C	5.277969	-2.235904	-1.620761
H	-0.580025	-5.613438	2.695437
H	5.151392	-2.304403	-2.695437
H	-3.222407	-4.69575	2.49296
H	-2.455435	-5.138561	-2.49296
C	1.702802	-5.567724	0.512528
C	0.702635	-5.688807	-1.620761
C	1.936356	-5.455718	-0.93047
C	2.653116	-5.109956	1.424088
C	3.756613	-4.404793	0.93047
C	3.098794	-4.852643	-1.424088
C	3.970389	-4.258532	-0.512528
H	0.580025	-5.613438	-2.695437
C	4.575334	-3.452903	1.620761
C	4.894924	-3.175116	-0.66965
C	5.197193	-2.65157	0.66965
H	2.455435	-5.138561	2.49296
H	3.222407	-4.69575	-2.49296

H	4.571367	-3.309035	2.695437

Table S 40. Coordinates of the calculated structure of the triplet of 6_6 (n=6) (TPSS-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.28742	-2.250625	1.612838
C	-5.71626	-1.05384	0.918182
C	-5.699342	-1.307562	-0.508328
C	-5.212219	-2.660752	-0.668952
C	-4.910388	-3.183538	0.668952
C	-5.771899	0.252879	1.417944
C	-5.699342	1.307562	0.508328
C	-5.71626	1.05384	-0.918182
C	-5.771899	-0.252879	-1.417944
C	-5.212219	2.660752	0.668952
C	-4.910388	3.183538	-0.668952
C	-5.28742	2.250625	-1.612838
C	-3.982053	4.281994	-0.508328
C	-3.770782	4.423506	0.918182
C	-4.592809	3.453728	1.612838
C	-2.66695	5.125051	1.417944
C	-1.717289	5.589556	0.508328
C	-1.945478	5.477346	-0.918182
C	-3.10495	4.872172	-1.417944
C	-0.301831	5.84429	0.668952
C	0.301831	5.84429	-0.668952
C	-0.694612	5.704353	-1.612838
C	1.717289	5.589556	-0.508328
C	1.945478	5.477346	0.918182
C	0.694612	5.704353	1.612838
C	3.10495	4.872172	1.417944
C	3.982053	4.281994	0.508328
C	3.770782	4.423506	-0.918182
C	2.66695	5.125051	-1.417944
C	4.592809	3.453728	-1.612838
C	5.212219	2.660752	-0.668952
C	4.910388	3.183538	0.668952
C	5.699342	1.307562	-0.508328
C	5.71626	1.05384	0.918182
C	5.28742	2.250625	1.612838
C	5.771899	0.252879	-1.417944
C	5.71626	-1.05384	-0.918182
C	5.699342	-1.307562	0.508328
C	5.771899	-0.252879	1.417944
C	-4.592809	-3.453728	-1.612838
H	3.223431	4.713823	2.487169
H	2.470575	5.148485	-2.487169
H	0.573542	5.622522	2.687608
H	-0.573542	5.622522	-2.687608
H	-2.470575	5.148485	2.487169
H	-3.223431	4.713823	-2.487169
H	-4.582476	3.307963	2.687608
H	-5.156018	2.314559	-2.687608
H	-5.694006	0.434662	2.487169
H	-5.694006	-0.434662	-2.487169
H	-5.156018	-2.314559	2.687608
H	-4.582476	-3.307963	-2.687608
H	5.694006	-0.434662	2.487169
H	5.694006	0.434662	-2.487169
H	5.156018	2.314559	2.687608
H	4.582476	3.307963	-2.687608
C	-3.982053	-4.281994	0.508328
C	-3.770782	-4.423506	-0.918182
C	-3.10495	-4.872172	1.417944
C	-2.66695	-5.125051	-1.417944
C	-1.717289	-5.589556	-0.508328
C	-1.945478	-5.477346	0.918182
C	-0.694612	-5.704353	1.612838
C	-0.301831	-5.84429	-0.668952
C	0.301831	-5.84429	0.668952
C	5.28742	-2.250625	-1.612838
H	-0.573542	-5.622522	2.687608
H	5.156018	-2.314559	-2.687608
H	-3.223431	-4.713823	2.487169
H	-2.470575	-5.148485	-2.487169
C	1.717289	-5.589556	0.508328
C	0.694612	-5.704353	-1.612838
C	1.945478	-5.477346	-0.918182
C	2.66695	-5.125051	1.417944
C	3.770782	-4.423506	0.918182
C	3.10495	-4.872172	-1.417944
C	3.982053	-4.281994	-0.508328
H	0.573542	-5.622522	-2.687608
C	4.592809	-3.453728	1.612838

C	4.910388	-3.183538	-0.668952
C	5.212219	-2.660752	0.668952
H	2.470575	-5.148485	2.487169
H	3.223431	-4.713823	-2.487169
H	4.582476	-3.307963	2.687608

Table S 41. Coordinates of the calculated structure of the open-shell singlet of 6_6 (n=6) (TDDFT, BP86-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.2777442	-2.2326849	1.6315843
C	-5.6843277	-1.0500952	0.9425551
C	-5.6638238	-1.3110404	-0.5140706
C	-5.1956262	-2.6493647	-0.6725599
C	-4.8922302	-3.1748619	0.6725599
C	-5.7454386	0.2604523	1.429983
C	-5.6638238	1.3110404	0.5140706
C	-5.6843277	1.0500952	-0.9425551
C	-5.7454386	-0.2604523	-1.429983
C	-5.1956262	2.6493647	0.6725599
C	-4.8922302	3.1748619	-0.6725599
C	-5.2777442	2.2326849	-1.6315843
C	-3.9673062	4.2494951	-0.5140706
C	-3.7515729	4.3977246	0.9425551
C	-4.5724339	3.4543181	1.6315843
C	-2.647161	5.1059219	1.429983
C	-1.6965176	5.5605355	0.5140706
C	-1.9327548	5.4478197	-0.9425551
C	-3.0982776	4.8454696	-1.429983
C	-0.3033959	5.8242266	0.6725599
C	0.3033959	5.8242266	-0.6725599
C	-0.7053102	5.687003	-1.6315843
C	1.6965176	5.5605355	-0.5140706
C	1.9327548	5.4478197	0.9425551
C	0.7053102	5.687003	1.6315843
C	3.0982776	4.8454696	1.429983
C	3.9673062	4.2494951	0.5140706
C	3.7515729	4.3977246	-0.9425551
C	2.647161	5.1059219	-1.429983
C	4.5724339	3.4543181	-1.6315843
C	5.1956262	2.6493647	-0.6725599
C	4.8922302	3.1748619	0.6725599
C	5.6638238	1.3110404	-0.5140706
C	5.6843277	1.0500952	0.9425551
C	5.2777442	2.2326849	1.6315843
C	5.7454386	0.2604523	-1.429983
C	5.6843277	-1.0500952	-0.9425551
C	5.6638238	-1.3110404	0.5140706
C	5.7454386	-0.2604523	1.429983
C	-4.5724339	-3.4543181	-1.6315843
H	3.2276041	4.6867378	2.5022662
H	2.4450319	5.1385561	-2.5022662
H	0.5791874	5.6108959	2.7095784
H	-0.5791874	5.6108959	-2.7095784
H	-2.4450319	5.1385561	2.5022662
H	-3.2276041	4.6867378	-2.5022662
H	-4.5695847	3.3070389	2.7095784
H	-5.1487721	2.303857	-2.7095784
H	-5.6726361	0.4518183	2.5022662
H	-5.6726361	-0.4518183	-2.5022662
H	-5.1487721	-2.303857	2.7095784
H	-4.5695847	-3.3070389	-2.7095784
H	5.6726361	-0.4518183	2.5022662
H	5.6726361	0.4518183	-2.5022662
H	5.1487721	2.303857	2.7095784
H	4.5695847	3.3070389	-2.7095784
C	-3.9673062	-4.2494951	0.5140706
C	-3.7515729	-4.3977246	-0.9425551
C	-3.0982776	-4.8454696	1.429983
C	-2.647161	-5.1059219	-1.429983
C	-1.6965176	-5.5605355	-0.5140706
C	-1.9327548	-5.4478197	0.9425551
C	-0.7053102	-5.687003	1.6315843
C	-0.3033959	-5.8242266	-0.6725599
C	0.3033959	-5.8242266	0.6725599
C	5.2777442	-2.2326849	-1.6315843
H	-0.5791874	-5.6108959	2.7095784
H	5.1487721	-2.303857	-2.7095784
H	-3.2276041	-4.6867378	2.5022662
H	-2.4450319	-5.1385561	-2.5022662
C	1.6965176	-5.5605355	0.5140706
C	0.7053102	-5.687003	-1.6315843
C	1.9327548	-5.4478197	-0.9425551
C	2.647161	-5.1059219	1.429983
C	3.7515729	-4.3977246	0.9425551

C	3.0982776	-4.8454696	-1.429983
C	3.9673062	-4.2494951	-0.5140706
H	0.5791874	-5.6108959	-2.7095784
C	4.5724339	-3.4543181	1.6315843
C	4.8922302	-3.1748619	-0.6725599
C	5.1956262	-2.6493647	0.6725599
H	2.4450319	-5.1385561	2.5022662
H	3.2276041	-4.6867378	-2.5022662
H	4.5695847	-3.3070389	2.7095784

Table S 42. Coordinates of the calculated structure of 6_7 (n=7) (TPSS-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.82614	-0.300825	-0.668826
C	6.61094	-1.735613	-0.505373
C	6.51408	-1.963389	0.906161
C	6.704096	-0.690257	1.60526
C	6.82614	0.300825	0.668826
C	6.202455	-2.712522	-1.413129
C	5.596501	-3.86876	-0.906161
C	5.478811	-4.086504	0.505373
C	5.987902	-3.158045	1.413129
C	4.7196	-4.811105	-1.60526
C	4.020834	-5.524452	-0.668826
C	4.491223	-5.149329	0.668826
C	2.764897	-6.250778	-0.505373
C	2.526423	-6.317065	0.906161
C	3.640271	-5.671842	1.60526
C	1.264337	-6.650539	1.413129
C	0.221025	-6.831401	0.505373
C	0.464643	-6.787653	-0.906161
C	1.746432	-6.540504	-1.413129
C	-0.818851	-6.689607	-1.60526
C	-1.812242	-6.588054	-0.668826
C	-1.225676	-6.721934	0.668826
C	-2.164753	-6.382414	1.60526
C	-3.363681	-5.913863	0.906161
C	-3.16317	-6.05898	-0.505373
C	-4.411299	-5.135042	1.413129
C	-5.203197	-4.432113	0.505373
C	-5.017101	-4.595305	-0.906161
C	-4.024689	-5.443353	-1.413129
C	-5.74069	-3.530699	-1.60526
C	-6.280662	-2.690717	-0.668826
C	-6.019616	-3.232785	0.668826
C	-6.339673	-2.286898	1.60526
C	-6.720865	-1.057401	0.906161
C	-6.709306	-1.304646	-0.505373
C	-6.765138	0.247246	1.413129
C	-6.709306	1.304646	0.505373
C	-6.720865	1.057401	-0.906161
C	-6.765138	-0.247246	-1.413129
C	-6.280662	2.690717	0.668826
C	-6.019616	3.232785	-0.668826
C	-6.339673	2.286898	-1.60526
C	-5.203197	4.432113	-0.505373
C	-5.017101	4.595305	0.906161
C	-5.74069	3.530699	1.60526
C	-4.024689	5.443353	1.413129
C	-3.16317	6.05898	0.505373
C	-3.363681	5.913863	-0.906161
C	-4.411299	5.135042	-1.413129
C	-2.164753	6.382414	-1.60526
C	-1.225676	6.721934	-0.668826
C	-1.812242	6.588054	0.668826
C	0.221025	6.831401	-0.505373
C	0.464643	6.787653	0.906161
C	-0.818851	6.689607	1.60526
C	1.746432	6.540504	1.413129
C	2.764897	6.250778	0.505373
C	2.526423	6.317065	-0.906161
C	1.264337	6.650539	-1.413129
C	6.704096	0.690257	-1.60526
H	1.904893	-6.432032	-2.483364
H	1.074505	-6.621563	2.483364
H	-0.914874	-6.589204	-2.681392
H	-2.034676	-6.333617	2.681392
H	-3.841084	-5.499612	-2.483364
H	-4.507003	-4.968558	2.483364
H	-5.722062	-3.393025	-2.681392
H	-6.220421	-2.358172	2.681392
H	-6.694646	-0.425872	-2.483364
H	-6.694646	0.425872	2.483364
H	-6.220421	2.358172	-2.681392

H	-5.722062	3.393025	2.681392
H	6.216446	-2.521001	-2.483364
H	5.846889	-3.288395	2.483364
H	4.581233	-4.823579	-2.681392
H	3.683221	-5.539719	2.681392
H	-2.034676	6.333617	-2.681392
H	6.627578	-0.5743	2.681392
H	-4.507003	4.968558	-2.483364
H	-3.841084	5.499612	2.483364
H	-0.914874	6.589204	2.681392
H	1.074505	6.621563	-2.483364
H	1.904893	6.432032	2.483364
H	6.627578	0.5743	-2.681392
C	3.640271	5.671842	-1.60526
C	4.020834	5.524452	0.668826
C	4.491223	5.149329	-0.668826
C	5.478811	4.086504	-0.505373
C	4.7196	4.811105	1.60526
C	5.596501	3.86876	0.906161
C	5.987902	3.158045	-1.413129
C	6.202455	2.712522	1.413129
C	6.51408	1.963389	-0.906161
C	6.61094	1.735613	0.505373
H	3.683221	5.539719	-2.681392
H	4.581233	4.823579	2.681392
H	5.846889	3.288395	-2.483364
H	6.216446	2.521001	2.483364

Table S 43. Coordinates of the calculated structure of the triplet of 6_7 (n=7) (TPSS-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.791899	-0.300478	-0.669281
C	6.570769	-1.712728	-0.512077
C	6.47396	-1.949134	0.925949
C	6.671184	-0.704535	1.617615
C	6.791899	0.300478	0.669281
C	6.171379	-2.688631	-1.422629
C	5.560343	-3.84628	-0.925949
C	5.435872	-4.069366	0.512077
C	5.949849	-3.148644	1.422629
C	4.710243	-4.776471	-1.617615
C	3.999756	-5.497466	-0.669281
C	4.469603	-5.122775	0.669281
C	2.757743	-6.205103	-0.512077
C	2.512553	-6.276811	0.925949
C	3.608587	-5.655012	1.617615
C	1.247961	-6.614927	1.422629
C	0.207653	-6.787144	0.512077
C	0.459674	-6.745368	-0.925949
C	1.745735	-6.501313	-1.422629
C	-0.797607	-6.660697	-1.617615
C	-1.804284	-6.554749	-0.669281
C	-1.218395	-6.688475	0.669281
C	-2.171349	-6.347149	1.617615
C	-3.340857	-5.877921	0.925949
C	-3.13192	-6.024908	-0.512077
C	-4.393667	-5.100034	1.422629
C	-5.176934	-4.394065	0.512077
C	-4.987139	-4.565055	-0.925949
C	-3.994483	-5.418373	-1.422629
C	-5.704843	-3.529282	-1.617615
C	-6.249662	-2.676173	-0.669281
C	-5.988917	-3.217616	0.669281
C	-6.316215	-2.259754	1.617615
C	-6.678534	-1.052837	0.925949
C	-6.663183	-1.307835	-0.512077
C	-6.726774	0.255288	1.422629
C	-6.663183	1.307835	0.512077
C	-6.678534	1.052837	-0.925949
C	-6.726774	-0.255288	-1.422629
C	-6.249662	2.676173	0.669281
C	-5.988917	3.217616	-0.669281
C	-6.316215	2.259754	-1.617615
C	-5.176934	4.394065	-0.512077
C	-4.987139	4.565055	0.925949
C	-5.704843	3.529282	1.617615
C	-3.994483	5.418373	1.422629
C	-3.13192	6.024908	0.512077
C	-3.340857	5.877921	-0.925949
C	-4.393667	5.100034	-1.422629
C	-2.171349	6.347149	-1.617615
C	-1.218395	6.688475	-0.669281
C	-1.804284	6.554749	0.669281
C	0.207653	6.787144	-0.512077

C	0.459674	6.745368	0.925949
C	-0.797607	6.660697	1.617615
C	1.745735	6.501313	1.422629
C	2.757743	6.205103	0.512077
C	2.512553	6.276811	-0.925949
C	1.247961	6.614927	-1.422629
C	6.671184	0.704535	-1.617615
H	1.911155	-6.39665	-2.492219
H	1.053511	-6.592401	2.492219
H	-0.897884	-6.5685	-2.693405
H	-2.041	-6.307591	2.693405
H	-3.809516	-5.482447	-2.492219
H	-4.497294	-4.933963	2.492219
H	-5.695282	-3.393399	-2.693405
H	-6.204016	-2.337001	2.693405
H	-6.661544	-0.43985	-2.492219
H	-6.661544	0.43985	2.492219
H	-6.204016	2.337001	-2.693405
H	-5.695282	3.393399	2.693405
H	6.192688	-2.494045	-2.492219
H	5.811	-3.286627	2.492219
H	4.575639	-4.797387	-2.693405
H	3.658931	-5.528437	2.693405

H	-2.041	6.307591	-2.693405
H	6.603612	-0.586257	2.693405
H	-4.497294	4.933963	-2.492219
H	-3.809516	5.482447	2.492219
H	-0.897884	6.5685	2.693405
H	1.053511	6.592401	-2.492219
H	1.911155	6.39665	2.492219
H	6.603612	0.586257	-2.693405
C	3.608587	5.655012	-1.617615
C	3.999756	5.497466	0.669281
C	4.469603	5.122775	-0.669281
C	5.435872	4.069366	-0.512077
C	4.710243	4.776471	1.617615
C	5.560343	3.84628	0.925949
C	5.949849	3.148644	-1.422629
C	6.171379	2.688631	1.422629
C	6.47396	1.949134	-0.925949
C	6.570769	1.712728	0.512077
H	3.658931	5.528437	-2.693405
H	4.575639	4.797387	2.693405
H	5.811	3.286627	-2.492219
H	6.192688	2.494045	2.492219

Table S 44. Coordinates of the calculated structure of the open-shell singlet of 6_7 (n=7) (TDDFT, BP86-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.8189243	-0.3020943	-0.6705655
C	6.5989033	-1.7263667	-0.5078977
C	6.5006802	-1.9588062	0.9177459
C	6.6952327	-0.6954097	1.6145098
C	6.8189243	0.3020943	0.6705655
C	6.194157	-2.704294	-1.4189975
C	5.5845642	-3.8611407	-0.9177459
C	5.4640768	-4.0828583	0.5078977
C	5.9762959	-3.1566872	1.4189975
C	4.7181025	-4.8009629	-1.6145098
C	4.0153429	-5.5196024	-0.6705655
C	4.4877166	-5.1428969	0.6705655
C	2.764621	-6.2356024	-0.5078977
C	2.5216514	-6.3037321	0.9177459
C	3.6307161	-5.6681246	1.6145098
C	1.2581621	-6.6406186	1.4189975
C	0.214689	-6.8176078	0.5078977

C	0.4631574	-6.77357	-0.9177459
C	1.7476915	-6.5288867	-1.4189975
C	-0.8118551	-6.6821125	-1.6145098
C	-1.8118736	-6.5807373	-0.6705655
C	-1.2228332	-6.7151819	0.6705655
C	-2.1678038	-6.3726261	1.6145098
C	-3.3562323	-5.9018192	0.9177459
C	-3.1514773	-6.0493023	-0.5078977
C	-4.4073935	-5.1240287	1.4189975
C	-5.196364	-4.4185595	0.5078977
C	-5.0070163	-4.5853629	-0.9177459
C	-4.0148213	-5.4370946	-1.4189975
C	-5.7304693	-3.5314951	-1.6145098
C	-6.2747123	-2.6864428	-0.6705655
C	-6.0125647	-3.230798	0.6705655
C	-6.3339232	-2.2784101	1.6145098
C	-6.7068046	-1.055716	0.9177459
C	-6.6944489	-1.3077542	-0.5078977

C	-6.7540919	0.2510593	1.4189975
C	-6.6944489	1.3077542	0.5078977
C	-6.7068046	1.055716	-0.9177459
C	-6.7540919	-0.2510593	-1.4189975
C	-6.2747123	2.6864428	0.6705655
C	-6.0125647	3.230798	-0.6705655
C	-6.3339232	2.2784101	-1.6145098
C	-5.196364	4.4185595	-0.5078977
C	-5.0070163	4.5853629	0.9177459
C	-5.7304693	3.5314951	1.6145098
C	-4.0148213	5.4370946	1.4189975
C	-3.1514773	6.0493023	0.5078977
C	-3.3562323	5.9018192	-0.9177459
C	-4.4073935	5.1240287	-1.4189975
C	-2.1678038	6.3726261	-1.6145098
C	-1.2228332	6.7151819	-0.6705655
C	-1.8118736	6.5807373	0.6705655
C	0.214689	6.8176078	-0.5078977
C	0.4631574	6.77357	0.9177459
C	-0.8118551	6.6821125	1.6145098
C	1.7476915	6.5288867	1.4189975
C	2.764621	6.2356024	0.5078977
C	2.5216514	6.3037321	-0.9177459
C	1.2581621	6.6406186	-1.4189975
C	6.6952327	0.6954097	-1.6145098
H	1.911032	-6.4201905	-2.4927847
H	1.0638359	-6.6135575	2.4927847
H	-0.9107941	-6.5817129	-2.6942288
H	-2.035101	-6.3250972	2.6942288
H	-3.8279981	-5.4970283	-2.4927847
H	-4.5073966	-4.955226	2.4927847
H	-5.7136612	-3.3915433	-2.6942288

H	-6.2140249	-2.3525275	2.6942288
H	-6.6844675	-0.4344917	-2.4927847
H	-6.6844675	0.4344917	2.4927847
H	-6.2140249	2.3525275	-2.6942288
H	-5.7136612	3.3915433	2.6942288
H	6.211016	-2.5088183	-2.4927847
H	5.8339783	-3.2917452	2.4927847
H	4.5779195	-4.8157184	-2.6942288
H	3.6762954	-5.5347397	2.6942288
H	-2.035101	6.3250972	-2.6942288
H	6.6193664	-0.5766103	2.6942288
H	-4.5073966	4.955226	-2.4927847
H	-3.8279981	5.4970283	2.4927847
H	-0.9107941	6.5817129	2.6942288
H	1.0638359	6.6135575	-2.4927847
H	1.911032	6.4201905	2.4927847
H	6.6193664	0.5766103	-2.6942288
C	3.6307161	5.6681246	-1.6145098
C	4.0153429	5.5196024	0.6705655
C	4.4877166	5.1428969	-0.6705655
C	5.4640768	4.0828583	-0.5078977
C	4.7181025	4.8009629	1.6145098
C	5.5845642	3.8611407	0.9177459
C	5.9762959	3.1566872	-1.4189975
C	6.194157	2.704294	1.4189975
C	6.5006802	1.9588062	-0.9177459
C	6.5989033	1.7263667	0.5078977
H	3.6762954	5.5347397	-2.6942288
H	4.5779195	4.8157184	2.6942288
H	5.8339783	3.2917452	-2.4927847
H	6.211016	2.5088183	2.4927847

Table S 45. Coordinates of the calculated structure of 6_8 (n=8) (TPSS-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.696737	0.253328	1.422367
C	-7.641616	1.307273	0.512369
C	-7.654445	1.053499	-0.923742
C	-7.696737	-0.253328	-1.422367
H	-7.638931	-0.437125	-2.492485
C	-7.641616	-1.307273	-0.512369
C	-7.654445	-1.053499	0.923742
C	-7.335301	-2.274722	1.615861

H	-7.235648	-2.35875	2.692453
C	-7.048456	-3.244841	0.669281
C	-7.27846	-2.689562	-0.669281
C	-6.795312	-3.57837	-1.615861
C	-6.327821	-4.479057	0.512369
C	-5.621545	-5.263285	1.422367
H	-5.710633	-5.092446	2.492485
H	-6.784263	-3.448488	-2.692453
C	-6.157447	-4.667573	-0.923742

C	-4.667573	-6.157447	0.923742
C	-4.479057	-6.327821	-0.512369
C	-5.263285	-5.621545	-1.422367
C	-3.57837	-6.795312	1.615861
C	-2.689562	-7.27846	0.669281
C	-3.244841	-7.048456	-0.669281
C	-2.274722	-7.335301	-1.615861
C	-1.053499	-7.654445	-0.923742
C	-1.307273	-7.641616	0.512369
C	-0.253328	-7.696737	1.422367
C	0.253328	-7.696737	-1.422367
C	1.307273	-7.641616	-0.512369
C	1.053499	-7.654445	0.923742
C	2.274722	-7.335301	1.615861
C	3.244841	-7.048456	0.669281
C	2.689562	-7.27846	-0.669281
C	3.57837	-6.795312	-1.615861
C	4.667573	-6.157447	-0.923742
C	4.479057	-6.327821	0.512369
C	5.263285	-5.621545	1.422367
C	5.621545	-5.263285	-1.422367
C	6.327821	-4.479057	-0.512369
C	6.157447	-4.667573	0.923742
C	6.795312	-3.57837	1.615861
C	7.048456	-3.244841	-0.669281
C	7.27846	-2.689562	0.669281
C	7.335301	-2.274722	-1.615861
C	7.654445	-1.053499	-0.923742
C	7.641616	-1.307273	0.512369
C	7.696737	-0.253328	1.422367
C	7.696737	0.253328	-1.422367
C	7.641616	1.307273	-0.512369
C	7.654445	1.053499	0.923742
C	7.27846	2.689562	-0.669281
C	7.335301	2.274722	1.615861
C	6.795312	3.57837	-1.615861
C	7.048456	3.244841	0.669281
C	6.157447	4.667573	-0.923742
C	6.327821	4.479057	0.512369
C	5.263285	5.621545	-1.422367
C	5.621545	5.263285	1.422367
C	4.667573	6.157447	0.923742
C	4.479057	6.327821	-0.512369
C	3.244841	7.048456	-0.669281

C	3.57837	6.795312	1.615861
C	2.689562	7.27846	0.669281
C	2.274722	7.335301	-1.615861
C	1.053499	7.654445	-0.923742
C	1.307273	7.641616	0.512369
C	0.253328	7.696737	1.422367
C	-0.253328	7.696737	-1.422367
C	-1.307273	7.641616	-0.512369
C	-1.053499	7.654445	0.923742
C	-2.274722	7.335301	1.615861
C	-7.27846	2.689562	0.669281
C	-7.335301	2.274722	-1.615861
C	-7.048456	3.244841	-0.669281
H	-7.638931	0.437125	2.492485
H	-3.448488	-6.784263	2.692453
H	-5.092446	-5.710633	-2.492485
H	-2.35875	-7.235648	-2.692453
H	-0.437125	-7.638931	2.492485
H	2.35875	-7.235648	2.692453
H	0.437125	-7.638931	-2.492485
H	3.448488	-6.784263	-2.692453
H	5.710633	-5.092446	-2.492485
H	5.092446	-5.710633	2.492485
H	6.784263	-3.448488	2.692453
H	7.235648	-2.35875	-2.692453
H	7.638931	0.437125	-2.492485
H	7.638931	-0.437125	2.492485
H	7.235648	2.35875	2.692453
H	6.784263	3.448488	-2.692453
H	5.092446	5.710633	-2.492485
H	5.710633	5.092446	2.492485
H	3.448488	6.784263	2.692453
H	2.35875	7.235648	-2.692453
H	-0.437125	7.638931	-2.492485
H	0.437125	7.638931	2.492485
C	-2.689562	7.27846	-0.669281
C	-3.244841	7.048456	0.669281
C	-3.57837	6.795312	-1.615861
C	-4.479057	6.327821	0.512369
C	-4.667573	6.157447	-0.923742
C	-5.263285	5.621545	1.422367
C	-5.621545	5.263285	-1.422367
C	-6.157447	4.667573	0.923742
C	-6.327821	4.479057	-0.512369

H	-5.092446	5.710633	2.492485
H	-5.710633	5.092446	-2.492485
H	-3.448488	6.784263	-2.692453
H	-2.35875	7.235648	2.692453

C	-6.795312	3.57837	1.615861
H	-6.784263	3.448488	2.692453
H	-7.235648	2.35875	-2.692453

Table S 46. Coordinates of the calculated structure of the triplet of 6_8 (n=8) (TPSS-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.717072	0.249793	1.417925
C	-7.665415	1.305603	0.509179
C	-7.67662	1.055655	-0.914545
C	-7.717072	-0.249793	-1.417925
H	-7.657132	-0.430907	-2.488364
C	-7.665415	-1.305603	-0.509179
C	-7.67662	-1.055655	0.914545
C	-7.349509	-2.287466	1.610233
H	-7.246852	-2.368863	2.68703
C	-7.065922	-3.251804	0.669015
C	-7.295734	-2.696989	-0.669015
C	-6.81437	-3.579404	-1.610233
C	-6.343467	-4.497066	0.509179
C	-5.633424	-5.280164	1.417925
H	-5.719107	-5.109713	2.488364
H	-6.799337	-3.44926	-2.68703
C	-6.174651	-4.68173	-0.914545
C	-4.68173	-6.174651	0.914545
C	-4.497066	-6.343467	-0.509179
C	-5.280164	-5.633424	-1.417925
C	-3.579404	-6.81437	1.610233
C	-2.696989	-7.295734	0.669015
C	-3.251804	-7.065922	-0.669015
C	-2.287466	-7.349509	-1.610233
C	-1.055655	-7.67662	-0.914545
C	-1.305603	-7.665415	0.509179
C	-0.249793	-7.717072	1.417925
C	0.249793	-7.717072	-1.417925
C	1.305603	-7.665415	-0.509179
C	1.055655	-7.67662	0.914545
C	2.287466	-7.349509	1.610233
C	3.251804	-7.065922	0.669015
C	2.696989	-7.295734	-0.669015
C	3.579404	-6.81437	-1.610233
C	4.68173	-6.174651	-0.914545
C	4.497066	-6.343467	0.509179

C	5.280164	-5.633424	1.417925
C	5.633424	-5.280164	-1.417925
C	6.343467	-4.497066	-0.509179
C	6.174651	-4.68173	0.914545
C	6.81437	-3.579404	1.610233
C	7.065922	-3.251804	-0.669015
C	7.295734	-2.696989	0.669015
C	7.349509	-2.287466	-1.610233
C	7.67662	-1.055655	-0.914545
C	7.665415	-1.305603	0.509179
C	7.717072	-0.249793	1.417925
C	7.717072	0.249793	-1.417925
C	7.665415	1.305603	-0.509179
C	7.67662	1.055655	0.914545
C	7.295734	2.696989	-0.669015
C	7.349509	2.287466	1.610233
C	6.81437	3.579404	-1.610233
C	7.065922	3.251804	0.669015
C	6.174651	4.68173	-0.914545
C	6.343467	4.497066	0.509179
C	5.280164	5.633424	-1.417925
C	5.633424	5.280164	1.417925
C	4.68173	6.174651	0.914545
C	4.497066	6.343467	-0.509179
C	3.251804	7.065922	-0.669015
C	3.579404	6.81437	1.610233
C	2.696989	7.295734	0.669015
C	2.287466	7.349509	-1.610233
C	1.055655	7.67662	-0.914545
C	1.305603	7.665415	0.509179
C	0.249793	7.717072	1.417925
C	-0.249793	7.717072	-1.417925
C	-1.305603	7.665415	-0.509179
C	-1.055655	7.67662	0.914545
C	-2.287466	7.349509	1.610233
C	-7.295734	2.696989	0.669015
C	-7.349509	2.287466	-1.610233

C	-7.065922	3.251804	-0.669015
H	-7.657132	0.430907	2.488364
H	-3.44926	-6.799337	2.68703
H	-5.109713	-5.719107	-2.488364
H	-2.368863	-7.246852	-2.68703
H	-0.430907	-7.657132	2.488364
H	2.368863	-7.246852	2.68703
H	0.430907	-7.657132	-2.488364
H	3.44926	-6.799337	-2.68703
H	5.719107	-5.109713	-2.488364
H	5.109713	-5.719107	2.488364
H	6.799337	-3.44926	2.68703
H	7.246852	-2.368863	-2.68703
H	7.657132	0.430907	-2.488364
H	7.657132	-0.430907	2.488364
H	7.246852	2.368863	2.68703
H	6.799337	3.44926	-2.68703
H	5.109713	5.719107	-2.488364
H	5.719107	5.109713	2.488364
H	3.44926	6.799337	2.68703

H	2.368863	7.246852	-2.68703
H	-0.430907	7.657132	-2.488364
H	0.430907	7.657132	2.488364
C	-2.696989	7.295734	-0.669015
C	-3.251804	7.065922	0.669015
C	-3.579404	6.81437	-1.610233
C	-4.497066	6.343467	0.509179
C	-4.68173	6.174651	-0.914545
C	-5.280164	5.633424	1.417925
C	-5.633424	5.280164	-1.417925
C	-6.174651	4.68173	0.914545
C	-6.343467	4.497066	-0.509179
H	-5.109713	5.719107	2.488364
H	-5.719107	5.109713	-2.488364
H	-3.44926	6.799337	-2.68703
H	-2.368863	7.246852	2.68703
C	-6.81437	3.579404	1.610233
H	-6.799337	3.44926	2.68703
H	-7.246852	2.368863	-2.68703

Table S 47. Coordinates of the calculated structure of the open-shell singlet of 6_8 (n=8) (TDDFT, BP86-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.6903084	0.2563219	1.4272932
C	-7.6334526	1.309641	0.5142882
C	-7.6468765	1.0527452	-0.933562
C	-7.6903084	-0.2563219	-1.4272932
H	-7.6327524	-0.4445423	-2.5010462
C	-7.6334526	-1.309641	-0.5142882
C	-7.6468765	-1.0527452	0.933562
C	-7.3328075	-2.2698569	1.6241916
H	-7.2319214	-2.3560762	2.7044276
C	-7.0445654	-3.2444095	0.6715754
C	-7.2754039	-2.687116	-0.6715754
C	-6.7901091	-3.5800467	-1.6241916
C	-6.3237221	-4.47161	0.5142882
C	-5.6191162	-5.2566223	1.4272932
H	-5.7115099	-5.0828322	2.5010462
H	-6.7797381	-3.4477432	-2.7044276
C	-6.1515615	-4.6627549	-0.933562
C	-4.6627549	-6.1515615	0.933562
C	-4.47161	-6.3237221	-0.5142882
C	-5.2566223	-5.6191162	-1.4272932

C	-3.5800467	-6.7901091	1.6241916
C	-2.687116	-7.2754039	0.6715754
C	-3.2444095	-7.0445654	-0.6715754
C	-2.2698569	-7.3328075	-1.6241916
C	-1.0527452	-7.6468765	-0.933562
C	-1.309641	-7.6334526	0.5142882
C	-0.2563219	-7.6903084	1.4272932
C	0.2563219	-7.6903084	-1.4272932
C	1.309641	-7.6334526	-0.5142882
C	1.0527452	-7.6468765	0.933562
C	2.2698569	-7.3328075	1.6241916
C	3.2444095	-7.0445654	0.6715754
C	2.687116	-7.2754039	-0.6715754
C	3.5800467	-6.7901091	-1.6241916
C	4.6627549	-6.1515615	-0.933562
C	4.47161	-6.3237221	0.5142882
C	5.2566223	-5.6191162	1.4272932
C	5.6191162	-5.2566223	-1.4272932
C	6.3237221	-4.47161	-0.5142882
C	6.1515615	-4.6627549	0.933562
C	6.7901091	-3.5800467	1.6241916

C	7.0445654	-3.2444095	-0.6715754
C	7.2754039	-2.687116	0.6715754
C	7.3328075	-2.2698569	-1.6241916
C	7.6468765	-1.0527452	-0.933562
C	7.6334526	-1.309641	0.5142882
C	7.6903084	-0.2563219	1.4272932
C	7.6903084	0.2563219	-1.4272932
C	7.6334526	1.309641	-0.5142882
C	7.6468765	1.0527452	0.933562
C	7.2754039	2.687116	-0.6715754
C	7.3328075	2.2698569	1.6241916
C	6.7901091	3.5800467	-1.6241916
C	7.0445654	3.2444095	0.6715754
C	6.1515615	4.6627549	-0.933562
C	6.3237221	4.47161	0.5142882
C	5.2566223	5.6191162	-1.4272932
C	5.6191162	5.2566223	1.4272932
C	4.6627549	6.1515615	0.933562
C	4.47161	6.3237221	-0.5142882
C	3.2444095	7.0445654	-0.6715754
C	3.5800467	6.7901091	1.6241916
C	2.687116	7.2754039	0.6715754
C	2.2698569	7.3328075	-1.6241916
C	1.0527452	7.6468765	-0.933562
C	1.309641	7.6334526	0.5142882
C	0.2563219	7.6903084	1.4272932
C	-0.2563219	7.6903084	-1.4272932
C	-1.309641	7.6334526	-0.5142882
C	-1.0527452	7.6468765	0.933562
C	-2.2698569	7.3328075	1.6241916
C	-7.2754039	2.687116	0.6715754
C	-7.3328075	2.2698569	-1.6241916
C	-7.0445654	3.2444095	-0.6715754
H	-7.6327524	0.4445423	2.5010462
H	-3.4477432	-6.7797381	2.7044276
H	-5.0828322	-5.7115099	-2.5010462
H	-2.3560762	-7.2319214	-2.7044276
H	-0.4445423	-7.6327524	2.5010462
H	2.3560762	-7.2319214	2.7044276
H	0.4445423	-7.6327524	-2.5010462
H	3.4477432	-6.7797381	-2.7044276
H	5.7115099	-5.0828322	-2.5010462
H	5.0828322	-5.7115099	2.5010462
H	6.7797381	-3.4477432	2.7044276
H	7.2319214	-2.3560762	-2.7044276
H	7.6327524	0.4445423	-2.5010462
H	7.6327524	-0.4445423	2.5010462
H	7.2319214	2.3560762	2.7044276
H	6.7797381	3.4477432	-2.7044276
H	5.0828322	5.7115099	-2.5010462
H	5.7115099	5.0828322	2.5010462
H	3.4477432	6.7797381	2.7044276
H	2.3560762	7.2319214	-2.7044276
H	-0.4445423	7.6327524	-2.5010462
H	0.4445423	7.6327524	2.5010462
C	-2.687116	7.2754039	-0.6715754
C	-3.2444095	7.0445654	0.6715754
C	-3.5800467	6.7901091	-1.6241916
C	-4.47161	6.3237221	0.5142882
C	-4.6627549	6.1515615	-0.933562
C	-5.2566223	5.6191162	1.4272932
C	-5.6191162	5.2566223	-1.4272932
C	-6.1515615	4.6627549	0.933562
C	-6.3237221	4.47161	-0.5142882
H	-5.0828322	5.7115099	2.5010462
H	-5.7115099	5.0828322	-2.5010462
H	-3.4477432	6.7797381	-2.7044276
H	-2.3560762	7.2319214	2.7044276
C	-6.7901091	3.5800467	1.6241916
H	-6.7797381	3.4477432	2.7044276
H	-7.2319214	2.3560762	-2.7044276

4.4 Calculated coordinates of methyl-substituted cyclacenes 10_n

Below can be found coordinates for the calculated structures of methyl-substituted $[5.5.6]_n$cyclacenes **10_n** as singlets and triplets at the TPSS-D3/def2-TZVP level of theory and of the open-shell singlets calculated using TDDFT at the BP86-D3/def2-TZVP level of theory, optimized in point group D_n.

Table S 48. Coordinates of the calculated structure of 10_3 (n=3) (TPSS-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.9351452	2.0584012	-1.6261152
C	-2.7438021	1.0503352	-0.9086222
C	-2.6982136	1.3142671	0.4960415
C	-1.7651815	2.439405	0.6666353
C	-1.229996	2.7483945	-0.6666353
C	-2.8793464	-0.2571951	-1.403642
C	-2.6982136	-1.3142671	-0.4960415
C	-2.7438021	-1.0503352	0.9086222
C	-2.8793464	0.2571951	1.403642
C	-1.7651815	-2.439405	-0.6666353
C	-1.229996	-2.7483945	0.6666353
C	-1.9351452	-2.0584012	1.6261152
C	0.2109181	-2.9938551	0.4960415
C	0.4622841	-2.90137	-0.9086222
C	-0.8150551	-2.7050855	-1.6261152
C	1.6624107	-2.3649896	-1.403642
C	2.4872955	-1.679588	-0.4960415
C	2.281518	-1.8510348	0.9086222
C	1.2169357	-2.6221847	1.403642
C	2.9951774	-0.3089895	-0.6666353
C	2.9951774	0.3089895	0.6666353
C	2.7502003	-0.6466843	1.6261152
C	2.4872955	1.679588	0.4960415
C	2.281518	1.8510348	-0.9086222
C	2.7502003	0.6466843	-1.6261152
C	1.2169357	2.6221847	-1.403642
C	0.2109181	2.9938551	-0.4960415
C	0.4622841	2.90137	0.9086222
C	1.6624107	2.3649896	1.403642
C	-0.8150551	2.7050855	1.6261152
H	1.008613	2.6083294	-2.4694675
H	1.754573	2.1776491	2.4694675
H	1.754573	-2.1776491	-2.4694675
H	1.008613	-2.6083294	2.4694675
H	-2.763186	-0.4306802	-2.4694675
H	-2.763186	0.4306802	2.4694675
C	-1.6789727	2.0198846	-3.0947195
H	-2.6051169	1.8600691	-3.6570682
H	-1.2158637	2.9453906	-3.4429269
H	-1.0035276	1.1869714	-3.3444966
C	-0.909785	2.4639753	3.0947195
H	-0.3083086	3.186132	3.6570682
H	-1.9428512	2.5256641	3.4429269
H	-0.5261836	1.4625661	3.3444966
C	2.5887577	0.4440907	-3.0947195
H	2.9134256	1.3260629	-3.6570682
H	3.1587149	-0.4197264	-3.4429269
H	1.5297112	0.2755947	-3.3444966
C	2.5887577	-0.4440907	3.0947195
H	2.9134256	-1.3260629	3.6570682
H	3.1587149	0.4197264	3.4429269
H	1.5297112	-0.2755947	3.3444966
C	-0.909785	-2.4639753	-3.0947195
H	-0.3083086	-3.186132	-3.6570682
H	-1.9428512	-2.5256641	-3.4429269
H	-0.5261836	-1.4625661	-3.3444966
C	-1.6789727	-2.0198846	3.0947195
H	-2.6051169	-1.8600691	3.6570682
H	-1.2158637	-2.9453906	3.4429269
H	-1.0035276	-1.1869714	3.3444966

Table S 49. Coordinates of the calculated structure of the triplet of 10_3 (n=3) (TPSS-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.9426095	2.0429982	-1.6420171
C	-2.7186976	1.0457769	-0.9290894
C	-2.6645242	1.3124245	0.5015092

C	-1.7602389	2.4326095	0.6699052
C	-1.2265821	2.7407164	-0.6699052
C	-2.861788	-0.2640559	-1.4143409
C	-2.6645242	-1.3124245	-0.5015092
C	-2.7186976	-1.0457769	0.9290894
C	-2.861788	0.2640559	1.4143409
C	-1.7602389	-2.4326095	-0.6699052
C	-1.2265821	-2.7407164	0.6699052
C	-1.9426095	-2.0429982	1.6420171
C	0.1956691	-2.9637579	0.5015092
C	0.4536795	-2.8773496	-0.9290894
C	-0.7979836	-2.7038483	-1.6420171
C	1.6595732	-2.3463532	-1.4143409
C	2.4688551	-1.6513334	-0.5015092
C	2.2650181	-1.8315727	0.9290894
C	1.2022149	-2.6104091	1.4143409
C	2.9868211	-0.3081069	-0.6699052
C	2.9868211	0.3081069	0.6699052
C	2.7405931	-0.6608501	1.6420171
C	2.4688551	1.6513334	0.5015092
C	2.2650181	1.8315727	-0.9290894
C	2.7405931	0.6608501	-1.6420171
C	1.2022149	2.6104091	-1.4143409
C	0.1956691	2.9637579	-0.5015092
C	0.4536795	2.8773496	0.9290894
C	1.6595732	2.3463532	1.4143409
C	-0.7979836	2.7038483	1.6420171
H	0.99348	2.612661	-2.4800762
H	1.7658908	2.1667094	2.4800762
H	1.7658908	-2.1667094	-2.4800762
H	0.99348	-2.612661	2.4800762
H	-2.7593708	-0.4459516	-2.4800762
H	-2.7593708	0.4459516	2.4800762
C	-1.6686356	2.0050436	-3.1078113
H	-2.5564977	1.7127957	-3.6768006
H	-1.3270728	2.9762168	-3.4741083
H	-0.8791489	1.2685607	-3.3333209
C	-0.9021009	2.4476026	3.1078113
H	-0.2050757	3.0703898	3.6768006
H	-1.9139429	2.6373872	3.4741083
H	-0.6590314	1.3956456	3.3333209
C	2.5707365	0.442559	-3.1078113
H	2.7615734	1.3575941	-3.6768006
H	3.2410158	-0.3388296	-3.4741083
H	1.5381803	0.1270849	-3.3333209
C	2.5707365	-0.442559	3.1078113
H	2.7615734	-1.3575941	3.6768006
H	3.2410158	0.3388296	3.4741083
H	1.5381803	-0.1270849	3.3333209
C	-0.9021009	-2.4476026	-3.1078113
H	-0.2050757	-3.0703898	-3.6768006
H	-1.9139429	-2.6373872	-3.4741083
H	-0.6590314	-1.3956456	-3.3333209
C	-1.6686356	-2.0050436	3.1078113
H	-2.5564977	-1.7127957	3.6768006
H	-1.3270728	-2.9762168	3.4741083
H	-0.8791489	-1.2685607	3.3333209

Table S 50. Coordinates of the calculated structure of the open-shell singlet of 10_3 (n=3) (TDDFT, BP86-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.9375465	2.0397634	-1.6458694
C	-2.715442	1.0441275	-0.9336127
C	-2.6633653	1.3154312	0.4994086
C	-1.7676038	2.4410139	0.6699006
C	-1.2301781	2.7512967	-0.6699006
C	-2.8612846	-0.2678659	-1.4152978
C	-2.6633653	-1.3154312	-0.4994086
C	-2.715442	-1.0441275	0.9336127
C	-2.8612846	0.2678659	1.4152978
C	-1.7676038	-2.4410139	-0.6699006
C	-1.2301781	-2.7512967	0.6699006
C	-1.9375465	-2.0397634	1.6458694
C	0.1924858	-2.9642576	0.4994086
C	0.4534801	-2.8737055	-0.9336127
C	-0.7977137	-2.6978462	-1.6458694
C	1.662621	-2.3440122	-1.4152978
C	2.4708795	-1.6488264	-0.4994086
C	2.2619619	-1.829578	0.9336127
C	1.1986636	-2.6118781	1.4152978
C	2.9977819	-0.3102828	-0.6699006
C	2.9977819	0.3102828	0.6699006
C	2.7352602	-0.6580828	1.6458694
C	2.4708795	1.6488264	0.4994086

C	2.2619619	1.829578	-0.9336127
C	2.7352602	0.6580828	-1.6458694
C	1.1986636	2.6118781	-1.4152978
C	0.1924858	2.9642576	-0.4994086
C	0.4534801	2.8737055	0.9336127
C	1.662621	2.3440122	1.4152978
C	-0.7977137	2.6978462	1.6458694
H	0.9866587	2.6170774	-2.4846878
H	1.7731262	2.1630102	2.4846878
H	1.7731262	-2.1630102	-2.4846878
H	0.9866587	-2.6170774	2.4846878
H	-2.7597848	-0.4540672	-2.4846878
H	-2.7597848	0.4540672	2.4846878
C	-1.6412456	1.9868353	-3.1028546
H	-2.5145115	1.6678452	-3.6875802
H	-1.3080533	2.9603261	-3.4827224
H	-0.8306132	1.2585515	-3.3060718
C	-0.900027	2.414778	3.1028546
H	-0.1871406	3.0115534	3.6875802
H	-1.909691	2.6129705	3.4827224
H	-0.674631	1.3486079	3.3060718
C	2.5412726	0.4279427	-3.1028546
H	2.7016521	1.3437082	-3.6875802
H	3.2177443	-0.3473557	-3.4827224
H	1.5052442	0.0900564	-3.3060718
C	2.5412726	-0.4279427	3.1028546
H	2.7016521	-1.3437082	3.6875802
H	3.2177443	0.3473557	3.4827224
H	1.5052442	-0.0900564	3.3060718
C	-0.900027	-2.414778	-3.1028546
H	-0.1871406	-3.0115534	-3.6875802
H	-1.909691	-2.6129705	-3.4827224
H	-0.674631	-1.3486079	-3.3060718
C	-1.6412456	-1.9868353	3.1028546
H	-2.5145115	-1.6678452	3.6875802
H	-1.3080533	-2.9603261	3.4827224
H	-0.8306132	-1.2585515	3.3060718

Table S 51. Coordinates of the calculated structure of 10_4 (n=4) (TPSS-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.701723	-1.047585	-0.943513
C	3.663077	-1.311710	0.510189
C	3.800928	0.262900	-1.425250
C	3.663077	1.311710	-0.510189
C	3.701723	1.047585	0.943513
C	3.800928	-0.262900	1.425250
C	3.115632	-2.145886	-1.646942
C	2.985135	-2.553697	0.670740
C	2.553697	-2.985135	-0.670740
C	2.145886	-3.115632	1.646942
C	1.311710	-3.663077	-0.510189
C	1.047585	-3.701723	0.943513
C	0.262900	-3.800928	-1.425250
C	-0.262900	-3.800928	1.425250
C	-1.047585	-3.701723	-0.943513
C	-1.311710	-3.663077	0.510189
C	-2.553697	-2.985135	0.670740
C	-2.145886	-3.115632	-1.646942
C	-2.985135	-2.553697	-0.670740
C	-3.115632	-2.145886	1.646942
C	-3.663077	-1.311710	-0.510189
C	-3.701723	-1.047585	0.943513
C	-3.800928	-0.262900	-1.425250
C	-3.800928	0.262900	1.425250
C	-3.663077	1.311710	0.510189
C	-3.701723	1.047585	-0.943513
C	-3.115632	2.145886	-1.646942
C	-2.985135	2.553697	0.670740
C	-2.553697	2.985135	-0.670740
C	-2.145886	3.115632	1.646942
C	-1.047585	3.701723	0.943513
C	-1.311710	3.663077	-0.510189
C	0.262900	3.800928	1.425250
C	-0.262900	3.800928	-1.425250
C	1.047585	3.701723	-0.943513
C	1.311710	3.663077	0.510189
C	2.145886	3.115632	-1.646942
C	2.553697	2.985135	0.670740
C	2.985135	2.553697	-0.670740
C	3.115632	2.145886	1.646942
H	-3.712663	0.453978	2.491058
H	-3.712663	-0.453978	-2.491058
H	-0.453978	-3.712663	2.491058

H	0.453978	-3.712663	-2.491058
H	3.712663	-0.453978	2.491058
H	3.712663	0.453978	-2.491058
H	0.453978	3.712663	2.491058
H	-0.453978	3.712663	-2.491058
C	-2.192488	2.863682	3.118798
H	-1.589414	3.588902	3.672197
H	-3.218087	2.911611	3.496993
H	-1.804908	1.859409	3.352566
C	-2.863682	2.192488	-3.118798
H	-3.588902	1.589414	-3.672197
H	-2.911611	3.218087	-3.496993
H	-1.859409	1.804908	-3.352566
C	-2.863682	-2.192488	3.118798
H	-3.588902	-1.589414	3.672197
H	-2.911611	-3.218087	3.496993
H	-1.859409	-1.804908	3.352566
C	-2.192488	-2.863682	-3.118798
H	-1.589414	-3.588902	-3.672197

H	-3.218087	-2.911611	-3.496993
H	-1.804908	-1.859409	-3.352566
C	2.192488	-2.863682	3.118798
H	1.589414	-3.588902	3.672197
H	3.218087	-2.911611	3.496993
H	1.804908	-1.859409	3.352566
C	2.863682	-2.192488	-3.118798
H	3.588902	-1.589414	-3.672197
H	2.911611	-3.218087	-3.496993
H	1.859409	-1.804908	-3.352566
C	2.192488	2.863682	-3.118798
H	1.589414	3.588902	-3.672197
H	3.218087	2.911611	-3.496993
H	1.804908	1.859409	-3.352566
C	2.863682	2.192488	3.118798
H	3.588902	1.589414	3.672197
H	2.911611	3.218087	3.496993
H	1.859409	1.804908	3.352566

Table S 52. Coordinates of the calculated structure of the triplet of 10_4 (n=4) (TPSS-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.726117	-1.050984	-0.924675
C	3.694962	-1.312365	0.504873
C	3.818376	0.257944	-1.415854
C	3.694962	1.312365	-0.504873
C	3.726117	1.050984	0.924675
C	3.818376	-0.257944	1.415854
C	3.113929	-2.160159	-1.633569
C	2.997275	-2.567473	0.667905
C	2.567473	-2.997275	-0.667905
C	2.160159	-3.113929	1.633569
C	1.312365	-3.694962	-0.504873
C	1.050984	-3.726117	0.924675
C	0.257944	-3.818376	-1.415854
C	-0.257944	-3.818376	1.415854
C	-1.050984	-3.726117	-0.924675
C	-1.312365	-3.694962	0.504873
C	-2.567473	-2.997275	0.667905
C	-2.160159	-3.113929	-1.633569
C	-2.997275	-2.567473	-0.667905
C	-3.113929	-2.160159	1.633569
C	-3.694962	-1.312365	-0.504873

C	-3.726117	-1.050984	0.924675
C	-3.818376	-0.257944	-1.415854
C	-3.818376	0.257944	1.415854
C	-3.694962	1.312365	0.504873
C	-3.726117	1.050984	-0.924675
C	-3.113929	2.160159	-1.633569
C	-2.997275	2.567473	0.667905
C	-2.567473	2.997275	-0.667905
C	-2.160159	3.113929	1.633569
C	-1.050984	3.726117	0.924675
C	-1.312365	3.694962	-0.504873
C	0.257944	3.818376	1.415854
C	-0.257944	3.818376	-1.415854
C	1.050984	3.726117	-0.924675
C	1.312365	3.694962	0.504873
C	2.160159	3.113929	-1.633569
C	2.567473	2.997275	0.667905
C	2.997275	2.567473	-0.667905
C	3.113929	2.160159	1.633569
H	-3.719203	0.440939	2.482153
H	-3.719203	-0.440939	-2.482153
H	-0.440939	-3.719203	2.482153

H	0.440939	-3.719203	-2.482153
H	3.719203	-0.440939	2.482153
H	3.719203	0.440939	-2.482153
H	0.440939	3.719203	2.482153
H	-0.440939	3.719203	-2.482153
C	-2.186811	2.859890	3.105549
H	-1.705062	3.669435	3.662425
H	-3.211179	2.752335	3.471538
H	-1.648477	1.929809	3.346363
C	-2.859890	2.186811	-3.105549
H	-3.669435	1.705062	-3.662425
H	-2.752335	3.211179	-3.471538
H	-1.929809	1.648477	-3.346363
C	-2.859890	-2.186811	3.105549
H	-3.669435	-1.705062	3.662425
H	-2.752335	-3.211179	3.471538
H	-1.929809	-1.648477	3.346363
C	-2.186811	-2.859890	-3.105549
H	-1.705062	-3.669435	-3.662425

H	-3.211179	-2.752335	-3.471538
H	-1.648477	-1.929809	-3.346363
C	2.186811	-2.859890	3.105549
H	1.705062	-3.669435	3.662425
H	3.211179	-2.752335	3.471538
H	1.648477	-1.929809	3.346363
C	2.859890	-2.186811	-3.105549
H	3.669435	-1.705062	-3.662425
H	2.752335	-3.211179	-3.471538
H	1.929809	-1.648477	-3.346363
C	2.186811	2.859890	-3.105549
H	1.705062	3.669435	-3.662425
H	3.211179	2.752335	-3.471538
H	1.648477	1.929809	-3.346363
C	2.859890	2.186811	3.105549
H	3.669435	1.705062	3.662425
H	2.752335	3.211179	3.471538
H	1.929809	1.648477	3.346363

Table S 53. Coordinates of the calculated structure of the open-shell singlet of 10_4 (n=4) (TPSS-D3/def2-TZVP) in C_1 geometry.

	x	y	z
C	3.120703	2.134538	1.648090
C	3.722776	1.045704	0.943812
C	3.693465	1.319784	-0.497320
C	3.006291	2.576826	-0.652436
C	2.577913	3.001460	0.668186
C	3.810264	-0.279407	1.418297
C	3.691452	-1.323536	0.501921
C	3.722880	-1.049487	-0.939174
C	3.812352	0.275538	-1.413562
C	3.002573	-2.579744	0.656154
C	2.575491	-3.003974	-0.665016
C	3.120637	-2.137731	-1.644246
C	1.318724	-3.691680	-0.509737
C	1.047180	-3.725195	0.931790
C	2.137275	-3.125287	1.635930
C	-0.277089	-3.813938	1.408373
C	-1.322836	-3.692725	0.494178
C	-1.051342	-3.720318	-0.947470
C	0.272848	-3.808229	-1.424463
C	-2.578828	-3.004345	0.652468
C	-3.005558	-2.574142	-0.666892

C	-2.141121	-3.116686	-1.649038
C	-3.692791	-1.317672	-0.507372
C	-3.723861	-1.049640	0.934850
C	-3.122721	-2.141503	1.635303
C	-3.811714	0.273486	1.414799
C	-3.691966	1.321471	0.502936
C	-3.721596	1.053475	-0.939345
C	-3.810041	-0.269545	-1.419409
C	-3.118559	2.144743	-1.639028
C	-2.574960	3.006999	-0.655517
C	-3.003698	2.577244	0.663305
C	-1.318391	3.693948	-0.495789
C	-1.048602	3.721363	0.946184
C	-2.139873	3.119042	1.646441
C	-0.271391	3.813708	-1.408748
C	1.052239	3.723978	-0.930529
C	1.321996	3.690315	0.511329
C	0.275117	3.807540	1.424785
C	2.142857	3.123383	-1.633319
C	2.855798	-2.184011	-3.109948
C	2.185586	-2.861454	3.101739
C	-2.189805	-2.847802	-3.113982

C	-2.857111	-2.193842	3.100666
C	-2.850594	2.196558	-3.103984
C	-2.190806	2.850294	3.111277
C	2.193367	2.860414	-3.099212
C	2.853270	2.180769	3.113316
H	-3.716842	0.464802	2.484991
H	-3.713033	-0.460908	-2.489408
H	-0.471014	-3.720779	2.478235
H	0.466882	-3.711273	-2.493986
H	3.714530	-0.475227	2.487586
H	3.718023	0.471453	-2.482969
H	0.467686	3.708613	2.494380
H	-0.464095	3.719730	-2.478772
H	-1.538375	3.528070	3.676327
H	-3.212984	2.954297	3.500584
H	-1.868012	1.815921	3.329274
H	-3.530179	1.546201	-3.669272
H	-2.952540	3.219354	-3.492191
H	-1.817091	1.871616	-3.322958
H	-3.536329	-1.542204	3.664918
H	-2.961627	-3.216452	3.488705
H	-1.823317	-1.870937	3.321228
H	-1.542761	-3.530967	-3.678780
H	-3.212684	-2.943740	-3.503406
H	-1.858498	-1.816126	-3.332223
H	1.532087	-3.541071	3.663334
H	3.207057	-2.966853	3.492529
H	1.862492	-1.827791	3.322621
H	3.535845	-1.530684	-3.671240
H	2.959652	-3.205157	-3.502017
H	1.822370	-1.859376	-3.329751
H	1.541009	3.540618	-3.661438
H	3.215498	2.965642	-3.488351
H	1.870231	1.826991	-3.321191
H	3.531137	1.526063	3.675621
H	2.958211	3.201591	3.505941
H	1.818877	1.857896	3.331088

Table S 54. Coordinates of the calculated structure of 10_5 (n=5) (TPSS-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	-4.232789	-2.238567	1.619675
C	-4.748863	-1.057580	0.904326
C	-4.729031	-1.309707	-0.504809
C	-4.144437	-2.639610	-0.667606
C	-3.791120	-3.125910	0.667606
C	-4.815332	0.246988	1.409407
C	-4.729031	1.309707	0.504809
C	-4.748863	1.057580	-0.904326
C	-4.815332	-0.246988	-1.409407
C	-4.144437	2.639610	0.667606
C	-3.791120	3.125910	-0.667606
C	-4.232789	2.238567	-1.619675
C	-2.706956	4.092855	-0.504809
C	-2.473298	4.189627	0.904326
C	-3.437008	3.333866	1.619675
C	-1.253120	4.655976	1.409407
C	-0.215746	4.902298	0.504809
C	-0.461661	4.843247	-0.904326
C	-1.722919	4.503329	-1.409407
C	1.229717	4.757278	0.667606
C	1.801396	4.571528	-0.667606
C	0.821000	4.717377	-1.619675
C	3.056041	3.839230	-0.504809
C	3.220281	3.646912	0.904326
C	2.108602	4.299010	1.619675
C	4.040861	2.630564	1.409407
C	4.595693	1.720080	0.504809
C	4.463541	1.935711	-0.904326
C	3.750509	3.030199	-1.409407
C	4.740195	0.676932	-1.619675
C	4.904444	-0.300550	-0.667606
C	4.904444	0.300550	0.667606
C	4.595693	-1.720080	-0.504809
C	4.463541	-1.935711	0.904326
C	4.740195	-0.676932	1.619675
C	4.040861	-2.630564	-1.409407
C	3.220281	-3.646912	-0.904326
C	3.056041	-3.839230	0.504809
C	3.750509	-3.030199	1.409407
C	-3.437008	-3.333866	-1.619675
H	4.070260	2.438070	2.478324
H	3.576522	3.117643	-2.478324
H	-1.060962	4.624453	2.478324

H	-1.859849	4.364879	-2.478324
H	-4.725971	0.419999	2.478324
H	-4.725971	-0.419999	-2.478324
H	3.576522	-3.117643	2.478324
H	4.070260	-2.438070	-2.478324
C	-2.706956	-4.092855	0.504809
C	-2.473298	-4.189627	-0.904326
C	-1.722919	-4.503329	1.409407
C	-1.253120	-4.655976	-1.409407
C	-0.215746	-4.902298	-0.504809
C	-0.461661	-4.843247	0.904326
C	0.821000	-4.717377	1.619675
C	1.229717	-4.757278	-0.667606
C	1.801396	-4.571528	0.667606
C	2.108602	-4.299010	-1.619675
H	-1.859849	-4.364879	2.478324
H	-1.060962	-4.624453	-2.478324
C	4.619031	-0.522373	3.099601
H	5.189292	-1.298391	3.623766
H	4.979966	0.452673	3.432530
H	3.571246	-0.628262	3.415939
C	4.619031	0.522373	-3.099601
H	5.189292	1.298391	-3.623766
H	4.979966	-0.452673	-3.432530
H	3.571246	0.628262	-3.415939
C	1.924166	-4.231537	-3.099601
H	2.838423	-4.534085	-3.623766
H	1.108377	-4.876113	-3.432530
H	1.701088	-3.202313	-3.415939
C	0.930553	-4.554382	3.099601
H	0.368736	-5.336535	3.623766
H	1.969412	-4.596345	3.432530
H	0.506063	-3.590600	3.415939
C	-3.429831	-3.137607	-3.099601
H	-3.435050	-4.100610	-3.623766
H	-4.294952	-2.560931	-3.432530
H	-2.519915	-2.607400	-3.415939
C	-4.043918	-2.292389	3.099601
H	-4.961400	-1.999769	3.623766
H	-3.762803	-3.293371	3.432530
H	-3.258481	-1.590851	3.415939
C	-4.043918	2.292389	-3.099601
H	-4.961400	1.999769	-3.623766
H	-3.762803	3.293371	-3.432530
H	-3.258481	1.590851	-3.415939
C	-3.429831	3.137607	3.099601
H	-3.435050	4.100610	3.623766
H	-4.294952	2.560931	3.432530
H	-2.519915	2.607400	3.415939
C	0.930553	4.554382	-3.099601
H	0.368736	5.336535	-3.623766
H	1.969412	4.596345	-3.432530
H	0.506063	3.590600	-3.415939
C	1.924166	4.231537	3.099601
H	2.838423	4.534085	3.623766
H	1.108377	4.876113	3.432530
H	1.701088	3.202313	3.415939

Table S 55. Coordinates of the calculated structure of the triplet of 10_5 (n=5) (TPSS-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	-4.221573	2.221269	-1.629066
C	-4.722803	1.054348	-0.920080
C	-4.701383	1.310714	0.507201
C	-4.132985	2.630932	0.667530
C	-3.779328	3.117699	-0.667530
C	-4.791059	-0.253532	-1.416360
C	-4.701383	-1.310714	-0.507201
C	-4.722803	-1.054348	0.920080
C	-4.791059	0.253532	1.416360
C	-4.132985	-2.630932	-0.667530
C	-3.779328	-3.117699	0.667530
C	-4.221573	-2.221269	1.629066
C	-2.699370	-4.066248	0.507201
C	-2.462171	-4.165841	-0.920080
C	-3.417090	-3.328545	-1.629066
C	-1.239395	-4.634913	-1.416360
C	-0.206245	-4.876314	-0.507201
C	-0.456682	-4.817464	0.920080
C	-1.721642	-4.478222	1.416360
C	1.225003	-4.743705	-0.667530
C	1.797232	-4.557777	0.667530
C	0.808015	-4.701364	1.629066
C	3.033081	-3.823793	0.507201

C	3.201098	-3.628980	-0.920080
C	2.109695	-4.278423	-1.629066
C	4.025070	-2.611002	-1.416360
C	4.573917	-1.703014	-0.507201
C	4.440559	-1.923008	0.920080
C	3.727025	-3.021225	1.416360
C	4.720954	-0.684334	1.629066
C	4.890078	0.300839	0.667530
C	4.890078	-0.300839	-0.667530
C	4.573917	1.703014	0.507201
C	4.440559	1.923008	-0.920080
C	4.720954	0.684334	-1.629066
C	4.025070	2.611002	1.416360
C	3.201098	3.628980	0.920080
C	3.033081	3.823793	-0.507201
C	3.727025	3.021225	-1.416360
C	-3.417090	3.328545	1.629066
H	4.061096	-2.412557	-2.484168
H	3.549426	-3.116810	2.484168
H	-1.039531	-4.607853	-2.484168
H	-1.867430	-4.338852	2.484168
H	-4.703561	-0.435252	-2.484168
H	-4.703561	0.435252	2.484168
H	3.549426	3.116810	-2.484168
H	4.061096	2.412557	2.484168
C	-2.699370	4.066248	-0.507201
C	-2.462171	4.165841	0.920080
C	-1.721642	4.478222	-1.416360
C	-1.239395	4.634913	1.416360
C	-0.206245	4.876314	0.507201
C	-0.456682	4.817464	-0.920080
C	0.808015	4.701364	-1.629066
C	1.225003	4.743705	0.667530
C	1.797232	4.557777	-0.667530
C	2.109695	4.278423	1.629066
H	-1.867430	4.338852	-2.484168
H	-1.039531	4.607853	2.484168
C	4.588029	0.505103	-3.106888
H	4.906873	1.400861	-3.649347
H	5.183885	-0.340708	-3.459428
H	3.540066	0.312190	-3.381314
C	4.588029	-0.505103	3.106888
H	4.906873	-1.400861	3.649347
H	5.183885	0.340708	3.459428
H	3.540066	-0.312190	3.381314
C	1.898160	4.207390	3.106888
H	2.848605	4.233824	3.649347
H	1.277876	5.035453	3.459428
H	1.390851	3.270331	3.381314
C	0.937398	4.519560	-3.106888
H	0.184009	5.099604	-3.649347
H	1.925941	4.824883	-3.459428
H	0.797030	3.463275	-3.381314
C	-3.414902	3.105412	3.106888
H	-3.146338	4.017508	3.649347
H	-4.394115	2.771373	3.459428
H	-2.680473	2.333366	3.381314
C	-4.008686	2.288139	-3.106888
H	-4.793149	1.750867	-3.649347
H	-3.993588	3.322650	-3.459428
H	-3.047474	1.828232	-3.381314
C	-4.008686	-2.288139	3.106888
H	-4.793149	-1.750867	3.649347
H	-3.993588	-3.322650	3.459428
H	-3.047474	-1.828232	3.381314
C	-3.414902	-3.105412	-3.106888
H	-3.146338	-4.017508	-3.649347
H	-4.394115	-2.771373	-3.459428
H	-2.680473	-2.333366	-3.381314
C	0.937398	-4.519560	3.106888
H	0.184009	-5.099604	3.649347
H	1.925941	-4.824883	3.459428
H	0.797030	-3.463275	3.381314
C	1.898160	-4.207390	-3.106888
H	2.848605	-4.233824	-3.649347
H	1.277876	-5.035453	-3.459428
H	1.390851	-3.270331	-3.381314

Table S 56. Coordinates of the calculated structure of the open-shell singlet of 10_5 (n=5) (TDDFT, BP86-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	-4.220947	-2.221518	1.632076
C	-4.723371	-1.054065	0.924136
C	-4.703997	-1.312982	-0.506314

C	-4.141016	-2.634963	-0.667863
C	-3.785643	-3.124092	0.667863
C	-4.790920	0.255916	1.417868
C	-4.703997	1.312982	0.506314
C	-4.723371	1.054065	-0.924136
C	-4.790920	-0.255916	-1.417868
C	-4.141016	2.634963	0.667863
C	-3.785643	3.124092	-0.667863
C	-4.220947	2.221518	-1.632076
C	-2.702335	4.068033	-0.506314
C	-2.462077	4.166469	0.924136
C	-3.417133	3.327872	1.632076
C	-1.237085	4.635518	1.417868
C	-0.204895	4.879501	0.506314
C	-0.457127	4.817917	-0.924136
C	-1.723866	4.477354	-1.417868
C	1.226354	4.752589	0.667863
C	1.801360	4.565758	-0.667863
C	0.808445	4.700846	-1.632076
C	3.033862	3.827165	-0.506314
C	3.201724	3.629084	0.924136
C	2.109043	4.278256	1.632076
C	4.026360	2.608992	1.417868
C	4.577365	1.702715	0.506314
C	4.440851	1.923572	-0.924136
C	3.725512	3.023073	-1.417868
C	4.720593	0.683765	-1.632076
C	4.898945	-0.302298	-0.667863
C	4.898945	0.302298	0.667863
C	4.577365	-1.702715	-0.506314
C	4.440851	-1.923572	0.924136
C	4.720593	-0.683765	1.632076
C	4.026360	-2.608992	-1.417868
C	3.201724	-3.629084	-0.924136
C	3.033862	-3.827165	0.506314
C	3.725512	-3.023073	1.417868
C	-3.417133	-3.327872	-1.632076
H	4.061658	2.405281	2.489305
H	3.542679	3.119594	-2.489305
H	-1.032437	4.606139	2.489305
H	-1.872162	4.333296	-2.489305
H	-4.699739	0.441470	2.489305
H	-4.699739	-0.441470	-2.489305
H	3.542679	-3.119594	2.489305

H	4.061658	-2.405281	-2.489305
C	-2.702335	-4.068033	0.506314
C	-2.462077	-4.166469	-0.924136
C	-1.723866	-4.477354	1.417868
C	-1.237085	-4.635518	-1.417868
C	-0.204895	-4.879501	-0.506314
C	-0.457127	-4.817917	0.924136
C	0.808445	-4.700846	1.632076
C	1.226354	-4.752589	-0.667863
C	1.801360	-4.565758	0.667863
C	2.109043	-4.278256	-1.632076
H	-1.872162	-4.333296	2.489305
H	-1.032437	-4.606139	-2.489305
C	4.576182	-0.496051	3.104454
H	4.870777	-1.397192	3.659710
H	5.186209	0.342503	3.463073
H	3.526124	-0.278841	3.369530
C	4.576182	0.496051	-3.104454
H	4.870777	1.397192	-3.659710
H	5.186209	-0.342503	-3.463073
H	3.526124	0.278841	-3.369530
C	1.885890	-4.198919	-3.104454
H	2.833961	-4.200628	-3.659710
H	1.276887	-5.038217	-3.463073
H	1.354825	-3.267377	-3.369530
C	0.942346	-4.505496	3.104454
H	0.176344	-5.064140	3.659710
H	1.928366	-4.826539	3.463073
H	0.824439	-3.439710	3.369530
C	-3.410638	-3.091126	-3.104454
H	-3.119292	-3.993323	-3.659710
H	-4.397049	-2.771287	-3.463073
H	-2.688796	-2.298191	-3.369530
C	-3.993780	-2.288499	3.104454
H	-4.761790	-1.732619	3.659710
H	-3.994413	-3.325468	3.463073
H	-3.016593	-1.847017	3.369530
C	-3.993780	2.288499	-3.104454
H	-4.761790	1.732619	-3.659710
H	-3.994413	3.325468	-3.463073
H	-3.016593	1.847017	-3.369530
C	-3.410638	3.091126	3.104454
H	-3.119292	3.993323	3.659710
H	-4.397049	2.771287	3.463073

H	-2.688796	2.298191	3.369530
C	0.942346	4.505496	-3.104454
H	0.176344	5.064140	-3.659710
H	1.928366	4.826539	-3.463073
H	0.824439	3.439710	-3.369530
C	1.885890	4.198919	3.104454
H	2.833961	4.200628	3.659710
H	1.276887	5.038217	3.463073
H	1.354825	3.267377	3.369530

Table S 57. Coordinates of the calculated structure of 10_6 (n=6) (TPSS-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.271556	-2.239588	1.635625
C	-5.682092	-1.052859	0.932428
C	-5.663717	-1.310444	-0.510826
C	-5.197560	-2.653445	-0.667563
C	-4.896731	-3.174496	0.667563
C	-5.741603	0.256235	1.422746
C	-5.663717	1.310444	0.510826
C	-5.682092	1.052859	-0.932428
C	-5.741603	-0.256235	-1.422746
C	-5.197560	2.653445	0.667563
C	-4.896731	3.174496	-0.667563
C	-5.271556	2.239588	-1.635625
C	-3.966736	4.249700	-0.510826
C	-3.752848	4.394406	0.932428
C	-4.575319	3.445507	1.635625
C	-2.648895	5.100492	1.422746
C	-1.696980	5.560145	0.510826
C	-1.929243	5.447265	-0.932428
C	-3.092708	4.844257	-1.422746
C	-0.300829	5.827941	0.667563
C	0.300829	5.827941	-0.667563
C	-0.696238	5.685096	-1.635625
C	1.696980	5.560145	-0.510826
C	1.929243	5.447265	0.932428
C	0.696238	5.685096	1.635625
C	3.092708	4.844257	1.422746
C	3.966736	4.249700	0.510826
C	3.752848	4.394406	-0.932428
C	2.648895	5.100492	-1.422746
C	4.575319	3.445507	-1.635625
C	5.197560	2.653445	-0.667563
C	4.896731	3.174496	0.667563
C	5.663717	1.310444	-0.510826
C	5.682092	1.052859	0.932428
C	5.271556	2.239588	1.635625
C	5.741603	0.256235	-1.422746
C	5.682092	-1.052859	-0.932428
C	5.663717	-1.310444	0.510826
C	5.741603	-0.256235	1.422746
C	-4.575319	-3.445507	-1.635625
H	3.221905	4.689193	2.490682
H	2.450007	5.134848	-2.490682
H	-2.450007	5.134848	2.490682
H	-3.221905	4.689193	-2.490682
H	-5.671912	0.445656	2.490682
H	-5.671912	-0.445656	-2.490682
H	5.671912	-0.445656	2.490682
H	5.671912	0.445656	-2.490682
C	-3.966736	-4.249700	0.510826
C	-3.752848	-4.394406	-0.932428
C	-3.092708	-4.844257	1.422746
C	-2.648895	-5.100492	-1.422746
C	-1.696980	-5.560145	-0.510826
C	-1.929243	-5.447265	0.932428
C	-0.696238	-5.685096	1.635625
C	-0.300829	-5.827941	-0.667563
C	0.300829	-5.827941	0.667563
C	5.271556	-2.239588	-1.635625
H	-3.221905	-4.689193	2.490682
H	-2.450007	-5.134848	-2.490682
C	1.696980	-5.560145	0.510826
C	0.696238	-5.685096	-1.635625
C	1.929243	-5.447265	-0.932428
C	2.648895	-5.100492	1.422746
C	3.752848	-4.394406	0.932428
C	3.092708	-4.844257	-1.422746
C	3.966736	-4.249700	-0.510826
C	4.575319	-3.445507	1.635625
C	4.896731	-3.174496	-0.667563
C	5.197560	-2.653445	0.667563
H	2.450007	-5.134848	2.490682

H	3.221905	-4.689193	-2.490682
C	0.508113	5.578064	3.114817
H	1.453927	5.691900	3.651745
H	-0.187193	6.340578	3.480217
H	0.086741	4.598249	3.383229
C	-0.508113	5.578064	-3.114817
H	-1.453927	5.691900	-3.651745
H	0.187193	6.340578	-3.480217
H	-0.086741	4.598249	-3.383229
C	-4.576688	3.229071	3.114817
H	-4.202367	4.105088	3.651745
H	-5.584698	3.008175	3.480217
H	-3.938830	2.374244	3.383229
C	-5.084802	2.348993	-3.114817
H	-5.656293	1.586812	-3.651745
H	-5.397505	3.332402	-3.480217
H	-4.025571	2.224005	-3.383229
C	4.576688	3.229071	-3.114817
H	4.202367	4.105088	-3.651745
H	5.584698	3.008175	-3.480217
H	3.938830	2.374244	-3.383229
C	5.084802	2.348993	3.114817
H	5.656293	1.586812	3.651745
H	5.397505	3.332402	3.480217
H	4.025571	2.224005	3.383229
C	-5.084802	-2.348993	3.114817
H	-5.656293	-1.586812	3.651745
H	-5.397505	-3.332402	3.480217
H	-4.025571	-2.224005	3.383229
C	-4.576688	-3.229071	-3.114817
H	-4.202367	-4.105088	-3.651745
H	-5.584698	-3.008175	-3.480217
H	-3.938830	-2.374244	-3.383229
C	-0.508113	-5.578064	3.114817
H	-1.453927	-5.691900	3.651745
H	0.187193	-6.340578	3.480217
H	-0.086741	-4.598249	3.383229
C	0.508113	-5.578064	-3.114817
H	1.453927	-5.691900	-3.651745
H	-0.187193	-6.340578	-3.480217
H	0.086741	-4.598249	-3.383229
C	4.576688	-3.229071	3.114817
H	4.202367	-4.105088	3.651745
H	5.584698	-3.008175	3.480217
H	3.938830	-2.374244	3.383229
C	5.084802	-2.348993	-3.114817
H	5.656293	-1.586812	-3.651745
H	5.397505	-3.332402	-3.480217
H	4.025571	-2.224005	-3.383229

Table S 58. Coordinates of the calculated structure of the triplet of 10_6 (n=6) (TPSS-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.288496	-2.255910	1.626212
C	-5.709994	-1.056013	0.916111
C	-5.692239	-1.309402	-0.509664
C	-5.213410	-2.664274	-0.668030
C	-4.914034	-3.182809	0.668030
C	-5.764597	0.249558	1.416604
C	-5.692239	1.309402	0.509664
C	-5.709994	1.056013	-0.916111
C	-5.764597	-0.249558	-1.416604
C	-5.213410	2.664274	0.668030
C	-4.914034	3.182809	-0.668030
C	-5.288496	2.255910	-1.626212
C	-3.980095	4.274923	-0.509664
C	-3.769531	4.416994	0.916111
C	-4.597924	3.452017	1.626212
C	-2.666175	5.117067	1.416604
C	-1.712144	5.584325	0.509664
C	-1.940463	5.473007	-0.916111
C	-3.098423	4.867509	-1.416604
C	-0.299376	5.847083	0.668030
C	0.299376	5.847083	-0.668030
C	-0.690573	5.707927	-1.626212
C	1.712144	5.584325	-0.509664
C	1.940463	5.473007	0.916111
C	0.690573	5.707927	1.626212
C	3.098423	4.867509	1.416604
C	3.980095	4.274923	0.509664
C	3.769531	4.416994	-0.916111
C	2.666175	5.117067	-1.416604
C	4.597924	3.452017	-1.626212
C	5.213410	2.664274	-0.668030

C	4.914034	3.182809	0.668030
C	5.692239	1.309402	-0.509664
C	5.709994	1.056013	0.916111
C	5.288496	2.255910	1.626212
C	5.764597	0.249558	-1.416604
C	5.709994	-1.056013	-0.916111
C	5.692239	-1.309402	0.509664
C	5.764597	-0.249558	1.416604
C	-4.597924	-3.452017	-1.626212
H	3.214720	4.711543	2.485801
H	2.472956	5.139800	-2.485801
H	-2.472956	5.139800	2.485801
H	-3.214720	4.711543	-2.485801
H	-5.687675	0.428258	2.485801
H	-5.687675	-0.428258	-2.485801
H	5.687675	-0.428258	2.485801
H	5.687675	0.428258	-2.485801
C	-3.980095	-4.274923	0.509664
C	-3.769531	-4.416994	-0.916111
C	-3.098423	-4.867509	1.416604
C	-2.666175	-5.117067	-1.416604
C	-1.712144	-5.584325	-0.509664
C	-1.940463	-5.473007	0.916111
C	-0.690573	-5.707927	1.626212
C	-0.299376	-5.847083	-0.668030
C	0.299376	-5.847083	0.668030
C	5.288496	-2.255910	-1.626212
H	-3.214720	-4.711543	2.485801
H	-2.472956	-5.139800	-2.485801
C	1.712144	-5.584325	0.509664
C	0.690573	-5.707927	-1.626212
C	1.940463	-5.473007	-0.916111
C	2.666175	-5.117067	1.416604
C	3.769531	-4.416994	0.916111
C	3.098423	-4.867509	-1.416604
C	3.980095	-4.274923	-0.509664
C	4.597924	-3.452017	1.626212
C	4.914034	-3.182809	-0.668030
C	5.213410	-2.664274	0.668030
H	2.472956	-5.139800	2.485801
H	3.214720	-4.711543	-2.485801
C	0.529185	5.601196	3.108078
H	1.369252	6.067687	3.634092
H	-0.394056	6.079268	3.443811
H	0.496759	4.547386	3.420847
C	-0.529185	5.601196	-3.108078
H	-1.369252	6.067687	-3.634092
H	0.394056	6.079268	-3.443811
H	-0.496759	4.547386	-3.420847
C	-4.586186	3.258885	3.108078
H	-4.570145	4.219650	3.634092
H	-5.461828	2.698371	3.443811
H	-3.689773	2.703899	3.420847
C	-5.115370	2.342311	-3.108078
H	-5.939397	1.848037	-3.634092
H	-5.067772	3.380897	-3.443811
H	-4.186532	1.843488	-3.420847
C	4.586186	3.258885	-3.108078
H	4.570145	4.219650	-3.634092
H	5.461828	2.698371	-3.443811
H	3.689773	2.703899	-3.420847
C	5.115370	2.342311	3.108078
H	5.939397	1.848037	3.634092
H	5.067772	3.380897	3.443811
H	4.186532	1.843488	3.420847
C	-5.115370	-2.342311	3.108078
H	-5.939397	-1.848037	3.634092
H	-5.067772	-3.380897	3.443811
H	-4.186532	-1.843488	3.420847
C	-4.586186	-3.258885	-3.108078
H	-4.570145	-4.219650	-3.634092
H	-5.461828	-2.698371	-3.443811
H	-3.689773	-2.703899	-3.420847
C	-0.529185	-5.601196	3.108078
H	-1.369252	-6.067687	3.634092
H	0.394056	-6.079268	3.443811
H	-0.496759	-4.547386	3.420847
C	0.529185	-5.601196	-3.108078
H	1.369252	-6.067687	-3.634092
H	-0.394056	-6.079268	-3.443811
H	0.496759	-4.547386	-3.420847
C	4.586186	-3.258885	3.108078
H	4.570145	-4.219650	3.634092
H	5.461828	-2.698371	3.443811
H	3.689773	-2.703899	3.420847
C	5.115370	-2.342311	-3.108078
H	5.939397	-1.848037	-3.634092
H	5.067772	-3.380897	-3.443811

H	4.186532	-1.843488	-3.420847

Table S 59. Coordinates of the calculated structure of the open-shell singlet of 10_6 (n=6) (TDDFT, BP86-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.268897	-2.236289	1.646172
C	-5.672259	-1.051968	0.945407
C	-5.653931	-1.312100	-0.511823
C	-5.197228	-2.651276	-0.670331
C	-4.894686	-3.175294	0.670331
C	-5.733192	0.259763	1.428794
C	-5.653931	1.312100	0.511823
C	-5.672259	1.051968	-0.945407
C	-5.733192	-0.259763	-1.428794
C	-5.197228	2.651276	0.670331
C	-4.894686	3.175294	-0.670331
C	-5.268897	2.236289	-1.646172
C	-3.963278	4.240398	-0.511823
C	-3.747161	4.386337	0.945407
C	-4.571132	3.444854	1.646172
C	-2.641635	5.094971	1.428794
C	-1.690654	5.552498	0.511823
C	-1.925099	5.438305	-0.945407
C	-3.091557	4.835208	-1.428794
C	-0.302542	5.826570	0.670331
C	0.302542	5.826570	-0.670331
C	-0.697765	5.681143	-1.646172
C	1.690654	5.552498	-0.511823
C	1.925099	5.438305	0.945407
C	0.697765	5.681143	1.646172
C	3.091557	4.835208	1.428794
C	3.963278	4.240398	0.511823
C	3.747161	4.386337	-0.945407
C	2.641635	5.094971	-1.428794
C	4.571132	3.444854	-1.646172
C	5.197228	2.651276	-0.670331
C	4.894686	3.175294	0.670331
C	5.653931	1.312100	-0.511823
C	5.672259	1.051968	0.945407
C	5.268897	2.236289	1.646172
C	5.733192	0.259763	-1.428794
C	5.672259	-1.051968	-0.945407
C	5.653931	-1.312100	0.511823
C	5.733192	-0.259763	1.428794
C	-4.571132	-3.444854	-1.646172
H	3.228641	4.677822	2.499946
H	2.436792	5.134996	-2.499946
H	-2.436792	5.134996	2.499946
H	-3.228641	4.677822	-2.499946
H	-5.665433	0.457174	2.499946
H	-5.665433	-0.457174	-2.499946
H	5.665433	-0.457174	2.499946
H	5.665433	0.457174	-2.499946
C	-3.963278	-4.240398	0.511823
C	-3.747161	-4.386337	-0.945407
C	-3.091557	-4.835208	1.428794
C	-2.641635	-5.094971	-1.428794
C	-1.690654	-5.552498	-0.511823
C	-1.925099	-5.438305	0.945407
C	-0.697765	-5.681143	1.646172
C	-0.302542	-5.826570	-0.670331
C	0.302542	-5.826570	0.670331
C	5.268897	-2.236289	-1.646172
H	-3.228641	-4.677822	2.499946
H	-2.436792	-5.134996	-2.499946
C	1.690654	-5.552498	0.511823
C	0.697765	-5.681143	-1.646172
C	1.925099	-5.438305	-0.945407
C	2.641635	-5.094971	1.428794
C	3.747161	-4.386337	0.945407
C	3.091557	-4.835208	-1.428794
C	3.963278	-4.240398	-0.511823
C	4.571132	-3.444854	1.646172
C	4.894686	-3.175294	-0.670331
C	5.197228	-2.651276	0.670331
H	2.436792	-5.134996	2.499946
H	3.228641	-4.677822	-2.499946
C	0.497176	5.571896	3.120160
H	1.446757	5.627925	3.667598
H	-0.157909	6.371785	3.493798
H	0.015985	4.613308	3.382519
C	-0.497176	5.571896	-3.120160
H	-1.446757	5.627925	-3.667598
H	0.157909	6.371785	-3.493798

H	-0.015985	4.613308	-3.382519
C	-4.576815	3.216515	3.120160
H	-4.150547	4.066890	3.667598
H	-5.597082	3.049139	3.493798
H	-3.987250	2.320497	3.382519
C	-5.073991	2.355381	-3.120160
H	-5.597304	1.561034	-3.667598
H	-5.439173	3.322646	-3.493798
H	-4.003234	2.292811	-3.382519
C	4.576815	3.216515	-3.120160
H	4.150547	4.066890	-3.667598
H	5.597082	3.049139	-3.493798
H	3.987250	2.320497	-3.382519
C	5.073991	2.355381	3.120160
H	5.597304	1.561034	3.667598
H	5.439173	3.322646	3.493798
H	4.003234	2.292811	3.382519
C	-5.073991	-2.355381	3.120160
H	-5.597304	-1.561034	3.667598
H	-5.439173	-3.322646	3.493798
H	-4.003234	-2.292811	3.382519
C	-4.576815	-3.216515	-3.120160
H	-4.150547	-4.066890	-3.667598
H	-5.597082	-3.049139	-3.493798
H	-3.987250	-2.320497	-3.382519
C	-0.497176	-5.571896	3.120160
H	-1.446757	-5.627925	3.667598
H	0.157909	-6.371785	3.493798
H	-0.015985	-4.613308	3.382519
C	0.497176	-5.571896	-3.120160
H	1.446757	-5.627925	-3.667598
H	-0.157909	-6.371785	-3.493798
H	0.015985	-4.613308	-3.382519
C	4.576815	-3.216515	3.120160
H	4.150547	-4.066890	3.667598
H	5.597082	-3.049139	3.493798
H	3.987250	-2.320497	3.382519
C	5.073991	-2.355381	-3.120160
H	5.597304	-1.561034	-3.667598
H	5.439173	-3.322646	-3.493798
H	4.003234	-2.292811	-3.382519

Table S 60. Coordinates of the calculated structure of 10_7 (n=7) (TPSS-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.829060	-0.297854	-0.668337
C	6.608459	-1.731564	-0.508183
C	6.512875	-1.960518	0.902077
C	6.710425	-0.687639	1.617882
C	6.829060	0.297854	0.668337
C	6.199522	-2.715657	-1.411284
C	5.593506	-3.869608	-0.902077
C	5.474098	-4.087089	0.508183
C	5.988525	-3.153797	1.411284
C	4.721500	-4.817686	-1.617882
C	4.024977	-5.524883	-0.668337
C	4.490721	-5.153465	0.668337
C	2.766516	-6.246313	-0.508183
C	2.527916	-6.314334	0.902077
C	3.646264	-5.675158	1.617882
C	1.268046	-6.648378	1.411284
C	0.217629	-6.828080	0.508183
C	0.462113	-6.785840	-0.902077
C	1.742153	-6.540166	-1.411284
C	-0.822812	-6.695195	-1.617882
C	-1.809995	-6.591563	-0.668337
C	-1.229222	-6.724120	0.668337
C	-2.163609	-6.389167	1.617882
C	-3.360615	-5.913328	0.902077
C	-3.158670	-6.057462	-0.508183
C	-4.407297	-5.136594	1.411284
C	-5.202718	-4.427388	0.508183
C	-5.017261	-4.592197	-0.902077
C	-4.027093	-5.439797	-1.411284
C	-5.747529	-3.531086	-1.617882
C	-6.282005	-2.694661	-0.668337
C	-6.023536	-3.231376	0.668337
C	-6.344240	-2.292003	1.617882
C	-6.718535	-1.059465	0.902077
C	-6.705313	-1.307218	-0.508183
C	-6.763856	0.243150	1.411284
C	-6.705313	1.307218	0.508183
C	-6.718535	1.059465	-0.902077
C	-6.763856	-0.243150	-1.411284

C	-6.282005	2.694661	0.668337
C	-6.023536	3.231376	-0.668337
C	-6.344240	2.292003	-1.617882
C	-5.202718	4.427388	-0.508183
C	-5.017261	4.592197	0.902077
C	-5.747529	3.531086	1.617882
C	-4.027093	5.439797	1.411284
C	-3.158670	6.057462	0.508183
C	-3.360615	5.913328	-0.902077
C	-4.407297	5.136594	-1.411284
C	-2.163609	6.389167	-1.617882
C	-1.229222	6.724120	-0.668337
C	-1.809995	6.591563	0.668337
C	0.217629	6.828080	-0.508183
C	0.462113	6.785840	0.902077
C	-0.822812	6.695195	1.617882
C	1.742153	6.540166	1.411284
C	2.766516	6.246313	0.508183
C	2.527916	6.314334	-0.902077
C	1.268046	6.648378	-1.411284
C	6.710425	0.687639	-1.617882
H	1.895043	-6.437334	-2.482150
H	1.085680	-6.622066	2.482150
H	-3.851370	-5.495216	-2.482150
H	-4.500429	-4.977609	2.482150
H	-6.697623	-0.415089	-2.482150
H	-6.697623	0.415089	2.482150
H	6.214450	-2.532008	-2.482150
H	5.854250	-3.279972	2.482150
H	-4.500429	4.977609	-2.482150
H	-3.851370	5.495216	2.482150
H	1.085680	6.622066	-2.482150
H	1.895043	6.437334	2.482150
C	3.646264	5.675158	-1.617882
C	4.024977	5.524883	0.668337
C	4.490721	5.153465	-0.668337
C	5.474098	4.087089	-0.508183
C	4.721500	4.817686	1.617882
C	5.593506	3.869608	0.902077
C	5.988525	3.153797	-1.411284
C	6.199522	2.715657	1.411284
C	6.512875	1.960518	-0.902077
C	6.608459	1.731564	0.508183
H	5.854250	3.279972	-2.482150

H	6.214450	2.532008	2.482150
C	4.562309	4.835928	3.102047
H	5.534282	4.950023	3.597788
H	3.913869	5.651320	3.428027
H	4.133391	3.889186	3.458805
C	3.699472	5.524017	-3.102047
H	3.594422	6.497009	-3.597788
H	4.638711	5.073278	-3.428027
H	2.871910	4.895183	-3.458805
C	6.625434	0.551805	-3.102047
H	5.617815	0.806747	-3.458805
H	7.320652	1.240587	-3.597788
H	6.858637	-0.463554	-3.428027
C	-0.936328	6.582109	3.102047
H	-0.419516	7.413164	3.597788
H	-1.978122	6.583527	3.428027
H	-0.463561	5.656483	3.458805
C	-2.012268	6.336532	-3.102047
H	-2.838481	6.861051	-3.597788
H	-1.074259	6.789827	-3.428027
H	-2.036602	5.297447	-3.458805
C	6.625434	-0.551805	3.102047
H	7.320652	-1.240587	3.597788
H	6.858637	0.463554	3.428027
H	5.617815	-0.806747	3.458805
C	3.699472	-5.524017	3.102047
H	3.594422	-6.497009	3.597788
H	4.638711	-5.073278	3.428027
H	2.871910	-4.895183	3.458805
C	4.562309	-4.835928	-3.102047
H	5.534282	-4.950023	-3.597788
H	3.913869	-5.651320	-3.428027
H	4.133391	-3.889186	-3.458805
C	-0.936328	-6.582109	-3.102047
H	-0.419516	-7.413164	-3.597788
H	-1.978122	-6.583527	-3.428027
H	-0.463561	-5.656483	-3.458805
C	-2.012268	-6.336532	3.102047
H	-2.838481	-6.861051	3.597788
H	-1.074259	-6.789827	3.428027
H	-2.036602	-5.297447	3.458805
C	-5.729891	-3.371827	-3.102047
H	-6.057409	-4.294042	-3.597788
H	-6.380547	-2.558204	-3.428027

H	-4.711442	-3.164333	-3.458805
C	-6.208729	-2.377509	3.102047
H	-7.133950	-2.058582	3.597788
H	-5.978290	-3.393499	3.428027
H	-5.411511	-1.710625	3.458805
C	-6.208729	2.377509	-3.102047
H	-7.133950	2.058582	-3.597788
H	-5.978290	3.393499	-3.428027
H	-5.411511	1.710625	-3.458805
C	-5.729891	3.371827	3.102047
H	-6.057409	4.294042	3.597788
H	-6.380547	2.558204	3.428027
H	-4.711442	3.164333	3.458805

Table S 61. Coordinates of the calculated structure of the triplet of 10_7 (n=7) (TPSS-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.810921	-0.297963	-0.668550
C	6.586764	-1.719789	-0.510878
C	6.491402	-1.952427	0.912600
C	6.692383	-0.694179	1.624058
C	6.810921	0.297963	0.668550
C	6.180677	-2.702216	-1.416182
C	5.573792	-3.857864	-0.912600
C	5.451366	-4.077468	0.510878
C	5.966266	-3.147444	1.416182
C	4.715363	-4.799502	-1.624058
C	4.013584	-5.510769	-0.668550
C	4.479497	-5.139216	0.668550
C	2.762195	-6.222011	-0.510878
C	2.520854	-6.292501	0.912600
C	3.629902	-5.665129	1.624058
C	1.259136	-6.627014	1.416182
C	0.210978	-6.804309	0.510878
C	0.459003	-6.763105	-0.912600
C	1.740912	-6.517052	-1.416182
C	-0.812421	-6.679060	-1.624058
C	-1.806065	-6.573854	-0.668550
C	-1.225081	-6.706460	0.668550
C	-2.165970	-6.370122	1.624058
C	-3.347948	-5.894193	0.912600
C	-3.142364	-6.038931	-0.510878
C	-4.396150	-5.116308	1.416182
C	-5.188281	-4.407367	0.510878
C	-5.001425	-4.575590	-0.912600
C	-4.009796	-5.424415	-1.416182
C	-5.728436	-3.529150	-1.624058
C	-6.265709	-2.686693	-0.668550
C	-6.007147	-3.223603	0.668550
C	-6.330822	-2.278283	1.624058
C	-6.695678	-1.057438	0.912600
C	-6.680658	-1.308413	-0.510878
C	-6.741045	0.247083	1.416182
C	-6.680658	1.308413	0.510878
C	-6.695678	1.057438	-0.912600
C	-6.741045	-0.247083	-1.416182
C	-6.265709	2.686693	0.668550
C	-6.007147	3.223603	-0.668550
C	-6.330822	2.278283	-1.624058
C	-5.188281	4.407367	-0.510878
C	-5.001425	4.575590	0.912600
C	-5.728436	3.529150	1.624058
C	-4.009796	5.424415	1.416182
C	-3.142364	6.038931	0.510878
C	-3.347948	5.894193	-0.912600
C	-4.396150	5.116308	-1.416182
C	-2.165970	6.370122	-1.624058
C	-1.225081	6.706460	-0.668550
C	-1.806065	6.573854	0.668550
C	0.210978	6.804309	-0.510878
C	0.459003	6.763105	0.912600
C	-0.812421	6.679060	1.624058
C	1.740912	6.517052	1.416182
C	2.762195	6.222011	0.510878
C	2.520854	6.292501	-0.912600
C	1.259136	6.627014	-1.416182
C	6.692383	0.694179	-1.624058
H	1.897853	-6.412327	-2.486355
H	1.072299	-6.600755	2.486355
H	-3.830068	-5.481822	-2.486355
H	-4.492111	-4.953860	2.486355
H	-6.673869	-0.423392	-2.486355
H	-6.673869	0.423392	2.486355
H	6.196651	-2.514220	-2.486355

H	5.829245	-3.277147	2.486355
H	-4.492111	4.953860	-2.486355
H	-3.830068	5.481822	2.486355
H	1.072299	6.600755	-2.486355
H	1.897853	6.412327	2.486355
C	3.629902	5.665129	-1.624058
C	4.013584	5.510769	0.668550
C	4.479497	5.139216	-0.668550
C	5.451366	4.077468	-0.510878
C	4.715363	4.799502	1.624058
C	5.573792	3.857864	0.912600
C	5.966266	3.147444	-1.416182
C	6.180677	2.702216	1.416182
C	6.491402	1.952427	-0.912600
C	6.586764	1.719789	0.510878
H	5.829245	3.277147	-2.486355
H	6.196651	2.514220	2.486355
C	4.544618	4.823146	3.108200
H	5.515026	4.802892	3.617613
H	4.004944	5.714557	3.434862
H	3.984520	3.941182	3.450256
C	3.690947	5.503926	-3.108200
H	3.455265	6.445497	-3.617613
H	4.680097	5.176140	-3.434862
H	2.955729	4.761615	-3.450256
C	6.604411	0.545943	-3.108200
H	5.565648	0.657936	-3.450256
H	7.193615	1.317267	-3.617613
H	6.964862	-0.431777	-3.434862
C	-0.937364	6.560308	3.108200
H	-0.316490	7.306376	3.617613
H	-1.970779	6.694159	3.434862
H	-0.597033	5.572510	3.450256
C	-2.001875	6.317340	-3.108200
H	-2.884970	6.720137	-3.617613
H	-1.128876	6.886318	-3.434862
H	-1.879914	5.279701	-3.450256
C	6.604411	-0.545943	3.108200
H	7.193615	-1.317267	3.617613
H	6.964862	0.431777	3.434862
H	5.565648	-0.657936	3.450256
C	3.690947	-5.503926	3.108200
H	3.455265	-6.445497	3.617613
H	4.680097	-5.176140	3.434862
H	2.955729	-4.761615	3.450256
C	4.544618	-4.823146	-3.108200
H	5.515026	-4.802892	-3.617613
H	4.004944	-5.714557	-3.434862
H	3.984520	-3.941182	-3.450256
C	-0.937364	-6.560308	-3.108200
H	-0.316490	-7.306376	-3.617613
H	-1.970779	-6.694159	-3.434862
H	-0.597033	-5.572510	-3.450256
C	-2.001875	-6.317340	3.108200
H	-2.884970	-6.720137	3.617613
H	-1.128876	-6.886318	3.434862
H	-1.879914	-5.279701	3.450256
C	-5.713492	-3.357424	-3.108200
H	-5.909683	-4.308009	-3.617613
H	-6.462465	-2.632923	-3.434862
H	-4.729007	-3.007624	-3.450256
C	-6.187244	-2.373668	3.108200
H	-7.052764	-1.934376	3.617613
H	-6.087783	-3.410958	3.434862
H	-5.299943	-1.822064	3.450256
C	-6.187244	2.373668	-3.108200
H	-7.052764	1.934376	-3.617613
H	-6.087783	3.410958	-3.434862
H	-5.299943	1.822064	-3.450256
C	-5.713492	3.357424	3.108200
H	-5.909683	4.308009	3.617613
H	-6.462465	2.632923	3.434862
H	-4.729007	3.007624	3.450256

Table S 62. Coordinates of the calculated structure of the open-shell singlet of 10_7 (n=7) (TDDFT, BP86-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.819786	-0.299076	-0.669208
C	6.592384	-1.720226	-0.510642
C	6.495026	-1.954215	0.915776
C	6.695075	-0.694777	1.626674
C	6.819786	0.299076	0.669208

C	6.184343	-2.701989	-1.417732
C	5.577450	-3.859583	-0.915776
C	5.455211	-4.081590	0.510642
C	5.968375	-3.150452	1.417732
C	4.717510	-4.801235	-1.626674
C	4.018240	-5.518395	-0.669208
C	4.485894	-5.145453	0.669208
C	2.765357	-6.226676	-0.510642
C	2.521715	-6.296449	0.915776
C	3.631113	-5.667607	1.626674
C	1.258099	-6.630538	1.417732
C	0.210153	-6.809885	0.510642
C	0.459940	-6.767036	-0.915776
C	1.743375	-6.519776	-1.417732
C	-0.812437	-6.681818	-1.626674
C	-1.809123	-6.582249	-0.669208
C	-1.225967	-6.715351	0.669208
C	-2.167152	-6.372614	1.626674
C	-3.350498	-5.897328	0.915776
C	-3.144040	-6.044312	-0.510642
C	-4.399551	-5.117694	1.417732
C	-5.193154	-4.410198	0.510642
C	-5.003914	-4.578773	-0.915776
C	-4.010390	-5.428039	-1.417732
C	-5.730602	-3.530857	-1.626674
C	-6.274180	-2.689536	-0.669208
C	-6.014651	-3.228453	0.669208
C	-6.333507	-2.278912	1.626674
C	-6.699719	-1.057399	0.915776
C	-6.685910	-1.310458	-0.510642
C	-6.744249	0.248878	1.417732
C	-6.685910	1.310458	0.510642
C	-6.699719	1.057399	-0.915776
C	-6.744249	-0.248878	-1.417732
C	-6.274180	2.689536	0.669208
C	-6.014651	3.228453	-0.669208
C	-6.333507	2.278912	-1.626674
C	-5.193154	4.410198	-0.510642
C	-5.003914	4.578773	0.915776
C	-5.730602	3.530857	1.626674
C	-4.010390	5.428039	1.417732
C	-3.144040	6.044312	0.510642
C	-3.350498	5.897328	-0.915776
C	-4.399551	5.117694	-1.417732

C	-2.167152	6.372614	-1.626674
C	-1.225967	6.715351	-0.669208
C	-1.809123	6.582249	0.669208
C	0.210153	6.809885	-0.510642
C	0.459940	6.767036	0.915776
C	-0.812437	6.681818	1.626674
C	1.743375	6.519776	1.417732
C	2.765357	6.226676	0.510642
C	2.521715	6.296449	-0.915776
C	1.258099	6.630538	-1.417732
C	6.695075	0.694777	-1.626674
H	1.902406	-6.411104	-2.491822
H	1.067666	-6.601628	2.491822
H	-3.826273	-5.484619	-2.491822
H	-4.495682	-4.950783	2.491822
H	-6.673690	-0.428104	-2.491822
H	-6.673690	0.428104	2.491822
H	6.198534	-2.509897	-2.491822
H	5.827040	-3.281314	2.491822
H	-4.495682	4.950783	-2.491822
H	-3.826273	5.484619	2.491822
H	1.067666	6.601628	-2.491822
H	1.902406	6.411104	2.491822
C	3.631113	5.667607	-1.626674
C	4.018240	5.518395	0.669208
C	4.485894	5.145453	-0.669208
C	5.455211	4.081590	-0.510642
C	4.717510	4.801235	1.626674
C	5.577450	3.859583	0.915776
C	5.968375	3.150452	-1.417732
C	6.184343	2.701989	1.417732
C	6.495026	1.954215	-0.915776
C	6.592384	1.720226	0.510642
H	5.827040	3.281314	-2.491822
H	6.198534	2.509897	2.491822
C	4.537829	4.821064	3.106586
H	5.506958	4.796968	3.627052
H	3.995696	5.715189	3.435637
H	3.972172	3.936472	3.446068
C	3.690427	5.496844	-3.106586
H	3.451284	6.436312	-3.627052
H	4.682771	5.167265	-3.435637
H	2.953885	4.748529	-3.446068
C	6.598550	0.541934	-3.106586

H	5.554267	0.651219	-3.446068
H	7.183952	1.314653	-3.627052
H	6.959590	-0.439401	-3.435637
C	-0.939969	6.553702	3.106586
H	-0.316888	7.296373	3.627052
H	-1.977039	6.687323	3.435637
H	-0.601049	5.559920	3.446068
C	-1.996662	6.312519	-3.106586
H	-2.880271	6.711298	-3.627052
H	-1.120270	6.882875	-3.435637
H	-1.870832	5.270100	-3.446068
C	6.598550	-0.541934	3.106586
H	7.183952	-1.314653	3.627052
H	6.959590	0.439401	3.435637
H	5.554267	-0.651219	3.446068
C	3.690427	-5.496844	3.106586
H	3.451284	-6.436312	3.627052
H	4.682771	-5.167265	3.435637
H	2.953885	-4.748529	3.446068
C	4.537829	-4.821064	-3.106586
H	5.506958	-4.796968	-3.627052
H	3.995696	-5.715189	-3.435637
H	3.972172	-3.936472	-3.446068
C	-0.939969	-6.553702	-3.106586
H	-0.316888	-7.296373	-3.627052
H	-1.977039	-6.687323	-3.435637
H	-0.601049	-5.559920	-3.446068
C	-1.996662	-6.312519	3.106586
H	-2.880271	-6.711298	3.627052
H	-1.120270	-6.882875	3.435637
H	-1.870832	-5.270100	3.446068
C	-5.709951	-3.351269	-3.106586
H	-5.902111	-4.301461	-3.627052
H	-6.461023	-2.623766	-3.435637
H	-4.721668	-2.996634	-3.446068
C	-6.180224	-2.374738	3.106586
H	-7.042924	-1.932539	3.627052
H	-6.079725	-3.415540	3.435637
H	-5.286775	-1.823178	3.446068
C	-6.180224	2.374738	-3.106586
H	-7.042924	1.932539	-3.627052
H	-6.079725	3.415540	-3.435637
H	-5.286775	1.823178	-3.446068
C	-5.709951	3.351269	3.106586
H	-5.902111	4.301461	3.627052
H	-6.461023	2.623766	3.435637
H	-4.721668	2.996634	3.446068

Table S 63. Coordinates of the calculated structure of 10_8 (n=8) (TPSS-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.737349	0.242179	1.411747
C	-7.686352	1.306501	0.508994
C	-7.697792	1.059885	-0.901469
C	-7.737349	-0.242179	-1.411747
H	-7.679468	-0.413777	-2.483176
C	-7.686352	-1.306501	-0.508994
C	-7.697792	-1.059885	0.901469
C	-7.369246	-2.305317	1.617448
C	-7.087124	-3.257260	0.668517
C	-7.314584	-2.708123	-0.668517
C	-6.840949	-3.580739	-1.617448
C	-6.358907	-4.511236	0.508994
C	-5.642379	-5.299886	1.411747
H	-5.722788	-5.137620	2.483176
C	-6.192613	-4.693709	-0.901469
C	-4.693709	-6.192613	0.901469
C	-4.511236	-6.358907	-0.508994
C	-5.299886	-5.642379	-1.411747
C	-3.580739	-6.840949	1.617448
C	-2.708123	-7.314584	0.668517
C	-3.257260	-7.087124	-0.668517
C	-2.305317	-7.369246	-1.617448
C	-1.059885	-7.697792	-0.901469
C	-1.306501	-7.686352	0.508994
C	-0.242179	-7.737349	1.411747
C	0.242179	-7.737349	-1.411747
C	1.306501	-7.686352	-0.508994
C	1.059885	-7.697792	0.901469
C	2.305317	-7.369246	1.617448
C	3.257260	-7.087124	0.668517
C	2.708123	-7.314584	-0.668517
C	3.580739	-6.840949	-1.617448
C	4.693709	-6.192613	-0.901469

C	4.511236	-6.358907	0.508994
C	5.299886	-5.642379	1.411747
C	5.642379	-5.299886	-1.411747
C	6.358907	-4.511236	-0.508994
C	6.192613	-4.693709	0.901469
C	6.840949	-3.580739	1.617448
C	7.087124	-3.257260	-0.668517
C	7.314584	-2.708123	0.668517
C	7.369246	-2.305317	-1.617448
C	7.697792	-1.059885	-0.901469
C	7.686352	-1.306501	0.508994
C	7.737349	-0.242179	1.411747
C	7.737349	0.242179	-1.411747
C	7.686352	1.306501	-0.508994
C	7.697792	1.059885	0.901469
C	7.314584	2.708123	-0.668517
C	7.369246	2.305317	1.617448
C	6.840949	3.580739	-1.617448
C	7.087124	3.257260	0.668517
C	6.192613	4.693709	-0.901469
C	6.358907	4.511236	0.508994
C	5.299886	5.642379	-1.411747
C	5.642379	5.299886	1.411747
C	4.693709	6.192613	0.901469
C	4.511236	6.358907	-0.508994
C	3.257260	7.087124	-0.668517
C	3.580739	6.840949	1.617448
C	2.708123	7.314584	0.668517
C	2.305317	7.369246	-1.617448
C	1.059885	7.697792	-0.901469
C	1.306501	7.686352	0.508994
C	0.242179	7.737349	1.411747
C	-0.242179	7.737349	-1.411747
C	-1.306501	7.686352	-0.508994
C	-1.059885	7.697792	0.901469
C	-2.305317	7.369246	1.617448
C	-7.314584	2.708123	0.668517
C	-7.369246	2.305317	-1.617448
C	-7.087124	3.257260	-0.668517
H	-7.679468	0.413777	2.483176
H	-5.137620	-5.722788	-2.483176
H	-0.413777	-7.679468	2.483176
H	0.413777	-7.679468	-2.483176
H	5.722788	-5.137620	-2.483176

H	5.137620	-5.722788	2.483176
H	7.679468	0.413777	-2.483176
H	7.679468	-0.413777	2.483176
H	5.137620	5.722788	-2.483176
H	5.722788	5.137620	2.483176
H	-0.413777	7.679468	-2.483176
H	0.413777	7.679468	2.483176
C	-2.708123	7.314584	-0.668517
C	-3.257260	7.087124	0.668517
C	-3.580739	6.840949	-1.617448
C	-4.511236	6.358907	0.508994
C	-4.693709	6.192613	-0.901469
C	-5.299886	5.642379	1.411747
C	-5.642379	5.299886	-1.411747
C	-6.192613	4.693709	0.901469
C	-6.358907	4.511236	-0.508994
H	-5.137620	5.722788	2.483176
H	-5.722788	5.137620	-2.483176
C	-6.840949	3.580739	1.617448
C	7.252096	2.398920	3.102692
H	8.178438	2.067802	3.588710
H	7.041288	3.419563	3.427332
H	6.449521	1.745591	3.471721
C	6.824299	3.431714	-3.102692
H	7.245186	4.320873	-3.588710
H	7.396939	2.560946	-3.427332
H	5.794819	3.326180	-3.471721
C	7.252096	-2.398920	-3.102692
H	8.178438	-2.067802	-3.588710
H	7.041288	-3.419563	-3.427332
H	6.449521	-1.745591	-3.471721
C	6.824299	-3.431714	3.102692
H	7.245186	-4.320873	3.588710
H	7.396939	-2.560946	3.427332
H	5.794819	-3.326180	3.471721
C	3.431714	-6.824299	-3.102692
H	4.320873	-7.245186	-3.588710
H	2.560946	-7.396939	-3.427332
H	3.326180	-5.794819	-3.471721
C	2.398920	-7.252096	3.102692
H	2.067802	-8.178438	3.588710
H	3.419563	-7.041288	3.427332
H	1.745591	-6.449521	3.471721
C	-2.398920	-7.252096	-3.102692

H	-2.067802	-8.178438	-3.588710
H	-3.419563	-7.041288	-3.427332
H	-1.745591	-6.449521	-3.471721
C	-3.431714	-6.824299	3.102692
H	-4.320873	-7.245186	3.588710
H	-2.560946	-7.396939	3.427332
H	-3.326180	-5.794819	3.471721
C	-6.824299	-3.431714	-3.102692
H	-7.245186	-4.320873	-3.588710
H	-7.396939	-2.560946	-3.427332
H	-5.794819	-3.326180	-3.471721
C	-7.252096	-2.398920	3.102692
H	-8.178438	-2.067802	3.588710
H	-7.041288	-3.419563	3.427332
H	-6.449521	-1.745591	3.471721
C	-7.252096	2.398920	-3.102692
H	-8.178438	2.067802	-3.588710
H	-7.041288	3.419563	-3.427332
H	-6.449521	1.745591	-3.471721
C	-6.824299	3.431714	3.102692

H	-7.245186	4.320873	3.588710
H	-7.396939	2.560946	3.427332
H	-5.794819	3.326180	3.471721
C	-3.431714	6.824299	-3.102692
H	-4.320873	7.245186	-3.588710
H	-2.560946	7.396939	-3.427332
H	-3.326180	5.794819	-3.471721
C	-2.398920	7.252096	3.102692
H	-2.067802	8.178438	3.588710
H	-3.419563	7.041288	3.427332
H	-1.745591	6.449521	3.471721
C	2.398920	7.252096	-3.102692
H	2.067802	8.178438	-3.588710
H	3.419563	7.041288	-3.427332
H	1.745591	6.449521	-3.471721
C	3.431714	6.824299	3.102692
H	4.320873	7.245186	3.588710
H	2.560946	7.396939	3.427332
H	3.326180	5.794819	3.471721

Table S 64. Coordinates of the calculated structure of the triplet of 10_8 (n=8) (TPSS-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.714585	0.245372	1.416135
C	-7.661466	1.307878	0.511832
C	-7.674594	1.058009	-0.910554
C	-7.714585	-0.245372	-1.416135
H	-7.656128	-0.420191	-2.487033
C	-7.661466	-1.307878	-0.511832
C	-7.674594	-1.058009	0.910554
C	-7.354070	-2.292392	1.622714
C	-7.068833	-3.250021	0.668840
C	-7.296532	-2.700308	-0.668840
C	-6.821078	-3.579147	-1.622714
C	-6.342284	-4.492665	0.511832
C	-5.628539	-5.281531	1.416135
H	-5.710820	-5.116580	2.487033
C	-6.174883	-4.678632	-0.910554
C	-4.678632	-6.174883	0.910554
C	-4.492665	-6.342284	-0.511832
C	-5.281531	-5.628539	-1.416135
C	-3.579147	-6.821078	1.622714
C	-2.700308	-7.296532	0.668840

C	-3.250021	-7.068833	-0.668840
C	-2.292392	-7.354070	-1.622714
C	-1.058009	-7.674594	-0.910554
C	-1.307878	-7.661466	0.511832
C	-0.245372	-7.714585	1.416135
C	0.245372	-7.714585	-1.416135
C	1.307878	-7.661466	-0.511832
C	1.058009	-7.674594	0.910554
C	2.292392	-7.354070	1.622714
C	3.250021	-7.068833	0.668840
C	2.700308	-7.296532	-0.668840
C	3.579147	-6.821078	-1.622714
C	4.678632	-6.174883	-0.910554
C	4.492665	-6.342284	0.511832
C	5.281531	-5.628539	1.416135
C	5.628539	-5.281531	-1.416135
C	6.342284	-4.492665	-0.511832
C	6.174883	-4.678632	0.910554
C	6.821078	-3.579147	1.622714
C	7.068833	-3.250021	-0.668840
C	7.296532	-2.700308	0.668840

C	7.354070	-2.292392	-1.622714
C	7.674594	-1.058009	-0.910554
C	7.661466	-1.307878	0.511832
C	7.714585	-0.245372	1.416135
C	7.714585	0.245372	-1.416135
C	7.661466	1.307878	-0.511832
C	7.674594	1.058009	0.910554
C	7.296532	2.700308	-0.668840
C	7.354070	2.292392	1.622714
C	6.821078	3.579147	-1.622714
C	7.068833	3.250021	0.668840
C	6.174883	4.678632	-0.910554
C	6.342284	4.492665	0.511832
C	5.281531	5.628539	-1.416135
C	5.628539	5.281531	1.416135
C	4.678632	6.174883	0.910554
C	4.492665	6.342284	-0.511832
C	3.250021	7.068833	-0.668840
C	3.579147	6.821078	1.622714
C	2.700308	7.296532	0.668840
C	2.292392	7.354070	-1.622714
C	1.058009	7.674594	-0.910554
C	1.307878	7.661466	0.511832
C	0.245372	7.714585	1.416135
C	-0.245372	7.714585	-1.416135
C	-1.307878	7.661466	-0.511832
C	-1.058009	7.674594	0.910554
C	-2.292392	7.354070	1.622714
C	-7.296532	2.700308	0.668840
C	-7.354070	2.292392	-1.622714
C	-7.068833	3.250021	-0.668840
H	-7.656128	0.420191	2.487033
H	-5.116580	-5.710820	-2.487033
H	-0.420191	-7.656128	2.487033
H	0.420191	-7.656128	-2.487033
H	5.710820	-5.116580	-2.487033
H	5.116580	-5.710820	2.487033
H	7.656128	0.420191	-2.487033
H	7.656128	-0.420191	2.487033
H	5.116580	5.710820	-2.487033
H	5.710820	5.116580	2.487033
H	-0.420191	7.656128	-2.487033
H	0.420191	7.656128	2.487033
C	-2.700308	7.296532	-0.668840

C	-3.250021	7.068833	0.668840
C	-3.579147	6.821078	-1.622714
C	-4.492665	6.342284	0.511832
C	-4.678632	6.174883	-0.910554
C	-5.281531	5.628539	1.416135
C	-5.628539	5.281531	-1.416135
C	-6.174883	4.678632	0.910554
C	-6.342284	4.492665	-0.511832
H	-5.116580	5.710820	2.487033
H	-5.710820	5.116580	-2.487033
C	-6.821078	3.579147	1.622714
C	7.233089	2.393696	3.108274
H	8.120923	1.982926	3.603899
H	7.109570	3.429290	3.431394
H	6.370287	1.816737	3.469550
C	6.807165	3.421967	-3.108274
H	7.144500	4.340220	-3.603899
H	7.452099	2.602351	-3.431394
H	5.789100	3.219846	-3.469550
C	7.233089	-2.393696	-3.108274
H	8.120923	-1.982926	-3.603899
H	7.109570	-3.429290	-3.431394
H	6.370287	-1.816737	-3.469550
C	6.807165	-3.421967	3.108274
H	7.144500	-4.340220	3.603899
H	7.452099	-2.602351	3.431394
H	5.789100	-3.219846	3.469550
C	3.421967	-6.807165	-3.108274
H	4.340220	-7.144500	-3.603899
H	2.602351	-7.452099	-3.431394
H	3.219846	-5.789100	-3.469550
C	2.393696	-7.233089	3.108274
H	1.982926	-8.120923	3.603899
H	3.429290	-7.109570	3.431394
H	1.816737	-6.370287	3.469550
C	-2.393696	-7.233089	-3.108274
H	-1.982926	-8.120923	-3.603899
H	-3.429290	-7.109570	-3.431394
H	-1.816737	-6.370287	-3.469550
C	-3.421967	-6.807165	3.108274
H	-4.340220	-7.144500	3.603899
H	-2.602351	-7.452099	3.431394
H	-3.219846	-5.789100	3.469550
C	-6.807165	-3.421967	-3.108274

H	-7.144500	-4.340220	-3.603899
H	-7.452099	-2.602351	-3.431394
H	-5.789100	-3.219846	-3.469550
C	-7.233089	-2.393696	3.108274
H	-8.120923	-1.982926	3.603899
H	-7.109570	-3.429290	3.431394
H	-6.370287	-1.816737	3.469550
C	-7.233089	2.393696	-3.108274
H	-8.120923	1.982926	-3.603899
H	-7.109570	3.429290	-3.431394
H	-6.370287	1.816737	-3.469550
C	-6.807165	3.421967	3.108274
H	-7.144500	4.340220	3.603899
H	-7.452099	2.602351	3.431394
H	-5.789100	3.219846	3.469550
C	-3.421967	6.807165	-3.108274

H	-4.340220	7.144500	-3.603899
H	-2.602351	7.452099	-3.431394
H	-3.219846	5.789100	-3.469550
C	-2.393696	7.233089	3.108274
H	-1.982926	8.120923	3.603899
H	-3.429290	7.109570	3.431394
H	-1.816737	6.370287	3.469550
C	2.393696	7.233089	-3.108274
H	1.982926	8.120923	-3.603899
H	3.429290	7.109570	-3.431394
H	1.816737	6.370287	-3.469550
C	3.421967	6.807165	3.108274
H	4.340220	7.144500	3.603899
H	2.602351	7.452099	3.431394
H	3.219846	5.789100	3.469550

Table S 65. Coordinates of the calculated structure of the open-shell singlet of 10_8 (n=8) (TDDFT, BP86-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.724769	0.246331	1.417017
C	-7.673830	1.309383	0.510757
C	-7.685439	1.058563	-0.912316
C	-7.724769	-0.246331	-1.417017
H	-7.663884	-0.423598	-2.491911
C	-7.673830	-1.309383	-0.510757
C	-7.685439	-1.058563	0.912316
C	-7.362125	-2.296975	1.625288
C	-7.081984	-3.256215	0.669763
C	-7.310211	-2.705227	-0.669763
C	-6.830015	-3.581602	-1.625288
C	-6.352090	-4.500344	0.510757
C	-5.636419	-5.288055	1.417017
H	-5.718713	-5.119655	2.491911
C	-6.182943	-4.685909	-0.912316
C	-4.685909	-6.182943	0.912316
C	-4.500344	-6.352090	-0.510757
C	-5.288055	-5.636419	-1.417017
C	-3.581602	-6.830015	1.625288
C	-2.705227	-7.310211	0.669763
C	-3.256215	-7.081984	-0.669763
C	-2.296975	-7.362125	-1.625288
C	-1.058563	-7.685439	-0.912316
C	-1.309383	-7.673830	0.510757

C	-0.246331	-7.724769	1.417017
C	0.246331	-7.724769	-1.417017
C	1.309383	-7.673830	-0.510757
C	1.058563	-7.685439	0.912316
C	2.296975	-7.362125	1.625288
C	3.256215	-7.081984	0.669763
C	2.705227	-7.310211	-0.669763
C	3.581602	-6.830015	-1.625288
C	4.685909	-6.182943	-0.912316
C	4.500344	-6.352090	0.510757
C	5.288055	-5.636419	1.417017
C	5.636419	-5.288055	-1.417017
C	6.352090	-4.500344	-0.510757
C	6.182943	-4.685909	0.912316
C	6.830015	-3.581602	1.625288
C	7.081984	-3.256215	-0.669763
C	7.310211	-2.705227	0.669763
C	7.362125	-2.296975	-1.625288
C	7.685439	-1.058563	-0.912316
C	7.673830	-1.309383	0.510757
C	7.724769	-0.246331	1.417017
C	7.724769	0.246331	-1.417017
C	7.673830	1.309383	-0.510757
C	7.685439	1.058563	0.912316
C	7.310211	2.705227	-0.669763

C	7.362125	2.296975	1.625288
C	6.830015	3.581602	-1.625288
C	7.081984	3.256215	0.669763
C	6.182943	4.685909	-0.912316
C	6.352090	4.500344	0.510757
C	5.288055	5.636419	-1.417017
C	5.636419	5.288055	1.417017
C	4.685909	6.182943	0.912316
C	4.500344	6.352090	-0.510757
C	3.256215	7.081984	-0.669763
C	3.581602	6.830015	1.625288
C	2.705227	7.310211	0.669763
C	2.296975	7.362125	-1.625288
C	1.058563	7.685439	-0.912316
C	1.309383	7.673830	0.510757
C	0.246331	7.724769	1.417017
C	-0.246331	7.724769	-1.417017
C	-1.309383	7.673830	-0.510757
C	-1.058563	7.685439	0.912316
C	-2.296975	7.362125	1.625288
C	-7.310211	2.705227	0.669763
C	-7.362125	2.296975	-1.625288
C	-7.081984	3.256215	-0.669763
H	-7.663884	0.423598	2.491911
H	-5.119655	-5.718713	-2.491911
H	-0.423598	-7.663884	2.491911
H	0.423598	-7.663884	-2.491911
H	5.718713	-5.119655	-2.491911
H	5.119655	-5.718713	2.491911
H	7.663884	0.423598	-2.491911
H	7.663884	-0.423598	2.491911
H	5.119655	5.718713	-2.491911
H	5.718713	5.119655	2.491911
H	-0.423598	7.663884	-2.491911
H	0.423598	7.663884	2.491911
C	-2.705227	7.310211	-0.669763
C	-3.256215	7.081984	0.669763
C	-3.581602	6.830015	-1.625288
C	-4.500344	6.352090	0.510757
C	-4.685909	6.182943	-0.912316
C	-5.288055	5.636419	1.417017
C	-5.636419	5.288055	-1.417017
C	-6.182943	4.685909	0.912316
C	-6.352090	4.500344	-0.510757

H	-5.119655	5.718713	2.491911
H	-5.718713	5.119655	-2.491911
C	-6.830015	3.581602	1.625288
C	7.233856	2.397576	3.106591
H	8.131325	2.006648	3.610626
H	7.085060	3.433746	3.431091
H	6.381458	1.799040	3.470200
C	6.810451	3.419766	-3.106591
H	7.168629	4.330801	-3.610626
H	7.437919	2.581868	-3.431091
H	5.784486	3.240259	-3.470200
C	7.233856	-2.397576	-3.106591
H	8.131325	-2.006648	-3.610626
H	7.085060	-3.433746	-3.431091
H	6.381458	-1.799040	-3.470200
C	6.810451	-3.419766	3.106591
H	7.168629	-4.330801	3.610626
H	7.437919	-2.581868	3.431091
H	5.784486	-3.240259	3.470200
C	3.419766	-6.810451	-3.106591
H	4.330801	-7.168629	-3.610626
H	2.581868	-7.437919	-3.431091
H	3.240259	-5.784486	-3.470200
C	2.397576	-7.233856	3.106591
H	2.006648	-8.131325	3.610626
H	3.433746	-7.085060	3.431091
H	1.799040	-6.381458	3.470200
C	-2.397576	-7.233856	-3.106591
H	-2.006648	-8.131325	-3.610626
H	-3.433746	-7.085060	-3.431091
H	-1.799040	-6.381458	-3.470200
C	-3.419766	-6.810451	3.106591
H	-4.330801	-7.168629	3.610626
H	-2.581868	-7.437919	3.431091
H	-3.240259	-5.784486	3.470200
C	-6.810451	-3.419766	-3.106591
H	-7.168629	-4.330801	-3.610626
H	-7.437919	-2.581868	-3.431091
H	-5.784486	-3.240259	-3.470200
C	-7.233856	-2.397576	3.106591
H	-8.131325	-2.006648	3.610626
H	-7.085060	-3.433746	3.431091
H	-6.381458	-1.799040	3.470200
C	-7.233856	2.397576	-3.106591

H	-8.131325	2.006648	-3.610626
H	-7.085060	3.433746	-3.431091
H	-6.381458	1.799040	-3.470200
C	-6.810451	3.419766	3.106591
H	-7.168629	4.330801	3.610626
H	-7.437919	2.581868	3.431091
H	-5.784486	3.240259	3.470200
C	-3.419766	6.810451	-3.106591
H	-4.330801	7.168629	-3.610626
H	-2.581868	7.437919	-3.431091
H	-3.240259	5.784486	-3.470200
C	-2.397576	7.233856	3.106591

H	-2.006648	8.131325	3.610626
H	-3.433746	7.085060	3.431091
H	-1.799040	6.381458	3.470200
C	2.397576	7.233856	-3.106591
H	2.006648	8.131325	-3.610626
H	3.433746	7.085060	-3.431091
H	1.799040	6.381458	-3.470200
C	3.419766	6.810451	3.106591
H	4.330801	7.168629	3.610626
H	2.581868	7.437919	3.431091
H	3.240259	5.784486	3.470200

4.5 Calculated coordinates of alkynyl-substituted cyclacenes 11_n

Below can be found coordinates for the calculated structures of alkynyl-substituted $[5.5.6]_n$cyclacenes $\mathbf{11_n}$ as singlets and triplets at the TPSS-D3/def2-TZVP level of theory and of the open-shell singlets calculated using TDDFT at the BP86-D3/def2-TZVP level of theory, optimized in point group D_n.

Table S 66. Coordinates of the calculated structure of 11_3 (n=3) (TPSS-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.932520	2.056052	-1.628015
C	-2.753917	1.040432	-0.912940
C	-2.705095	1.312098	0.487104
C	-1.767930	2.426960	0.657568
C	-1.217844	2.744553	-0.657568
C	-2.874855	-0.263362	-1.407527
C	-2.705095	-1.312098	-0.487104
C	-2.753917	-1.040432	0.912940
C	-2.874855	0.263362	1.407527
C	-1.767930	-2.426960	-0.657568
C	-1.217844	-2.744553	0.657568
C	-1.932520	-2.056052	1.628015
C	0.216238	-2.998730	0.487104
C	0.475918	-2.905178	-0.912940
C	-0.814334	-2.701637	-1.628015
C	1.665505	-2.358016	-1.407527
C	2.488857	-1.686633	-0.487104
C	2.277999	-1.864746	0.912940
C	1.209350	-2.621378	1.407527
C	2.985774	-0.317593	-0.657568
C	2.985774	0.317593	0.657568
C	2.746854	-0.645585	1.628015
C	2.488857	1.686633	0.487104
C	2.277999	1.864746	-0.912940
C	2.746854	0.645585	-1.628015
C	1.209350	2.621378	-1.407527
C	0.216238	2.998730	-0.487104
C	0.475918	2.905178	0.912940
C	1.665505	2.358016	1.407527
C	-0.814334	2.701637	1.628015
H	0.983424	2.586905	-2.469250
H	1.748613	2.145123	2.469250
H	1.748613	-2.145123	-2.469250
H	0.983424	-2.586905	2.469250
H	-2.732037	-0.441782	-2.469250
H	-2.732037	0.441782	2.469250
C	-1.491122	-2.008078	4.203710
C	-1.690921	-2.039260	3.007422
H	-1.312866	-1.998712	5.254001
C	-0.993486	-2.295389	-4.203710
C	-0.920590	-2.484011	-3.007422
H	-1.074503	-2.136332	-5.254001
C	2.484608	-0.287310	4.203710
C	2.611511	-0.444751	3.007422
H	2.387369	-0.137619	5.254001
C	2.484608	0.287310	-4.203710
C	2.611511	0.444751	-3.007422
H	2.387369	0.137619	-5.254001
C	-0.993486	2.295389	4.203710
C	-0.920590	2.484011	3.007422
H	-1.074503	2.136332	5.254001
C	-1.491122	2.008078	-4.203710
C	-1.690921	2.039260	-3.007422
H	-1.312866	1.998712	-5.254001

Table S 67. Coordinates of the calculated structure of the triplet of 11_3 (n=3) (TPSS-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.935032	2.0410281	-1.6438603
C	-2.7262165	1.034194	-0.9317848
C	-2.6725407	1.3100012	0.4906126
C	-1.7652704	2.4239179	0.6597523
C	-1.2165393	2.740728	-0.6597523
C	-2.8580542	-0.2699813	-1.4178536
C	-2.6725407	-1.3100012	-0.4906126
C	-2.7262165	-1.034194	0.9317848
C	-2.8580542	0.2699813	1.4178536
C	-1.7652704	-2.4239179	-0.6597523
C	-1.2165393	-2.740728	0.6597523

C	-1.935032	-2.0410281	1.6438603
C	0.2017761	-2.9694888	0.4906126
C	0.4674699	-2.8780698	-0.9317848
C	-0.8000662	-2.6963009	-1.6438603
C	1.6628378	-2.3401569	-1.4178536
C	2.4707647	-1.6594876	-0.4906126
C	2.2587466	-1.8438757	0.9317848
C	1.1952165	-2.6101382	1.4178536
C	2.9818097	-0.3168101	-0.6597523
C	2.9818097	0.3168101	0.6597523
C	2.7350981	-0.6552728	1.6438603
C	2.4707647	1.6594876	0.4906126
C	2.2587466	1.8438757	-0.9317848
C	2.7350981	0.6552728	-1.6438603
C	1.1952165	2.6101382	-1.4178536
C	0.2017761	2.9694888	-0.4906126
C	0.4674699	2.8780698	0.9317848
C	1.6628378	2.3401569	1.4178536
C	-0.8000662	2.6963009	1.6438603
H	0.9681874	2.5897466	-2.4794978
H	1.7586927	2.1333482	2.4794978
H	1.7586927	-2.1333482	-2.4794978
H	0.9681874	-2.5897466	2.4794978
H	-2.72688	-0.4563985	-2.4794978
H	-2.72688	0.4563985	2.4794978
C	-1.4573105	-1.9795374	4.2119107
C	-1.6812296	-2.0209736	3.0194437
H	-1.2667932	-1.9662445	5.2598701
C	-0.9856744	-2.2518366	-4.2119107
C	-0.9095997	-2.4664743	-3.0194437
H	-1.0694211	-2.0801974	-5.2598701
C	2.4429849	-0.2722992	4.2119107
C	2.5908292	-0.4455007	3.0194437
H	2.3362143	-0.1139528	5.2598701
C	2.4429849	0.2722992	-4.2119107
C	2.5908292	0.4455007	-3.0194437
H	2.3362143	0.1139528	-5.2598701
C	-0.9856744	2.2518366	4.2119107
C	-0.9095997	2.4664743	3.0194437
H	-1.0694211	2.0801974	5.2598701
C	-1.4573105	1.9795374	-4.2119107
C	-1.6812296	2.0209736	-3.0194437
H	-1.2667932	1.9662445	-5.2598701

Table S 68. Coordinates of the calculated structure of the open-shell singlet of 11_3 (n=3) (TDDFT, BP86-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.9333242	2.0600284	-1.6503063
C	-2.7135065	1.0292575	-0.9344817
C	-2.6698667	1.3131999	0.4838144
C	-1.7827776	2.4499335	0.6560022
C	-1.2303159	2.7688974	-0.6560022
C	-2.8500216	-0.2747197	-1.4189117
C	-2.6698667	-1.3131999	-0.4838144
C	-2.7135065	-1.0292575	0.9344817
C	-2.8500216	0.2747197	1.4189117
C	-1.7827776	-2.4499335	-0.6560022
C	-1.2303159	-2.7688974	0.6560022
C	-1.9333242	-2.0600284	1.6503063
C	0.1976689	-2.9687724	0.4838144
C	0.4653901	-2.8645943	-0.9344817
C	-0.8173748	-2.7043221	-1.6503063
C	1.6629251	-2.3308313	-1.4189117
C	2.4721978	-1.6555725	-0.4838144
C	2.2481164	-1.8353368	0.9344817
C	1.1870966	-2.605551	1.4189117
C	3.0130935	-0.3189639	-0.6560022
C	3.0130935	0.3189639	0.6560022
C	2.750699	-0.6442937	1.6503063
C	2.4721978	1.6555725	0.4838144
C	2.2481164	1.8353368	-0.9344817
C	2.750699	0.6442937	-1.6503063
C	1.1870966	2.605551	-1.4189117
C	0.1976689	2.9687724	-0.4838144
C	0.4653901	2.8645943	0.9344817
C	1.6629251	2.3308313	1.4189117
C	-0.8173748	2.7043221	1.6503063
H	0.9524659	2.585172	-2.4835781
H	1.7625916	2.1174457	2.4835781
H	1.7625916	-2.1174457	-2.4835781
H	0.9524659	-2.585172	2.4835781
H	-2.7150576	-0.4677263	-2.4835781
H	-2.7150576	0.4677263	2.4835781
C	-1.4783751	-2.0372418	4.2238049
C	-1.685464	-2.0548649	3.022104
H	-1.2918176	-2.0359124	5.2768244
C	-1.0251156	-2.2989313	-4.2238049
C	-0.9368332	-2.4870871	-3.022104

H	-1.117243	-2.1367031	-5.2768244
C	2.5034907	-0.2616895	4.2238049
C	2.6222972	-0.4322222	3.022104
H	2.4090607	-0.1007907	5.2768244
C	2.5034907	0.2616895	-4.2238049
C	2.6222972	0.4322222	-3.022104
H	2.4090607	0.1007907	-5.2768244

C	-1.0251156	2.2989313	4.2238049
C	-0.9368332	2.4870871	3.022104
H	-1.117243	2.1367031	5.2768244
C	-1.4783751	2.0372418	-4.2238049
C	-1.685464	2.0548649	-3.022104
H	-1.2918176	2.0359124	-5.2768244

Table S 69. Coordinates of the calculated structure of 11_4 (n=4) (TPSS-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.705776	-1.035595	-0.942424
C	3.668253	-1.308456	0.501704
C	3.798944	0.267229	-1.429381
C	3.668253	1.308456	-0.501704
C	3.705776	1.035595	0.942424
C	3.798944	-0.267229	1.429381
C	3.110947	-2.146043	-1.646739
C	2.990021	-2.548610	0.661250
C	2.548610	-2.990021	-0.661250
C	2.146043	-3.110947	1.646739
C	1.308456	-3.668253	-0.501704
C	1.035595	-3.705776	0.942424
C	0.267229	-3.798944	-1.429381
C	-0.267229	-3.798944	1.429381
C	-1.035595	-3.705776	-0.942424
C	-1.308456	-3.668253	0.501704
C	-2.548610	-2.990021	0.661250
C	-2.146043	-3.110947	-1.646739
C	-2.990021	-2.548610	-0.661250
C	-3.110947	-2.146043	1.646739
C	-3.668253	-1.308456	-0.501704
C	-3.705776	-1.035595	0.942424
C	-3.798944	-0.267229	-1.429381
C	-3.798944	0.267229	1.429381
C	-3.668253	1.308456	0.501704
C	-3.705776	1.035595	-0.942424
C	-3.110947	2.146043	-1.646739
C	-2.990021	2.548610	0.661250
C	-2.548610	2.990021	-0.661250
C	-2.146043	3.110947	1.646739
C	-1.035595	3.705776	0.942424
C	-1.308456	3.668253	-0.501704
C	0.267229	3.798944	1.429381

C	-0.267229	3.798944	-1.429381
C	1.035595	3.705776	-0.942424
C	1.308456	3.668253	0.501704
C	2.146043	3.110947	-1.646739
C	2.548610	2.990021	0.661250
C	2.990021	2.548610	-0.661250
C	3.110947	2.146043	1.646739
H	-3.692184	0.459486	2.492712
H	-3.692184	-0.459486	-2.492712
H	-0.459486	-3.692184	2.492712
H	0.459486	-3.692184	-2.492712
H	3.692184	-0.459486	2.492712
H	3.692184	0.459486	-2.492712
H	0.459486	3.692184	2.492712
H	-0.459486	3.692184	-2.492712
C	-2.236785	2.684580	4.225184
C	-2.199707	2.886902	3.029173
H	-2.281487	2.514786	5.275928
C	-2.684580	2.236785	-4.225184
C	-2.886902	2.199707	-3.029173
H	-2.514786	2.281487	-5.275928
C	2.236785	2.684580	-4.225184
C	2.199707	2.886902	-3.029173
H	2.281487	2.514786	-5.275928
C	2.684580	2.236785	4.225184
C	2.886902	2.199707	3.029173
H	2.514786	2.281487	5.275928
C	2.684580	-2.236785	-4.225184
C	2.886902	-2.199707	-3.029173
H	2.514786	-2.281487	-5.275928
C	2.236785	-2.684580	4.225184
C	2.199707	-2.886902	3.029173
H	2.281487	-2.514786	5.275928
C	-2.236785	-2.684580	-4.225184

C	-2.199707	-2.886902	-3.029173
H	-2.281487	-2.514786	-5.275928
C	-2.684580	-2.236785	4.225184
C	-2.886902	-2.199707	3.029173
H	-2.514786	-2.281487	5.275928

Table S 70. Coordinates of the calculated structure of the triplet of 11_4 (n=4) (TPSS-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.731309	-1.039740	-0.926108
C	3.698993	-1.309060	0.496471
C	3.817314	0.262624	-1.420301
C	3.698993	1.309060	-0.496471
C	3.731309	1.039740	0.926108
C	3.817314	-0.262624	1.420301
C	3.110922	-2.160278	-1.634801
C	2.999101	-2.558305	0.659045
C	2.558305	-2.999101	-0.659045
C	2.160278	-3.110922	1.634801
C	1.309060	-3.698993	-0.496471
C	1.039740	-3.731309	0.926108
C	0.262624	-3.817314	-1.420301
C	-0.262624	-3.817314	1.420301
C	-1.039740	-3.731309	-0.926108
C	-1.309060	-3.698993	0.496471
C	-2.558305	-2.999101	0.659045
C	-2.160278	-3.110922	-1.634801
C	-2.999101	-2.558305	-0.659045
C	-3.110922	-2.160278	1.634801
C	-3.698993	-1.309060	-0.496471
C	-3.731309	-1.039740	0.926108
C	-3.817314	-0.262624	-1.420301
C	-3.817314	0.262624	1.420301
C	-3.698993	1.309060	0.496471
C	-3.731309	1.039740	-0.926108
C	-3.110922	2.160278	-1.634801
C	-2.999101	2.558305	0.659045
C	-2.558305	2.999101	-0.659045
C	-2.160278	3.110922	1.634801
C	-1.039740	3.731309	0.926108
C	-1.309060	3.698993	-0.496471
C	0.262624	3.817314	1.420301
C	-0.262624	3.817314	-1.420301
C	1.039740	3.731309	-0.926108
C	1.309060	3.698993	0.496471
C	2.160278	3.110922	-1.634801
C	2.558305	2.999101	0.659045
C	2.999101	2.558305	-0.659045
C	3.110922	2.160278	1.634801
H	-3.703147	0.448969	2.483968
H	-3.703147	-0.448969	-2.483968
H	-0.448969	-3.703147	2.483968
H	0.448969	-3.703147	-2.483968
H	3.703147	-0.448969	2.483968
H	3.703147	0.448969	-2.483968
H	0.448969	3.703147	2.483968
H	-0.448969	3.703147	-2.483968
C	-2.226866	2.690402	4.214900
C	-2.203733	2.886043	3.017459
H	-2.260931	2.522990	5.266482
C	-2.690402	2.226866	-4.214900
C	-2.886043	2.203733	-3.017459
H	-2.522990	2.260931	-5.266482
C	2.226866	2.690402	-4.214900
C	2.203733	2.886043	-3.017459
H	2.260931	2.522990	-5.266482
C	2.690402	2.226866	4.214900
C	2.886043	2.203733	3.017459
H	2.522990	2.260931	5.266482
C	2.690402	-2.226866	-4.214900
C	2.886043	-2.203733	-3.017459
H	2.522990	-2.260931	-5.266482
C	2.226866	-2.690402	4.214900
C	2.203733	-2.886043	3.017459
H	2.260931	-2.522990	5.266482
C	-2.226866	-2.690402	-4.214900
C	-2.203733	-2.886043	-3.017459
H	-2.260931	-2.522990	-5.266482
C	-2.690402	-2.226866	4.214900
C	-2.886043	-2.203733	3.017459
H	-2.522990	-2.260931	5.266482

Table S 71. Coordinates of the calculated structure of the open-Shell singlet of 11_4 (n=4) (TDDFT, BP86-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.698356	-1.033399	-0.946195
C	3.669670	-1.311783	0.495202
C	3.794341	0.270820	-1.429782
C	3.669670	1.311783	-0.495202
C	3.698356	1.033399	0.946195
C	3.794341	-0.270820	1.429782
C	3.111786	-2.157638	-1.654290
C	3.010033	-2.564989	0.658315
C	2.564989	-3.010033	-0.658315
C	2.157638	-3.111786	1.654290
C	1.311783	-3.669670	-0.495202
C	1.033399	-3.698356	0.946195
C	0.270820	-3.794341	-1.429782
C	-0.270820	-3.794341	1.429782
C	-1.033399	-3.698356	-0.946195
C	-1.311783	-3.669670	0.495202
C	-2.564989	-3.010033	0.658315
C	-2.157638	-3.111786	-1.654290
C	-3.010033	-2.564989	-0.658315
C	-3.111786	-2.157638	1.654290
C	-3.669670	-1.311783	-0.495202
C	-3.698356	-1.033399	0.946195
C	-3.794341	-0.270820	-1.429782
C	-3.794341	0.270820	1.429782
C	-3.669670	1.311783	0.495202
C	-3.698356	1.033399	-0.946195
C	-3.111786	2.157638	-1.654290
C	-3.010033	2.564989	0.658315
C	-2.564989	3.010033	-0.658315
C	-2.157638	3.111786	1.654290
C	-1.033399	3.698356	0.946195
C	-1.311783	3.669670	-0.495202
C	0.270820	3.794341	1.429782
C	-0.270820	3.794341	-1.429782
C	1.033399	3.698356	-0.946195
C	1.311783	3.669670	0.495202
C	2.157638	3.111786	-1.654290
C	2.564989	3.010033	0.658315
C	3.010033	2.564989	-0.658315
C	3.111786	2.157638	1.654290
H	-3.684425	0.469980	2.496361
H	-3.684425	-0.469980	-2.496361
H	-0.469980	-3.684425	2.496361
H	0.469980	-3.684425	-2.496361
H	3.684425	-0.469980	2.496361
H	3.684425	0.469980	-2.496361
H	0.469980	3.684425	2.496361
H	-0.469980	3.684425	-2.496361
C	-2.261467	2.692620	4.234085
C	-2.217692	2.888377	3.031556
H	-2.311286	2.524334	5.289120
C	-2.692620	2.261467	-4.234085
C	-2.888377	2.217692	-3.031556
H	-2.524334	2.311286	-5.289120
C	2.261467	2.692620	-4.234085
C	2.217692	2.888377	-3.031556
H	2.311286	2.524334	-5.289120
C	2.692620	2.261467	4.234085
C	2.888377	2.217692	3.031556
H	2.524334	2.311286	5.289120
C	2.692620	-2.261467	-4.234085
C	2.888377	-2.217692	-3.031556
H	2.524334	-2.311286	-5.289120
C	2.261467	-2.692620	4.234085
C	2.217692	-2.888377	3.031556
H	2.311286	-2.524334	5.289120
C	-2.261467	-2.692620	-4.234085
C	-2.217692	-2.888377	-3.031556
H	-2.311286	-2.524334	-5.289120
C	-2.692620	-2.261467	4.234085
C	-2.888377	-2.217692	3.031556
H	-2.524334	-2.311286	5.289120

Table S 72. Coordinates of the calculated structure of 11_5 (n=5) (TPSS-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	-4.222855	-2.235348	1.621372

C	-4.747446	-1.045958	0.909334
C	-4.728531	-1.306772	-0.495874
C	-4.145547	-2.629953	-0.658316
C	-3.782278	-3.129949	0.658316
C	-4.807769	0.254199	1.414714
C	-4.728531	1.306772	0.495874
C	-4.747446	1.045958	-0.909334
C	-4.807769	-0.254199	-1.414714
C	-4.145547	2.629953	0.658316
C	-3.782278	3.129949	-0.658316
C	-4.222855	2.235348	-1.621372
C	-2.704011	4.093286	-0.495874
C	-2.461807	4.191871	0.909334
C	-3.430877	3.325413	1.621372
C	-1.243925	4.651012	1.414714
C	-0.218382	4.900915	0.495874
C	-0.472276	4.838309	-0.909334
C	-1.727440	4.493908	-1.414714
C	1.220189	4.755349	0.658316
C	1.807971	4.564368	-0.658316
C	0.821009	4.706935	-1.621372
C	3.057361	3.836562	-0.495874
C	3.225966	3.636677	0.909334
C	2.102457	4.290567	1.621372
C	4.038982	2.620284	1.414714
C	4.593564	1.722160	0.495874
C	4.455564	1.944281	-0.909334
C	3.740153	3.031587	-1.414714
C	4.730267	0.673697	-1.621372
C	4.899665	-0.309015	-0.658316
C	4.899665	0.309015	0.658316
C	4.593564	-1.722160	-0.495874
C	4.455564	-1.944281	0.909334
C	4.730267	-0.673697	1.621372
C	4.038982	-2.620284	-1.414714
C	3.225966	-3.636677	-0.909334
C	3.057361	-3.836562	0.495874
C	3.740153	-3.031587	1.414714
C	-3.430877	-3.325413	-1.621372
H	4.063579	2.414544	2.480752
H	3.552083	3.118558	-2.480752
H	-1.040653	4.610829	2.480752
H	-1.868271	4.341919	-2.480752
H	-4.706738	0.435105	2.480752

H	-4.706738	-0.435105	-2.480752
H	3.552083	-3.118558	2.480752
H	4.063579	-2.414544	-2.480752
C	-2.704011	-4.093286	0.495874
C	-2.461807	-4.191871	-0.909334
C	-1.727440	-4.493908	1.414714
C	-1.243925	-4.651012	-1.414714
C	-0.218382	-4.900915	-0.495874
C	-0.472276	-4.838309	0.909334
C	0.821009	-4.706935	1.621372
C	1.220189	-4.755349	-0.658316
C	1.807971	-4.564368	0.658316
C	2.102457	-4.290567	-1.621372
H	-1.868271	-4.341919	2.480752
H	-1.040653	-4.610829	-2.480752
C	4.505600	0.376869	-4.210697
C	4.613320	0.503186	-3.009016
H	4.419733	0.255326	-5.265724
C	4.505600	-0.376869	4.210697
C	4.613320	-0.503186	3.009016
H	4.419733	-0.255326	5.265724
C	1.750730	-4.168621	-4.210697
C	1.904153	-4.232035	-3.009016
H	1.608602	-4.124516	-5.265724
C	1.033884	-4.401539	4.210697
C	0.947036	-4.543021	3.009016
H	1.122944	-4.282316	5.265724
C	-3.423589	-2.953218	-4.210697
C	-3.436489	-3.118728	-3.009016
H	-3.425563	-2.804417	-5.265724
C	-3.866624	-2.343432	4.210697
C	-4.028020	-2.304556	3.009016
H	-3.725716	-2.391291	5.265724
C	-3.866624	2.343432	-4.210697
C	-4.028020	2.304556	-3.009016
H	-3.725716	2.391291	-5.265724
C	-3.423589	2.953218	4.210697
C	-3.436489	3.118728	3.009016
H	-3.425563	2.804417	5.265724
C	1.033884	4.401539	-4.210697
C	0.947036	4.543021	-3.009016
H	1.122944	4.282316	-5.265724
C	1.750730	4.168621	4.210697
C	1.904153	4.232035	3.009016

H	1.608602	4.124516	5.265724

Table S 73. Coordinates of the calculated structure of the triplet of 11_5 (n=5) (TPSS-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	-4.212031	-2.206906	1.638629
C	-4.705429	-1.040376	0.933747
C	-4.680572	-1.307725	-0.502918
C	-4.123761	-2.615469	-0.659992
C	-3.761771	-3.113706	0.659992
C	-4.772784	0.262852	1.427181
C	-4.680572	1.307725	0.502918
C	-4.705429	1.040376	-0.933747
C	-4.772784	-0.262852	-1.427181
C	-4.123761	2.615469	0.659992
C	-3.761771	3.113706	-0.659992
C	-4.212031	2.206906	-1.638629
C	-2.690097	4.047379	-0.502918
C	-2.443514	4.153635	0.933747
C	-3.400481	3.323908	1.638629
C	-1.224885	4.620413	1.427181
C	-0.202656	4.855598	0.502918
C	-0.464601	4.796623	-0.933747
C	-1.724858	4.457962	-1.427181
C	1.213146	4.730154	0.659992
C	1.798859	4.539845	-0.659992
C	0.797303	4.687851	-1.638629
C	3.018001	3.809143	-0.502918
C	3.195255	3.607464	0.933747
C	2.110418	4.261194	1.638629
C	4.015764	2.592721	1.427181
C	4.555324	1.693199	0.502918
C	4.418290	1.924100	-0.933747
C	3.706763	3.018023	-1.427181
C	4.704791	0.690345	-1.638629
C	4.873527	-0.307927	-0.659992
C	4.873527	0.307927	0.659992
C	4.555324	-1.693199	-0.502918
C	4.418290	-1.924100	0.933747
C	4.704791	-0.690345	1.638629
C	4.015764	-2.592721	-1.427181
C	3.195255	-3.607464	-0.933747
C	3.018001	-3.809143	0.502918
C	3.706763	-3.018023	1.427181
C	-3.400481	-3.323908	-1.638629
H	4.053603	2.385528	2.492460
H	3.521404	3.118037	-2.492460
H	-1.016140	4.592374	2.492460
H	-1.877256	4.312580	-2.492460
H	-4.681611	0.452716	2.492460
H	-4.681611	-0.452716	-2.492460
H	3.521404	-3.118037	2.492460
H	4.053603	-2.385528	-2.492460
C	-2.690097	-4.047379	0.502918
C	-2.443514	-4.153635	-0.933747
C	-1.724858	-4.457962	1.427181
C	-1.224885	-4.620413	-1.427181
C	-0.202656	-4.855598	-0.502918
C	-0.464601	-4.796623	0.933747
C	0.797303	-4.687851	1.638629
C	1.213146	-4.730154	-0.659992
C	1.798859	-4.539845	0.659992
C	2.110418	-4.261194	-1.638629
H	-1.877256	-4.312580	2.492460
H	-1.016140	-4.592374	-2.492460
C	4.506434	0.357443	-4.225575
C	4.602021	0.509099	-3.025437
H	4.431478	0.219997	-5.279379
C	4.506434	-0.357443	4.225575
C	4.602021	-0.509099	3.025437
H	4.431478	-0.219997	5.279379
C	1.732513	-4.175418	-4.225575
C	1.906284	-4.219461	-3.025437
H	1.578631	-4.146603	-5.279379
C	1.052617	-4.396329	4.225575
C	0.937921	-4.534102	3.025437
H	1.160173	-4.282569	5.279379
C	-3.435682	-2.937993	-4.225575
C	-3.423872	-3.116870	-3.025437
H	-3.455830	-2.782738	-5.279379
C	-3.855881	-2.359638	4.225575
C	-4.022354	-2.293130	3.025437
H	-3.714452	-2.426776	5.279379
C	-3.855881	2.359638	-4.225575

C	-4.022354	2.293130	-3.025437
H	-3.714452	2.426776	-5.279379
C	-3.435682	2.937993	4.225575
C	-3.423872	3.116870	3.025437
H	-3.455830	2.782738	5.279379
C	1.052617	4.396329	-4.225575
C	0.937921	4.534102	-3.025437
H	1.160173	4.282569	-5.279379
C	1.732513	4.175418	4.225575
C	1.906284	4.219461	3.025437
H	1.578631	4.146603	5.279379

Table S 74. Coordinates of the calculated structure of the open-shell singlet of 11_5 (n=5) (TDDFT, BP86-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	-4.216414	-2.227115	1.633654
C	-4.727538	-1.042052	0.923737
C	-4.709791	-1.308954	-0.496742
C	-4.146262	-2.628824	-0.658855
C	-3.781426	-3.130978	0.658855
C	-4.793651	0.259564	1.422140
C	-4.709791	1.308954	0.496742
C	-4.727538	1.042052	-0.923737
C	-4.793651	-0.259564	-1.422140
C	-4.146262	2.628824	0.658855
C	-3.781426	3.130978	-0.658855
C	-4.216414	2.227115	-1.633654
C	-2.700294	4.074788	-0.496742
C	-2.451940	4.174144	0.923737
C	-3.421056	3.321831	1.633654
C	-1.234460	4.639242	1.422140
C	-0.210516	4.883766	0.496742
C	-0.469839	4.818168	-0.923737
C	-1.728180	4.478823	-1.422140
C	1.218895	4.755681	0.658855
C	1.809212	4.563875	-0.658855
C	0.815169	4.698264	-1.633654
C	3.040917	3.827311	-0.496742
C	3.212156	3.621815	0.923737
C	2.102085	4.280120	1.633654
C	4.030713	2.607646	1.422140
C	4.579684	1.709380	0.496742
C	4.437162	1.935739	-0.923737
C	3.725577	3.027629	-1.422140
C	4.720216	0.676572	-1.633654
C	4.899581	-0.310348	-0.658855
C	4.899581	0.310348	0.658855
C	4.579684	-1.709380	-0.496742
C	4.437162	-1.935739	0.923737
C	4.720216	-0.676572	1.633654
C	4.030713	-2.607646	-1.422140
C	3.212156	-3.621815	-0.923737
C	3.040917	-3.827311	0.496742
C	3.725577	-3.027629	1.422140
C	-3.421056	-3.321831	-1.633654
H	4.060541	2.395456	2.491552
H	3.532990	3.121568	-2.491552
H	-1.023438	4.602041	2.491552
H	-1.877033	4.324691	-2.491552
H	-4.693061	0.448762	2.491552
H	-4.693061	-0.448762	-2.491552
H	3.532990	-3.121568	2.491552
H	4.060541	-2.395456	-2.491552
C	-2.700294	-4.074788	0.496742
C	-2.451940	-4.174144	-0.923737
C	-1.728180	-4.478823	1.422140
C	-1.234460	-4.639242	-1.422140
C	-0.210516	-4.883766	-0.496742
C	-0.469839	-4.818168	0.923737
C	0.815169	-4.698264	1.633654
C	1.218895	-4.755681	-0.658855
C	1.809212	-4.563875	0.658855
C	2.102085	-4.280120	-1.633654
H	-1.877033	-4.324691	2.491552
H	-1.023438	-4.602041	-2.491552
C	4.483988	0.353744	-4.220705
C	4.597962	0.496074	-3.016623
H	4.392735	0.220327	-5.278092
C	4.483988	-0.353744	4.220705
C	4.597962	-0.496074	3.016623
H	4.392735	-0.220327	5.278092
C	1.722059	-4.155213	-4.220705
C	1.892643	-4.219626	-3.016623
H	1.566973	-4.109655	-5.278092

C	1.049199	-4.373839	4.220705
C	0.949054	-4.526217	3.016623
H	1.147887	-4.245824	5.278092
C	-3.419697	-2.921807	-4.220705
C	-3.428244	-3.103946	-3.016623
H	-3.424293	-2.760233	-5.278092
C	-3.835548	-2.349438	4.220705
C	-4.011414	-2.301282	3.016623
H	-3.683303	-2.403737	5.278092
C	-3.835548	2.349438	-4.220705
C	-4.011414	2.301282	-3.016623
H	-3.683303	2.403737	-5.278092
C	-3.419697	2.921807	4.220705
C	-3.428244	3.103946	3.016623
H	-3.424293	2.760233	5.278092
C	1.049199	4.373839	-4.220705
C	0.949054	4.526217	-3.016623
H	1.147887	4.245824	-5.278092
C	1.722059	4.155213	4.220705
C	1.892643	4.219626	3.016623
H	1.566973	4.109655	5.278092

Table S 75. Coordinates of the calculated structure of 11_6 (n=6) (TPSS-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.270872	-2.240333	1.634655
C	-5.686994	-1.041679	0.929782
C	-5.667747	-1.307097	-0.504733
C	-5.200645	-2.647692	-0.659651
C	-4.893290	-3.180045	0.659651
C	-5.742739	0.259119	1.427142
C	-5.667747	1.307097	0.504733
C	-5.686994	1.041679	-0.929782
C	-5.742739	-0.259119	-1.427142
C	-5.200645	2.647692	0.659651
C	-4.893290	3.180045	-0.659651
C	-5.270872	2.240333	-1.634655
C	-3.965852	4.254864	-0.504733
C	-3.745618	4.404241	0.929782
C	-4.575621	3.444542	1.634655
C	-2.646966	5.102917	1.427142
C	-1.701895	5.561961	0.504733
C	-1.941376	5.445921	-0.929782
C	-3.095773	4.843798	-1.427142
C	-0.307354	5.827736	0.659651
C	0.307354	5.827736	-0.659651
C	-0.695250	5.684875	-1.634655
C	1.701895	5.561961	-0.504733
C	1.941376	5.445921	0.929782
C	0.695250	5.684875	1.634655
C	3.095773	4.843798	1.427142
C	3.965852	4.254864	0.504733
C	3.745618	4.404241	-0.929782
C	2.646966	5.102917	-1.427142
C	4.575621	3.444542	-1.634655
C	5.200645	2.647692	-0.659651
C	4.893290	3.180045	0.659651
C	5.667747	1.307097	-0.504733
C	5.686994	1.041679	0.929782
C	5.270872	2.240333	1.634655
C	5.742739	0.259119	-1.427142
C	5.686994	-1.041679	-0.929782
C	5.667747	-1.307097	0.504733
C	5.742739	-0.259119	1.427142
C	-4.575621	-3.444542	-1.634655
H	3.219645	4.682003	2.493852
H	2.444911	5.129296	-2.493852
H	-2.444911	5.129296	2.493852
H	-3.219645	4.682003	-2.493852
H	-5.664556	0.447293	2.493852
H	-5.664556	-0.447293	-2.493852
H	5.664556	-0.447293	2.493852
H	5.664556	0.447293	-2.493852
C	-3.965852	-4.254864	0.504733
C	-3.745618	-4.404241	-0.929782
C	-3.095773	-4.843798	1.427142
C	-2.646966	-5.102917	-1.427142
C	-1.701895	-5.561961	-0.504733
C	-1.941376	-5.445921	0.929782
C	-0.695250	-5.684875	1.634655
C	-0.307354	-5.827736	-0.659651
C	0.307354	-5.827736	0.659651
C	5.270872	-2.240333	-1.634655
H	-3.219645	-4.682003	2.493852

H	-2.444911	-5.129296	-2.493852
C	1.701895	-5.561961	0.504733
C	0.695250	-5.684875	-1.634655
C	1.941376	-5.445921	-0.929782
C	2.646966	-5.102917	1.427142
C	3.745618	-4.404241	0.929782
C	3.095773	-4.843798	-1.427142
C	3.965852	-4.254864	-0.504733
C	4.575621	-3.444542	1.634655
C	4.893290	-3.180045	-0.659651
C	5.200645	-2.647692	0.659651
H	2.444911	-5.129296	2.493852
H	3.219645	-4.682003	-2.493852
C	-0.381001	5.517876	-4.226416
C	-0.523239	5.597770	-3.024110
H	-0.250950	5.454399	-5.281947
C	0.381001	5.517876	4.226416
C	0.523239	5.597770	3.024110
H	0.250950	5.454399	5.281947
C	4.588120	3.088894	-4.226416
C	4.586191	3.252023	-3.024110
H	4.598173	2.944529	-5.281947
C	4.969121	2.428981	4.226416
C	5.109430	2.345747	3.024110
H	4.849123	2.509870	5.281947
C	4.969121	-2.428981	-4.226416
C	5.109430	-2.345747	-3.024110
H	4.849123	-2.509870	-5.281947
C	4.588120	-3.088894	4.226416
C	4.586191	-3.252023	3.024110
H	4.598173	-2.944529	5.281947
C	0.381001	-5.517876	-4.226416
C	0.523239	-5.597770	-3.024110
H	0.250950	-5.454399	-5.281947
C	-0.381001	-5.517876	4.226416
C	-0.523239	-5.597770	3.024110
H	-0.250950	-5.454399	5.281947
C	-4.588120	-3.088894	-4.226416
C	-4.586191	-3.252023	-3.024110
H	-4.598173	-2.944529	-5.281947
C	-4.969121	-2.428981	4.226416
C	-5.109430	-2.345747	3.024110
H	-4.849123	-2.509870	5.281947
C	-4.969121	2.428981	-4.226416
C	-5.109430	2.345747	-3.024110
H	-4.849123	2.509870	-5.281947
C	-4.588120	3.088894	4.226416
C	-4.586191	3.252023	3.024110
H	-4.598173	2.944529	5.281947

Table S 76. Coordinates of the calculated structure of the triplet of 11_6 (n=6) (TPSS-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.280152	-2.254225	1.627277
C	-5.709149	-1.044304	0.918666
C	-5.692448	-1.306128	-0.501201
C	-5.214496	-2.655991	-0.658911
C	-4.907404	-3.187890	0.658911
C	-5.761598	0.255487	1.421432
C	-5.692448	1.306128	0.501201
C	-5.709149	1.044304	-0.918666
C	-5.761598	-0.255487	-1.421432
C	-5.214496	2.655991	0.658911
C	-4.907404	3.187890	-0.658911
C	-5.280152	2.254225	-1.627277
C	-3.977364	4.276741	-0.501201
C	-3.758968	4.422116	0.918666
C	-4.592293	3.445633	1.627277
C	-2.659541	5.117434	1.421432
C	-1.715084	5.582868	0.501201
C	-1.950181	5.466420	-0.918666
C	-3.102057	4.861947	-1.421432
C	-0.307092	5.843881	0.658911
C	0.307092	5.843881	-0.658911
C	-0.687860	5.699859	-1.627277
C	1.715084	5.582868	-0.501201
C	1.950181	5.466420	0.918666
C	0.687860	5.699859	1.627277
C	3.102057	4.861947	1.421432
C	3.977364	4.276741	0.501201
C	3.758968	4.422116	-0.918666
C	2.659541	5.117434	-1.421432
C	4.592293	3.445633	-1.627277
C	5.214496	2.655991	-0.658911

C	4.907404	3.187890	0.658911
C	5.692448	1.306128	-0.501201
C	5.709149	1.044304	0.918666
C	5.280152	2.254225	1.627277
C	5.761598	0.255487	-1.421432
C	5.709149	-1.044304	-0.918666
C	5.692448	-1.306128	0.501201
C	5.761598	-0.255487	1.421432
C	-4.592293	-3.445633	-1.627277
H	3.220720	4.698821	2.488563
H	2.458939	5.138636	-2.488563
H	-2.458939	5.138636	2.488563
H	-3.220720	4.698821	-2.488563
H	-5.679659	0.439815	2.488563
H	-5.679659	-0.439815	-2.488563
H	5.679659	-0.439815	2.488563
H	5.679659	0.439815	-2.488563
C	-3.977364	-4.276741	0.501201
C	-3.758968	-4.422116	-0.918666
C	-3.102057	-4.861947	1.421432
C	-2.659541	-5.117434	-1.421432
C	-1.715084	-5.582868	-0.501201
C	-1.950181	-5.466420	0.918666
C	-0.687860	-5.699859	1.627277
C	-0.307092	-5.843881	-0.658911
C	0.307092	-5.843881	0.658911
C	5.280152	-2.254225	-1.627277
H	-3.220720	-4.698821	2.488563
H	-2.458939	-5.138636	-2.488563
C	1.715084	-5.582868	0.501201
C	0.687860	-5.699859	-1.627277
C	1.950181	-5.466420	-0.918666
C	2.659541	-5.117434	1.421432
C	3.758968	-4.422116	0.918666
C	3.102057	-4.861947	-1.421432
C	3.977364	-4.276741	-0.501201
C	4.592293	-3.445633	1.627277
C	4.907404	-3.187890	-0.658911
C	5.214496	-2.655991	0.658911
H	2.458939	-5.138636	2.488563
H	3.220720	-4.698821	-2.488563
C	-0.390670	5.519149	-4.220084
C	-0.520979	5.605706	-3.016954
H	-0.268302	5.449996	-5.276212
C	0.390670	5.519149	4.220084
C	0.520979	5.605706	3.016954
H	0.268302	5.449996	5.276212
C	4.584388	3.097904	-4.220084
C	4.594194	3.254034	-3.016954
H	4.585684	2.957355	-5.276212
C	4.975058	2.421245	4.220084
C	5.115174	2.351672	3.016954
H	4.853986	2.492642	5.276212
C	4.975058	-2.421245	-4.220084
C	5.115174	-2.351672	-3.016954
H	4.853986	-2.492642	-5.276212
C	4.584388	-3.097904	4.220084
C	4.594194	-3.254034	3.016954
H	4.585684	-2.957355	5.276212
C	0.390670	-5.519149	-4.220084
C	0.520979	-5.605706	-3.016954
H	0.268302	-5.449996	-5.276212
C	-0.390670	-5.519149	4.220084
C	-0.520979	-5.605706	3.016954
H	-0.268302	-5.449996	5.276212
C	-4.584388	-3.097904	-4.220084
C	-4.594194	-3.254034	-3.016954
H	-4.585684	-2.957355	-5.276212
C	-4.975058	-2.421245	4.220084
C	-5.115174	-2.351672	3.016954
H	-4.853986	-2.492642	5.276212
C	-4.975058	2.421245	-4.220084
C	-5.115174	2.351672	-3.016954
H	-4.853986	2.492642	-5.276212
C	-4.584388	3.097904	4.220084
C	-4.594194	3.254034	3.016954
H	-4.585684	2.957355	5.276212

Table S 77. Coordinates of the calculated structure of the open-shell singlet of 11_6 (n=6) (TDDFT, BP86-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.266953	-2.236657	1.645182
C	-5.676227	-1.040196	0.941732
C	-5.657561	-1.308380	-0.505532

C	-5.200168	-2.645992	-0.661817
C	-4.891580	-3.180481	0.661817
C	-5.732834	0.262545	1.433232
C	-5.657561	1.308380	0.505532
C	-5.676227	1.040196	-0.941732
C	-5.732834	-0.262545	-1.433232
C	-5.200168	2.645992	0.661817
C	-4.891580	3.180481	-0.661817
C	-5.266953	2.236657	-1.645182
C	-3.961871	4.245402	-0.505532
C	-3.738950	4.395659	0.941732
C	-4.570478	3.442987	1.645182
C	-2.639046	5.096052	1.433232
C	-1.695691	5.553782	0.505532
C	-1.937277	5.435855	-0.941732
C	-3.093787	4.833507	-1.433232
C	-0.308588	5.826473	0.661817
C	0.308588	5.826473	-0.661817
C	-0.696475	5.679644	-1.645182
C	1.695691	5.553782	-0.505532
C	1.937277	5.435855	0.941732
C	0.696475	5.679644	1.645182
C	3.093787	4.833507	1.433232
C	3.961871	4.245402	0.505532
C	3.738950	4.395659	-0.941732
C	2.639046	5.096052	-1.433232
C	4.570478	3.442987	-1.645182
C	5.200168	2.645992	-0.661817
C	4.891580	3.180481	0.661817
C	5.657561	1.308380	-0.505532
C	5.676227	1.040196	0.941732
C	5.266953	2.236657	1.645182
C	5.732834	0.262545	-1.433232
C	5.676227	-1.040196	-0.941732
C	5.657561	-1.308380	0.505532
C	5.732834	-0.262545	1.433232
C	-4.570478	-3.442987	-1.645182
H	3.223354	4.667055	2.503364
H	2.430111	5.125034	-2.503364
H	-2.430111	5.125034	2.503364
H	-3.223354	4.667055	-2.503364
H	-5.653465	0.457979	2.503364
H	-5.653465	-0.457979	-2.503364
H	5.653465	-0.457979	2.503364

H	5.653465	0.457979	-2.503364
C	-3.961871	-4.245402	0.505532
C	-3.738950	-4.395659	-0.941732
C	-3.093787	-4.833507	1.433232
C	-2.639046	-5.096052	-1.433232
C	-1.695691	-5.553782	-0.505532
C	-1.937277	-5.435855	0.941732
C	-0.696475	-5.679644	1.645182
C	-0.308588	-5.826473	-0.661817
C	0.308588	-5.826473	0.661817
C	5.266953	-2.236657	-1.645182
H	-3.223354	-4.667055	2.503364
H	-2.430111	-5.125034	-2.503364
C	1.695691	-5.553782	0.505532
C	0.696475	-5.679644	-1.645182
C	1.937277	-5.435855	-0.941732
C	2.639046	-5.096052	1.433232
C	3.738950	-4.395659	0.941732
C	3.093787	-4.833507	-1.433232
C	3.961871	-4.245402	-0.505532
C	4.570478	-3.442987	1.645182
C	4.891580	-3.180481	-0.661817
C	5.200168	-2.645992	0.661817
H	2.430111	-5.125034	2.503364
H	3.223354	-4.667055	-2.503364
C	-0.359764	5.503185	-4.236215
C	-0.515186	5.587857	-3.031579
H	-0.219644	5.435571	-5.294484
C	0.359764	5.503185	4.236215
C	0.515186	5.587857	3.031579
H	0.219644	5.435571	5.294484
C	4.586016	3.063157	-4.236215
C	4.581633	3.240093	-3.031579
H	4.597520	2.908003	-5.294484
C	4.945780	2.440028	4.236215
C	5.096819	2.347764	3.031579
H	4.817164	2.527568	5.294484
C	4.945780	-2.440028	-4.236215
C	5.096819	-2.347764	-3.031579
H	4.817164	-2.527568	-5.294484
C	4.586016	-3.063157	4.236215
C	4.581633	-3.240093	3.031579
H	4.597520	-2.908003	5.294484
C	0.359764	-5.503185	-4.236215

C	0.515186	-5.587857	-3.031579
H	0.219644	-5.435571	-5.294484
C	-0.359764	-5.503185	4.236215
C	-0.515186	-5.587857	3.031579
H	-0.219644	-5.435571	5.294484
C	-4.586016	-3.063157	-4.236215
C	-4.581633	-3.240093	-3.031579
H	-4.597520	-2.908003	-5.294484
C	-4.945780	-2.440028	4.236215
C	-5.096819	-2.347764	3.031579
H	-4.817164	-2.527568	5.294484
C	-4.945780	2.440028	-4.236215
C	-5.096819	2.347764	-3.031579
H	-4.817164	2.527568	-5.294484
C	-4.586016	3.063157	4.236215
C	-4.581633	3.240093	3.031579
H	-4.597520	2.908003	5.294484

Table S 78. Coordinates of the calculated structure of 11_7 (n=7) (TPSS-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.822614	-0.306074	-0.658862
C	6.602501	-1.732396	-0.499360
C	6.501817	-1.968215	0.907393
C	6.697552	-0.684574	1.619708
C	6.822614	0.306074	0.658862
C	6.192895	-2.704447	-1.417049
C	5.592629	-3.856163	-0.907393
C	5.471034	-4.081911	0.499360
C	5.975629	-3.155605	1.417049
C	4.711077	-4.809532	-1.619708
C	4.014532	-5.524968	-0.658862
C	4.493129	-5.143300	0.658862
C	2.762150	-6.242174	-0.499360
C	2.515004	-6.310487	0.907393
C	3.640634	-5.663183	1.619708
C	1.258592	-6.639422	1.417049
C	0.219767	-6.822457	0.499360
C	0.472078	-6.776772	-0.907393
C	1.746785	-6.527995	-1.417049
C	-0.822935	-6.681963	-1.619708
C	-1.816575	-6.583449	-0.658862
C	-1.219774	-6.719664	0.658862
C	-2.157756	-6.377299	1.619708
C	-3.365658	-5.900833	0.907393
C	-3.158156	-6.051468	-0.499360
C	-4.406190	-5.123619	1.417049
C	-5.196989	-4.425553	0.499360
C	-5.003958	-4.594333	-0.907393
C	-4.014690	-5.435830	-1.417049
C	-5.737261	-3.522739	-1.619708
C	-6.279763	-2.684458	-0.658862
C	-6.014162	-3.235985	0.658862
C	-6.331312	-2.289179	1.619708
C	-6.711911	-1.047732	0.907393
C	-6.700306	-1.303882	-0.499360
C	-6.753021	0.250374	1.417049
C	-6.700306	1.303882	0.499360
C	-6.711911	1.047732	-0.907393
C	-6.753021	-0.250374	-1.417049
C	-6.279763	2.684458	0.658862
C	-6.014162	3.235985	-0.658862
C	-6.331312	2.289179	-1.619708
C	-5.196989	4.425553	-0.499360
C	-5.003958	4.594333	0.907393
C	-5.737261	3.522739	1.619708
C	-4.014690	5.435830	1.417049
C	-3.158156	6.051468	0.499360
C	-3.365658	5.900833	-0.907393
C	-4.406190	5.123619	-1.417049
C	-2.157756	6.377299	-1.619708
C	-1.219774	6.719664	-0.658862
C	-1.816575	6.583449	0.658862
C	0.219767	6.822457	-0.499360
C	0.472078	6.776772	0.907393
C	-0.822935	6.681963	1.619708
C	1.746785	6.527995	1.417049
C	2.762150	6.242174	0.499360
C	2.515004	6.310487	-0.907393
C	1.258592	6.639422	-1.417049
C	6.697552	0.684574	-1.619708
H	1.906211	-6.415285	-2.485379
H	1.066051	-6.607046	2.485379
H	-3.827168	-5.490201	-2.485379

H	-4.500925	-4.952898	2.485379
H	-6.678612	-0.430883	-2.485379
H	-6.678612	0.430883	2.485379
H	6.204175	-2.509529	-2.485379
H	5.830268	-3.285954	2.485379
H	-4.500925	4.952898	-2.485379
H	-3.827168	5.490201	2.485379
H	1.066051	6.607046	-2.485379
H	1.906211	6.415285	2.485379
C	3.640634	5.663183	-1.619708
C	4.014532	5.524968	0.658862
C	4.493129	5.143300	-0.658862
C	5.471034	4.081911	-0.499360
C	4.711077	4.809532	1.619708
C	5.592629	3.856163	0.907393
C	5.975629	3.155605	-1.417049
C	6.192895	2.704447	1.417049
C	6.501817	1.968215	-0.907393
C	6.602501	1.732396	0.499360
H	5.830268	3.285954	-2.485379
H	6.204175	2.509529	2.485379
C	4.395148	4.845126	4.216587
C	4.533516	4.838252	3.011506
H	4.268689	4.862431	5.274409
C	3.745636	5.363094	-4.216587
C	3.708145	5.496464	-3.011506
H	3.790647	5.243657	-5.274409
C	6.528402	0.415379	-4.216587
C	6.609299	0.527845	-3.011506
H	6.463086	0.305719	-5.274409
C	6.528402	-0.415379	4.216587
C	6.609299	-0.527845	3.011506
H	6.463086	-0.305719	5.274409
C	4.395148	-4.845126	-4.216587
C	4.533516	-4.838252	-3.011506
H	4.268689	-4.862431	-5.274409
C	3.745636	-5.363094	4.216587
C	3.708145	-5.496464	3.011506
H	3.790647	-5.243657	5.274409
C	-1.047742	-6.457151	-4.216587
C	-0.956097	-6.561046	-3.011506
H	-1.140118	-6.369072	-5.274409
C	-1.857670	-6.272291	4.216587
C	-1.985318	-6.326133	3.011506
H	-1.736226	-6.233014	5.274409
C	-5.701661	-3.206810	-4.216587
C	-5.725749	-3.343239	-3.011506
H	-5.690393	-3.079671	-5.274409
C	-6.062113	-2.458324	4.216587
C	-6.183796	-2.392096	3.011506
H	-5.955686	-2.528784	5.274409
C	-6.062113	2.458324	-4.216587
C	-6.183796	2.392096	-3.011506
H	-5.955686	2.528784	-5.274409
C	-5.701661	3.206810	4.216587
C	-5.725749	3.343239	3.011506
H	-5.690393	3.079671	5.274409
C	-1.857670	6.272291	-4.216587
C	-1.985318	6.326133	-3.011506
H	-1.736226	6.233014	-5.274409
C	-1.047742	6.457151	4.216587
C	-0.956097	6.561046	3.011506
H	-1.140118	6.369072	5.274409

Table S 79. Coordinates of the calculated structure of the triplet of 11_7 (n=7) (TPSS-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.790956	-0.305555	-0.659457
C	6.564010	-1.711675	-0.504775
C	6.463726	-1.954412	0.925359
C	6.666279	-0.697421	1.631547
C	6.790956	0.305555	0.659457
C	6.163307	-2.682949	-1.425859
C	5.558089	-3.834989	-0.925359
C	5.430835	-4.064738	0.504775
C	5.940373	-3.145876	1.425859
C	4.701623	-4.777071	-1.631547
C	3.995200	-5.499893	-0.659457
C	4.472984	-5.118873	0.659457
C	2.754352	-6.199162	-0.504775
C	2.502046	-6.272101	0.925359
C	3.611091	-5.646742	1.631547
C	1.244217	-6.605793	1.425859
C	0.208130	-6.780320	0.504775

C	0.467097	-6.736565	-0.925359
C	1.745145	-6.491459	-1.425859
C	-0.803451	-6.654332	-1.631547
C	-1.809024	-6.552700	-0.659457
C	-1.213236	-6.688685	0.659457
C	-2.163322	-6.343950	1.631547
C	-3.343726	-5.866770	0.925359
C	-3.129390	-6.018553	-0.504775
C	-4.388860	-5.091413	1.425859
C	-5.171301	-4.390183	0.504775
C	-4.975629	-4.565370	-0.925359
C	-3.987147	-5.411768	-1.425859
C	-5.703510	-3.520745	-1.631547
C	-6.251015	-2.671190	-0.659457
C	-5.985865	-3.221781	0.659457
C	-6.308709	-2.264035	1.631547
C	-6.671604	-1.043641	0.925359
C	-6.656637	-1.305851	-0.504775
C	-6.717036	0.256905	1.425859
C	-6.656637	1.305851	0.504775
C	-6.671604	1.043641	-0.925359
C	-6.717036	-0.256905	-1.425859
C	-6.251015	2.671190	0.659457
C	-5.985865	3.221781	-0.659457
C	-6.308709	2.264035	-1.631547
C	-5.171301	4.390183	-0.504775
C	-4.975629	4.565370	0.925359
C	-5.703510	3.520745	1.631547
C	-3.987147	5.411768	1.425859
C	-3.129390	6.018553	0.504775
C	-3.343726	5.866770	-0.925359
C	-4.388860	5.091413	-1.425859
C	-2.163322	6.343950	-1.631547
C	-1.213236	6.688685	-0.659457
C	-1.809024	6.552700	0.659457
C	0.208130	6.780320	-0.504775
C	0.467097	6.736565	0.925359
C	-0.803451	6.654332	1.631547
C	1.745145	6.491459	1.425859
C	2.754352	6.199162	0.504775
C	2.502046	6.272101	-0.925359
C	1.244217	6.605793	-1.425859
C	6.666279	0.697421	-1.631547
H	1.911900	-6.382774	-2.493435

H	1.046819	-6.580223	2.493435
H	-3.798204	-5.474378	-2.493435
H	-4.491945	-4.921138	2.493435
H	-6.648183	-0.443664	-2.493435
H	-6.648183	0.443664	2.493435
H	6.182304	-2.484811	-2.493435
H	5.797307	-3.284266	2.493435
H	-4.491945	4.921138	-2.493435
H	-3.798204	5.474378	2.493435
H	1.046819	6.580223	-2.493435
H	1.911900	6.382774	2.493435
C	3.611091	5.646742	-1.631547
C	3.995200	5.499893	0.659457
C	4.472984	5.118873	-0.659457
C	5.430835	4.064738	-0.504775
C	4.701623	4.777071	1.631547
C	5.558089	3.834989	0.925359
C	5.940373	3.145876	-1.425859
C	6.163307	2.682949	1.425859
C	6.463726	1.954412	-0.925359
C	6.564010	1.711675	0.504775
H	5.797307	3.284266	-2.493435
H	6.182304	2.484811	2.493435
C	4.374629	4.846008	4.226333
C	4.523469	4.818935	3.022503
H	4.242636	4.877753	5.283075
C	3.751062	5.343286	-4.226333
C	3.691547	5.482370	-3.022503
H	3.811382	5.221667	-5.283075
C	6.516298	0.398786	-4.226333
C	6.587932	0.532034	-3.022503
H	6.458821	0.275798	-5.283075
C	6.516298	-0.398786	4.226333
C	6.587932	-0.532034	3.022503
H	6.458821	-0.275798	5.283075
C	4.374629	-4.846008	-4.226333
C	4.523469	-4.818935	-3.022503
H	4.242636	-4.877753	-5.283075
C	3.751062	-5.343286	4.226333
C	3.691547	-5.482370	3.022503
H	3.811382	-5.221667	5.283075
C	-1.061225	-6.441659	-4.226333
C	-0.947258	-6.541147	-3.022503
H	-1.168340	-6.358256	-5.283075

C	-1.838801	-6.264183	4.226333
C	-1.984648	-6.304370	3.022503
H	-1.706106	-6.235514	5.283075
C	-5.697955	-3.186610	-4.226333
C	-5.704680	-3.337743	-3.022503
H	-5.699533	-3.050863	-5.283075
C	-6.044009	-2.468022	4.226333
C	-6.166362	-2.379050	3.022503
H	-5.938861	-2.553892	5.283075
C	-6.044009	2.468022	-4.226333
C	-6.166362	2.379050	-3.022503
H	-5.938861	2.553892	-5.283075
C	-5.697955	3.186610	4.226333
C	-5.704680	3.337743	3.022503
H	-5.699533	3.050863	5.283075
C	-1.838801	6.264183	-4.226333
C	-1.984648	6.304370	-3.022503
H	-1.706106	6.235514	-5.283075
C	-1.061225	6.441659	4.226333
C	-0.947258	6.541147	3.022503
H	-1.168340	6.358256	5.283075

Table S 80. Coordinates of the calculated structure of the open-shell singlet of 11_7 (n=7) (TDDFT, BP86-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.817862	-0.307224	-0.659760
C	6.590275	-1.723657	-0.500972
C	6.486961	-1.963694	0.918705
C	6.686035	-0.688698	1.628615
C	6.817862	0.307224	0.659760
C	6.183078	-2.695040	-1.422922
C	5.579832	-3.847367	-0.918705
C	5.456578	-4.077802	0.500972
C	5.962153	-3.153795	1.422922
C	4.707120	-4.797956	-1.628615
C	4.010670	-5.521971	-0.659760
C	4.491065	-5.138868	0.659760
C	2.761360	-6.227167	-0.500972
C	2.509277	-6.296054	0.918705
C	3.630228	-5.656749	1.628615
C	1.251605	-6.627758	1.422922
C	0.213967	-6.808593	0.500972
C	0.470975	-6.761283	-0.918705
C	1.748019	-6.514455	-1.422922
C	-0.816351	-6.671652	-1.628615
C	-1.816639	-6.578560	-0.659760
C	-1.217595	-6.715288	0.659760
C	-2.159214	-6.365152	1.628615
C	-3.357945	-5.887357	0.918705
C	-3.146916	-6.041493	-0.500972
C	-4.401427	-5.110884	1.422922
C	-5.189766	-4.412374	0.500972
C	-4.992535	-4.583814	-0.918705
C	-4.003334	-5.428353	-1.422922
C	-5.725094	-3.521457	-1.628615
C	-6.275981	-2.681360	-0.659760
C	-6.009382	-3.234959	0.659760
C	-6.322724	-2.280466	1.628615
C	-6.696565	-1.045360	0.918705
C	-6.685499	-1.306452	-0.500972
C	-6.740095	0.254590	1.422922
C	-6.685499	1.306452	0.500972
C	-6.696565	1.045360	-0.918705
C	-6.740095	-0.254590	-1.422922
C	-6.275981	2.681360	0.659760
C	-6.009382	3.234959	-0.659760
C	-6.322724	2.280466	-1.628615
C	-5.189766	4.412374	-0.500972
C	-4.992535	4.583814	0.918705
C	-5.725094	3.521457	1.628615
C	-4.003334	5.428353	1.422922
C	-3.146916	6.041493	0.500972
C	-3.357945	5.887357	-0.918705
C	-4.401427	5.110884	-1.422922
C	-2.159214	6.365152	-1.628615
C	-1.217595	6.715288	-0.659760
C	-1.816639	6.578560	0.659760
C	0.213967	6.808593	-0.500972
C	0.470975	6.761283	0.918705
C	-0.816351	6.671652	1.628615
C	1.748019	6.514455	1.422922
C	2.761360	6.227167	0.500972
C	2.509277	6.296054	-0.918705
C	1.251605	6.627758	-1.422922

C	6.686035	0.688698	-1.628615
H	1.913271	-6.399353	-2.494843
H	1.052778	-6.595755	2.494843
H	-3.810311	-5.485787	-2.494843
H	-4.500372	-4.935481	2.494843
H	-6.664651	-0.441311	-2.494843
H	-6.664651	0.441311	2.494843
H	6.196120	-2.494076	-2.494843
H	5.813165	-3.289291	2.494843
H	-4.500372	4.935481	-2.494843
H	-3.810311	5.485787	2.494843
H	1.052778	6.595755	-2.494843
H	1.913271	6.399353	2.494843
C	3.630228	5.656749	-1.628615
C	4.010670	5.521971	0.659760
C	4.491065	5.138868	-0.659760
C	5.456578	4.077802	-0.500972
C	4.707120	4.797956	1.628615
C	5.579832	3.847367	0.918705
C	5.962153	3.153795	-1.422922
C	6.183078	2.695040	1.422922
C	6.486961	1.963694	-0.918705
C	6.590275	1.723657	0.500972
H	5.813165	3.289291	-2.494843
H	6.196120	2.494076	2.494843
C	4.367654	4.837470	4.225087
C	4.520133	4.827087	3.017383
H	4.230417	4.856483	5.285822
C	3.744290	5.334586	-4.225087
C	3.700238	5.480932	-3.017383
H	3.793364	5.205020	-5.285822
C	6.505274	0.398656	-4.225087
C	6.592226	0.524343	-3.017383
H	6.434573	0.279506	-5.285822
C	6.505274	-0.398656	4.225087
C	6.592226	-0.524343	3.017383
H	6.434573	-0.279506	5.285822
C	4.367654	-4.837470	-4.225087
C	4.520133	-4.827087	-3.017383
H	4.230417	-4.856483	-5.285822
C	3.744290	-5.334586	4.225087
C	3.700238	-5.480932	3.017383
H	3.793364	-5.205020	5.285822
C	-1.058899	-6.430882	-4.225087
C	-0.955712	-6.543622	-3.017383
H	-1.159329	-6.335440	-5.285822
C	-1.836221	-6.253464	4.225087
C	-1.978105	-6.310268	3.017383
H	-1.704325	-6.211049	5.285822
C	-5.688079	-3.181709	-4.225087
C	-5.711886	-3.332676	-3.017383
H	-5.676077	-3.043682	-5.285822
C	-6.034020	-2.463356	4.225087
C	-6.166894	-2.387843	3.017383
H	-5.918622	-2.540031	5.285822
C	-6.034020	2.463356	-4.225087
C	-6.166894	2.387843	-3.017383
H	-5.918622	2.540031	-5.285822
C	-5.688079	3.181709	4.225087
C	-5.711886	3.332676	3.017383
H	-5.676077	3.043682	5.285822
C	-1.836221	6.253464	-4.225087
C	-1.978105	6.310268	-3.017383
H	-1.704325	6.211049	-5.285822
C	-1.058899	6.430882	4.225087
C	-0.955712	6.543622	3.017383
H	-1.159329	6.335440	5.285822

Table S 81. Coordinates of the calculated structure of 11_8 (n=8) (TPSS-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.686908	0.255069	1.425662
C	-7.634564	1.305400	0.505390
C	-7.647108	1.044267	-0.923111
C	-7.686908	-0.255069	-1.425662
H	-7.625953	-0.440864	-2.493850
C	-7.634564	-1.305400	-0.505390
C	-7.647108	-1.044267	0.923111
C	-7.327615	-2.278557	1.629628
C	-7.044569	-3.248557	0.659412
C	-7.278339	-2.684186	-0.659412
C	-6.792589	-3.570223	-1.629628
C	-6.321509	-4.475395	0.505390
C	-5.615826	-5.255104	1.425662

H	-5.704101	-5.080626	2.493850
C	-6.145730	-4.668914	-0.923111
C	-4.668914	-6.145730	0.923111
C	-4.475395	-6.321509	-0.505390
C	-5.255104	-5.615826	-1.425662
C	-3.570223	-6.792589	1.629628
C	-2.684186	-7.278339	0.659412
C	-3.248557	-7.044569	-0.659412
C	-2.278557	-7.327615	-1.629628
C	-1.044267	-7.647108	-0.923111
C	-1.305400	-7.634564	0.505390
C	-0.255069	-7.686908	1.425662
C	0.255069	-7.686908	-1.425662
C	1.305400	-7.634564	-0.505390
C	1.044267	-7.647108	0.923111
C	2.278557	-7.327615	1.629628
C	3.248557	-7.044569	0.659412
C	2.684186	-7.278339	-0.659412
C	3.570223	-6.792589	-1.629628
C	4.668914	-6.145730	-0.923111
C	4.475395	-6.321509	0.505390
C	5.255104	-5.615826	1.425662
C	5.615826	-5.255104	-1.425662
C	6.321509	-4.475395	-0.505390
C	6.145730	-4.668914	0.923111
C	6.792589	-3.570223	1.629628
C	7.044569	-3.248557	-0.659412
C	7.278339	-2.684186	0.659412
C	7.327615	-2.278557	-1.629628
C	7.647108	-1.044267	-0.923111
C	7.634564	-1.305400	0.505390
C	7.686908	-0.255069	1.425662
C	7.686908	0.255069	-1.425662
C	7.634564	1.305400	-0.505390
C	7.647108	1.044267	0.923111
C	7.278339	2.684186	-0.659412
C	7.327615	2.278557	1.629628
C	6.792589	3.570223	-1.629628
C	7.044569	3.248557	0.659412
C	6.145730	4.668914	-0.923111
C	6.321509	4.475395	0.505390
C	5.255104	5.615826	-1.425662
C	5.615826	5.255104	1.425662
C	4.668914	6.145730	0.923111

C	4.475395	6.321509	-0.505390
C	3.248557	7.044569	-0.659412
C	3.570223	6.792589	1.629628
C	2.684186	7.278339	0.659412
C	2.278557	7.327615	-1.629628
C	1.044267	7.647108	-0.923111
C	1.305400	7.634564	0.505390
C	0.255069	7.686908	1.425662
C	-0.255069	7.686908	-1.425662
C	-1.305400	7.634564	-0.505390
C	-1.044267	7.647108	0.923111
C	-2.278557	7.327615	1.629628
C	-7.278339	2.684186	0.659412
C	-7.327615	2.278557	-1.629628
C	-7.044569	3.248557	-0.659412
H	-7.625953	0.440864	2.493850
H	-5.080626	-5.704101	-2.493850
H	-0.440864	-7.625953	2.493850
H	0.440864	-7.625953	-2.493850
H	5.704101	-5.080626	-2.493850
H	5.080626	-5.704101	2.493850
H	7.625953	0.440864	-2.493850
H	7.625953	-0.440864	2.493850
H	5.080626	5.704101	-2.493850
H	5.704101	5.080626	2.493850
H	-0.440864	7.625953	-2.493850
H	0.440864	7.625953	2.493850
C	-2.684186	7.278339	-0.659412
C	-3.248557	7.044569	0.659412
C	-3.570223	6.792589	-1.629628
C	-4.475395	6.321509	0.505390
C	-4.668914	6.145730	-0.923111
C	-5.255104	5.615826	1.425662
C	-5.615826	5.255104	-1.425662
C	-6.145730	4.668914	0.923111
C	-6.321509	4.475395	-0.505390
H	-5.080626	5.704101	2.493850
H	-5.704101	5.080626	-2.493850
C	-6.792589	3.570223	1.629628
C	6.780458	3.252953	-4.226633
C	6.790057	3.395163	-3.021782
H	6.778768	3.123796	-5.284217
C	7.094693	2.494322	4.226633
C	7.202038	2.400553	3.021782

H	7.002170	2.584456	5.284217
C	7.094693	-2.494322	-4.226633
C	7.202038	-2.400553	-3.021782
H	7.002170	-2.584456	-5.284217
C	6.780458	-3.252953	4.226633
C	6.790057	-3.395163	3.021782
H	6.778768	-3.123796	5.284217
C	3.252953	-6.780458	-4.226633
C	3.395163	-6.790057	-3.021782
H	3.123796	-6.778768	-5.284217
C	2.494322	-7.094693	4.226633
C	2.400553	-7.202038	3.021782
H	2.584456	-7.002170	5.284217
C	-2.494322	-7.094693	-4.226633
C	-2.400553	-7.202038	-3.021782
H	-2.584456	-7.002170	-5.284217
C	-3.252953	-6.780458	4.226633
C	-3.395163	-6.790057	3.021782
H	-3.123796	-6.778768	5.284217
C	-6.780458	-3.252953	-4.226633
C	-6.790057	-3.395163	-3.021782
H	-6.778768	-3.123796	-5.284217

C	-7.094693	-2.494322	4.226633
C	-7.202038	-2.400553	3.021782
H	-7.002170	-2.584456	5.284217
C	-7.094693	2.494322	-4.226633
C	-7.202038	2.400553	-3.021782
H	-7.002170	2.584456	-5.284217
C	-6.780458	3.252953	4.226633
C	-6.790057	3.395163	3.021782
H	-6.778768	3.123796	5.284217
C	-3.252953	6.780458	-4.226633
C	-3.395163	6.790057	-3.021782
H	-3.123796	6.778768	-5.284217
C	-2.494322	7.094693	4.226633
C	-2.400553	7.202038	3.021782
H	-2.584456	7.002170	5.284217
C	2.494322	7.094693	-4.226633
C	2.400553	7.202038	-3.021782
H	2.584456	7.002170	-5.284217
C	3.252953	6.780458	4.226633
C	3.395163	6.790057	3.021782
H	3.123796	6.778768	5.284217

Table S 82. Coordinates of the calculated structure of the triplet of 11_8 (n=8) (TPSS-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.705969	0.252196	1.421567
C	-7.656980	1.304278	0.502777
C	-7.668108	1.046193	-0.914783
C	-7.705969	-0.252196	-1.421567
H	-7.642803	-0.435162	-2.490129
C	-7.656980	-1.304278	-0.502777
C	-7.668108	-1.046193	0.914783
C	-7.341144	-2.290406	1.624320
C	-7.060734	-3.255100	0.659098
C	-7.294396	-2.690990	-0.659098
C	-6.810535	-3.571411	-1.624320
C	-6.336567	-4.492039	0.502777
C	-5.627272	-5.270614	1.421567
H	-5.711983	-5.096572	2.490129
C	-6.161941	-4.682401	-0.914783
C	-4.682401	-6.161941	0.914783
C	-4.492039	-6.336567	-0.502777
C	-5.270614	-5.627272	-1.421567

C	-3.571411	-6.810535	1.624320
C	-2.690990	-7.294396	0.659098
C	-3.255100	-7.060734	-0.659098
C	-2.290406	-7.341144	-1.624320
C	-1.046193	-7.668108	-0.914783
C	-1.304278	-7.656980	0.502777
C	-0.252196	-7.705969	1.421567
C	0.252196	-7.705969	-1.421567
C	1.304278	-7.656980	-0.502777
C	1.046193	-7.668108	0.914783
C	2.290406	-7.341144	1.624320
C	3.255100	-7.060734	0.659098
C	2.690990	-7.294396	-0.659098
C	3.571411	-6.810535	-1.624320
C	4.682401	-6.161941	-0.914783
C	4.492039	-6.336567	0.502777
C	5.270614	-5.627272	1.421567
C	5.627272	-5.270614	-1.421567
C	6.336567	-4.492039	-0.502777

C	6.161941	-4.682401	0.914783
C	6.810535	-3.571411	1.624320
C	7.060734	-3.255100	-0.659098
C	7.294396	-2.690990	0.659098
C	7.341144	-2.290406	-1.624320
C	7.668108	-1.046193	-0.914783
C	7.656980	-1.304278	0.502777
C	7.705969	-0.252196	1.421567
C	7.705969	0.252196	-1.421567
C	7.656980	1.304278	-0.502777
C	7.668108	1.046193	0.914783
C	7.294396	2.690990	-0.659098
C	7.341144	2.290406	1.624320
C	6.810535	3.571411	-1.624320
C	7.060734	3.255100	0.659098
C	6.161941	4.682401	-0.914783
C	6.336567	4.492039	0.502777
C	5.270614	5.627272	-1.421567
C	5.627272	5.270614	1.421567
C	4.682401	6.161941	0.914783
C	4.492039	6.336567	-0.502777
C	3.255100	7.060734	-0.659098
C	3.571411	6.810535	1.624320
C	2.690990	7.294396	0.659098
C	2.290406	7.341144	-1.624320
C	1.046193	7.668108	-0.914783
C	1.304278	7.656980	0.502777
C	0.252196	7.705969	1.421567
C	-0.252196	7.705969	-1.421567
C	-1.304278	7.656980	-0.502777
C	-1.046193	7.668108	0.914783
C	-2.290406	7.341144	1.624320
C	-7.294396	2.690990	0.659098
C	-7.341144	2.290406	-1.624320
C	-7.060734	3.255100	-0.659098
H	-7.642803	0.435162	2.490129
H	-5.096572	-5.711983	-2.490129
H	-0.435162	-7.642803	2.490129
H	0.435162	-7.642803	-2.490129
H	5.711983	-5.096572	-2.490129
H	5.096572	-5.711983	2.490129
H	7.642803	0.435162	-2.490129
H	7.642803	-0.435162	2.490129
H	5.096572	5.711983	-2.490129

H	5.711983	5.096572	2.490129
H	-0.435162	7.642803	-2.490129
H	0.435162	7.642803	2.490129
C	-2.690990	7.294396	-0.659098
C	-3.255100	7.060734	0.659098
C	-3.571411	6.810535	-1.624320
C	-4.492039	6.336567	0.502777
C	-4.682401	6.161941	-0.914783
C	-5.270614	5.627272	1.421567
C	-5.627272	5.270614	-1.421567
C	-6.161941	4.682401	0.914783
C	-6.336567	4.492039	-0.502777
H	-5.096572	5.711983	2.490129
H	-5.711983	5.096572	-2.490129
C	-6.810535	3.571411	1.624320
C	6.785169	3.263976	-4.222401
C	6.802378	3.398625	-3.016842
H	6.777774	3.139476	-5.280551
C	7.105818	2.489859	4.222401
C	7.213199	2.406817	3.016842
H	7.012555	2.572665	5.280551
C	7.105818	-2.489859	-4.222401
C	7.213199	-2.406817	-3.016842
H	7.012555	-2.572665	-5.280551
C	6.785169	-3.263976	4.222401
C	6.802378	-3.398625	3.016842
H	6.777774	-3.139476	5.280551
C	3.263976	-6.785169	-4.222401
C	3.398625	-6.802378	-3.016842
H	3.139476	-6.777774	-5.280551
C	2.489859	-7.105818	4.222401
C	2.406817	-7.213199	3.016842
H	2.572665	-7.012555	5.280551
C	-2.489859	-7.105818	-4.222401
C	-2.406817	-7.213199	-3.016842
H	-2.572665	-7.012555	-5.280551
C	-3.263976	-6.785169	4.222401
C	-3.398625	-6.802378	3.016842
H	-3.139476	-6.777774	5.280551
C	-6.785169	-3.263976	-4.222401
C	-6.802378	-3.398625	-3.016842
H	-6.777774	-3.139476	-5.280551
C	-7.105818	-2.489859	4.222401
C	-7.213199	-2.406817	3.016842

H	-7.012555	-2.572665	5.280551
C	-7.105818	2.489859	-4.222401
C	-7.213199	2.406817	-3.016842
H	-7.012555	2.572665	-5.280551
C	-6.785169	3.263976	4.222401
C	-6.802378	3.398625	3.016842
H	-6.777774	3.139476	5.280551
C	-3.263976	6.785169	-4.222401
C	-3.398625	6.802378	-3.016842
H	-3.139476	6.777774	-5.280551
C	-2.489859	7.105818	4.222401
C	-2.406817	7.213199	3.016842
H	-2.572665	7.012555	5.280551
C	2.489859	7.105818	-4.222401
C	2.406817	7.213199	-3.016842
H	2.572665	7.012555	-5.280551
C	3.263976	6.785169	4.222401
C	3.398625	6.802378	3.016842
H	3.123796	6.778768	5.284217

Table S 83. Coordinates of the calculated structure of the open-shell singlet of 11_8 (n=8) (TDDFT, BP86-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.677845	0.258380	1.430774
C	-7.625659	1.307175	0.506572
C	-7.637637	1.042955	-0.932938
C	-7.677845	-0.258380	-1.430774
H	-7.615121	-0.450026	-2.502605
C	-7.625659	-1.307175	-0.506572
C	-7.637637	-1.042955	0.932938
C	-7.321817	-2.273535	1.637634
C	-7.041406	-3.248478	0.661028
C	-7.276046	-2.682005	-0.661028
C	-6.784938	-3.569674	-1.637634
C	-6.316467	-4.467843	0.506572
C	-5.611759	-5.246354	1.430774
H	-5.702920	-5.066488	2.502605
C	-6.138105	-4.663144	-0.932938
C	-4.663144	-6.138105	0.932938
C	-4.467843	-6.316467	-0.506572
C	-5.246354	-5.611759	-1.430774
C	-3.569674	-6.784938	1.637634
C	-2.682005	-7.276046	0.661028
C	-3.248478	-7.041406	-0.661028
C	-2.273535	-7.321817	-1.637634
C	-1.042955	-7.637637	-0.932938
C	-1.307175	-7.625659	0.506572
C	-0.258380	-7.677845	1.430774
C	0.258380	-7.677845	-1.430774
C	1.307175	-7.625659	-0.506572
C	1.042955	-7.637637	0.932938
C	2.273535	-7.321817	1.637634
C	3.248478	-7.041406	0.661028
C	2.682005	-7.276046	-0.661028
C	3.569674	-6.784938	-1.637634
C	4.663144	-6.138105	-0.932938
C	4.467843	-6.316467	0.506572
C	5.246354	-5.611759	1.430774
C	5.611759	-5.246354	-1.430774
C	6.316467	-4.467843	-0.506572
C	6.138105	-4.663144	0.932938
C	6.784938	-3.569674	1.637634
C	7.041406	-3.248478	-0.661028
C	7.276046	-2.682005	0.661028
C	7.321817	-2.273535	-1.637634
C	7.637637	-1.042955	-0.932938
C	7.625659	-1.307175	0.506572
C	7.677845	-0.258380	1.430774
C	7.677845	0.258380	-1.430774
C	7.625659	1.307175	-0.506572
C	7.637637	1.042955	0.932938
C	7.276046	2.682005	-0.661028
C	7.321817	2.273535	1.637634
C	6.784938	3.569674	-1.637634
C	7.041406	3.248478	0.661028
C	6.138105	4.663144	-0.932938
C	6.316467	4.467843	0.506572
C	5.246354	5.611759	-1.430774
C	5.611759	5.246354	1.430774
C	4.663144	6.138105	0.932938
C	4.467843	6.316467	-0.506572
C	3.248478	7.041406	-0.661028
C	3.569674	6.784938	1.637634
C	2.682005	7.276046	0.661028

C	2.273535	7.321817	-1.637634
C	1.042955	7.637637	-0.932938
C	1.307175	7.625659	0.506572
C	0.258380	7.677845	1.430774
C	-0.258380	7.677845	-1.430774
C	-1.307175	7.625659	-0.506572
C	-1.042955	7.637637	0.932938
C	-2.273535	7.321817	1.637634
C	-7.276046	2.682005	0.661028
C	-7.321817	2.273535	-1.637634
C	-7.041406	3.248478	-0.661028
H	-7.615121	0.450026	2.502605
H	-5.066488	-5.702920	-2.502605
H	-0.450026	-7.615121	2.502605
H	0.450026	-7.615121	-2.502605
H	5.702920	-5.066488	-2.502605
H	5.066488	-5.702920	2.502605
H	7.615121	0.450026	-2.502605
H	7.615121	-0.450026	2.502605
H	5.066488	5.702920	-2.502605
H	5.702920	5.066488	2.502605
H	-0.450026	7.615121	-2.502605
H	0.450026	7.615121	2.502605
C	-2.682005	7.276046	-0.661028
C	-3.248478	7.041406	0.661028
C	-3.569674	6.784938	-1.637634
C	-4.467843	6.316467	0.506572
C	-4.663144	6.138105	-0.932938
C	-5.246354	5.611759	1.430774
C	-5.611759	5.246354	-1.430774
C	-6.138105	4.663144	0.932938
C	-6.316467	4.467843	-0.506572
H	-5.066488	5.702920	2.502605
H	-5.702920	5.066488	-2.502605
C	-6.784938	3.569674	1.637634
C	6.770307	3.228896	-4.234644
C	6.780348	3.384963	-3.027412
H	6.767490	3.088849	-5.295135
C	7.070504	2.504156	4.234644
C	7.187960	2.400899	3.027412
H	6.969484	2.601192	5.295135
C	7.070504	-2.504156	-4.234644
C	7.187960	-2.400899	-3.027412
H	6.969484	-2.601192	-5.295135
C	6.770307	-3.228896	4.234644
C	6.780348	-3.384963	3.027412
H	6.767490	-3.088849	5.295135
C	3.228896	-6.770307	-4.234644
C	3.384963	-6.780348	-3.027412
H	3.088849	-6.767490	-5.295135
C	2.504156	-7.070504	4.234644
C	2.400899	-7.187960	3.027412
H	2.601192	-6.969484	5.295135
C	-2.504156	-7.070504	-4.234644
C	-2.400899	-7.187960	-3.027412
H	-2.601192	-6.969484	-5.295135
C	-3.228896	-6.770307	4.234644
C	-3.384963	-6.780348	3.027412
H	-3.088849	-6.767490	5.295135
C	-6.770307	-3.228896	-4.234644
C	-6.780348	-3.384963	-3.027412
H	-6.767490	-3.088849	-5.295135
C	-7.070504	-2.504156	4.234644
C	-7.187960	-2.400899	3.027412
H	-6.969484	-2.601192	5.295135
C	-7.070504	2.504156	-4.234644
C	-7.187960	2.400899	-3.027412
H	-6.969484	2.601192	-5.295135
C	-6.770307	3.228896	4.234644
C	-6.780348	3.384963	3.027412
H	-6.767490	3.088849	5.295135
C	-3.228896	6.770307	-4.234644
C	-3.384963	6.780348	-3.027412
H	-3.088849	6.767490	-5.295135
C	-2.504156	7.070504	4.234644
C	-2.400899	7.187960	3.027412
H	-2.601192	6.969484	5.295135
C	2.504156	7.070504	-4.234644
C	2.400899	7.187960	-3.027412
H	2.601192	6.969484	-5.295135
C	3.228896	6.770307	4.234644
C	3.384963	6.780348	3.027412
H	3.088849	6.767490	5.295135

4.6 Calculated coordinates of thiomethyl-substituted cyclacenes 12_n

Below can be found coordinates for the calculated structures of thiomethyl-substituted $[5.5.6]_n$cyclacenes **12_n** as singlets and triplets at the TPSS-D3/def2-TZVP level of theory and of the open-shell singlets calculated using TDDFT at the BP86-D3/def2-TZVP level of theory, optimized in point group D_n.

Table S 84. Coordinates of the calculated structure of 12_3 (n=3) (TPSS-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.950700	2.080710	-1.620348
C	-2.717532	1.041584	-0.912602
C	-2.675970	1.322020	0.492811
C	-1.800713	2.484695	0.659985
C	-1.251453	2.801811	-0.659985
C	-2.837732	-0.265656	-1.404641
C	-2.675970	-1.322020	-0.492811
C	-2.717532	-1.041584	0.912602
C	-2.837732	0.265656	1.404641
C	-1.800713	-2.484695	-0.659985
C	-1.251453	-2.801811	0.659985
C	-1.950700	-2.080710	1.620348
C	0.193082	-2.978468	0.492811
C	0.456728	-2.874244	-0.912602
C	-0.826598	-2.729711	-1.620348
C	1.648931	-2.324720	-1.404641
C	2.482888	-1.656448	-0.492811
C	2.260804	-1.832660	0.912602
C	1.188801	-2.590376	1.404641
C	3.052166	-0.317115	-0.659985
C	3.052166	0.317115	0.659985
C	2.777298	-0.649001	1.620348
C	2.482888	1.656448	0.492811
C	2.260804	1.832660	-0.912602
C	2.777298	0.649001	-1.620348
C	1.188801	2.590376	-1.404641
C	0.193082	2.978468	-0.492811
C	0.456728	2.874244	0.912602
C	1.648931	2.324720	1.404641
C	-0.826598	2.729711	1.620348
H	0.966383	2.536957	-2.466767
H	1.713878	2.105391	2.466767
H	1.713878	-2.105391	-2.466767
H	0.966383	-2.536957	2.466767
H	-2.680261	-0.431566	-2.466767
H	-2.680261	0.431566	2.466767
S	-0.926023	2.523924	3.336444
C	-2.667485	2.954309	3.654485
H	-2.774463	2.970912	4.741392
H	-2.872491	3.943179	3.241037
H	-3.352622	2.220071	3.229935
C	-1.224764	3.787265	-3.654485
S	-1.722771	2.063921	-3.336444
H	-1.185653	3.888211	-4.741392
H	-0.246327	4.013491	-3.229935
H	-1.978647	4.459240	-3.241037
C	3.892250	-0.832955	-3.654485
S	2.648794	0.460003	-3.336444
H	3.960116	-0.917300	-4.741392
H	3.598949	-1.793420	-3.229935
H	4.851138	-0.516061	-3.241037
C	-2.667485	-2.954309	-3.654485
S	-0.926023	-2.523924	-3.336444
H	-2.774463	-2.970912	-4.741392
H	-3.352622	-2.220071	-3.229935
H	-2.872491	-3.943179	-3.241037
C	3.892250	0.832955	3.654485
S	2.648794	-0.460003	3.336444
H	3.960116	0.917300	4.741392
H	3.598949	1.793420	3.229935
H	4.851138	0.516061	3.241037
C	-1.224764	-3.787265	3.654485
S	-1.722771	-2.063921	3.336444
H	-1.185653	-3.888211	4.741392
H	-0.246327	-4.013491	3.229935
H	-1.978647	-4.459240	3.241037

Table S 85. Coordinates of the calculated structure of the triplet of 12_3 (n=3) (TPSS-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.965395	2.061940	-1.628019
C	-2.709830	1.039835	-0.925038
C	-2.664818	1.327160	0.489614
C	-1.801547	2.493614	0.649927
C	-1.258759	2.806992	-0.649927
C	-2.823597	-0.281250	-1.404022
C	-2.664818	-1.327160	-0.489614
C	-2.709830	-1.039835	0.925038
C	-2.823597	0.281250	1.404022
C	-1.801547	-2.493614	-0.649927
C	-1.258759	-2.806992	0.649927
C	-1.965395	-2.061940	1.628019
C	0.183055	-2.971380	0.489614
C	0.454392	-2.866699	-0.925038
C	-0.802995	-2.733052	-1.628019
C	1.655368	-2.304682	-1.404022
C	2.481763	-1.644220	-0.489614
C	2.255439	-1.826864	0.925038
C	1.168230	-2.585932	1.404022
C	3.060306	-0.313379	-0.649927
C	3.060306	0.313379	0.649927
C	2.768390	-0.671112	1.628019
C	2.481763	1.644220	0.489614
C	2.255439	1.826864	-0.925038
C	2.768390	0.671112	-1.628019
C	1.168230	2.585932	-1.404022
C	0.183055	2.971380	-0.489614
C	0.454392	2.866699	0.925038
C	1.655368	2.304682	1.404022
C	-0.802995	2.733052	1.628019
H	0.943399	2.544735	-2.466654
H	1.732106	2.089375	2.466654
H	1.732106	-2.089375	-2.466654
H	0.943399	-2.544735	2.466654
H	-2.675505	-0.455360	-2.466654
H	-2.675505	0.455360	2.466654
S	-0.928547	2.515954	3.341072
C	-2.657480	3.007771	3.640498
H	-2.813250	2.904532	4.716635
H	-2.797538	4.047256	3.339566
H	-3.354826	2.363158	3.104417
C	-1.276066	3.805330	-3.640498
S	-1.714606	2.062122	-3.341072
H	-1.108773	3.888611	-4.716635
H	-0.369142	4.086943	-3.104417
H	-2.106258	4.446367	-3.339566
C	3.933546	-0.797559	-3.640498
S	2.643153	0.453832	-3.341072
H	3.922023	-0.984080	-4.716635
H	3.723968	-1.723785	-3.104417
H	4.903796	-0.399111	-3.339566
C	-2.657480	-3.007771	-3.640498
S	-0.928547	-2.515954	-3.341072
H	-2.813250	-2.904532	-4.716635
H	-3.354826	-2.363158	-3.104417
H	-2.797538	-4.047256	-3.339566
C	3.933546	0.797559	3.640498
S	2.643153	-0.453832	3.341072
H	3.922023	0.984080	4.716635
H	3.723968	1.723785	3.104417
H	4.903796	0.399111	3.339566
C	-1.276066	-3.805330	3.640498
S	-1.714606	-2.062122	3.341072
H	-1.108773	-3.888611	4.716635
H	-0.369142	-4.086943	3.104417
H	-2.106258	-4.446367	3.339566

Table S 86. Coordinates of the calculated structure of the open-shell singlet of 12_3 (n=3) (TDDFT, BP86-D3/def2-TZVP) in D_3 geometry.

	x	y	z
C	-1.946863	2.059986	-1.640741
C	-2.696080	1.037025	-0.935788
C	-2.648563	1.321475	0.495396
C	-1.799141	2.478222	0.665074
C	-1.246633	2.797213	-0.665074
C	-2.829604	-0.274171	-1.415219
C	-2.648563	-1.321475	-0.495396

C	-2.696080	-1.037025	0.935788
C	-2.829604	0.274171	1.415219
C	-1.799141	-2.478222	-0.665074
C	-1.246633	-2.797213	0.665074
C	-1.946863	-2.059986	1.640741
C	0.179851	-2.954460	0.495396
C	0.449950	-2.853386	-0.935788
C	-0.810569	-2.716026	-1.640741
C	1.652241	-2.313423	-1.415219
C	2.468712	-1.632985	-0.495396
C	2.246129	-1.816361	0.935788
C	1.177363	-2.587594	1.415219
C	3.045774	-0.318991	-0.665074
C	3.045774	0.318991	0.665074
C	2.757432	-0.656040	1.640741
C	2.468712	1.632985	0.495396
C	2.246129	1.816361	-0.935788
C	2.757432	0.656040	-1.640741
C	1.177363	2.587594	-1.415219
C	0.179851	2.954460	-0.495396
C	0.449950	2.853386	0.935788
C	1.652241	2.313423	1.415219
C	-0.810569	2.716026	1.640741
H	0.953994	2.556924	-2.482546
H	1.737364	2.104645	2.482546
H	1.737364	-2.104645	-2.482546
H	0.953994	-2.556924	2.482546
H	-2.691358	-0.452279	-2.482546
H	-2.691358	0.452279	2.482546
S	-0.904453	2.411594	3.344573
C	-2.607806	2.932941	3.714475
H	-2.731122	2.811987	4.797508
H	-2.741234	3.985472	3.440152
H	-3.346946	2.313873	3.193818
C	-1.236099	3.724896	-3.714475
S	-1.636275	1.989076	-3.344573
H	-1.069691	3.771214	-4.797508
H	-0.330399	4.055477	-3.193818
H	-2.080903	4.366714	-3.440152
C	3.843904	-0.791955	-3.714475
S	2.540728	0.422518	-3.344573
H	3.800813	-0.959227	-4.797508
H	3.677346	-1.741604	-3.193818
H	4.822137	-0.381242	-3.440152
C	-2.607806	-2.932941	-3.714475
S	-0.904453	-2.411594	-3.344573
H	-2.731122	-2.811987	-4.797508
H	-3.346946	-2.313873	-3.193818
H	-2.741234	-3.985472	-3.440152
C	3.843904	0.791955	3.714475
S	2.540728	-0.422518	3.344573
H	3.800813	0.959227	4.797508
H	3.677346	1.741604	3.193818
H	4.822137	0.381242	3.440152
C	-1.236099	-3.724896	3.714475
S	-1.636275	-1.989076	3.344573
H	-1.069691	-3.771214	4.797508
H	-0.330399	-4.055477	3.193818
H	-2.080903	-4.366714	3.440152

Table S 87. Coordinates of the calculated structure of 12_4 (n=4) (TPSS-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.733611	-1.047038	-0.909212
C	3.714450	-1.317882	0.498126
C	3.809041	0.258649	-1.407825
C	3.714450	1.317882	-0.498126
C	3.733611	1.047038	0.909212
C	3.809041	-0.258649	1.407825
C	3.137136	-2.191569	-1.615704
C	3.044253	-2.605853	0.660205
C	2.605853	-3.044253	-0.660205
C	2.191569	-3.137136	1.615704
C	1.317882	-3.714450	-0.498126
C	1.047038	-3.733611	0.909212
C	0.258649	-3.809041	-1.407825
C	-0.258649	-3.809041	1.407825
C	-1.047038	-3.733611	-0.909212
C	-1.317882	-3.714450	0.498126
C	-2.605853	-3.044253	0.660205
C	-2.191569	-3.137136	-1.615704
C	-3.044253	-2.605853	-0.660205
C	-3.137136	-2.191569	1.615704
C	-3.714450	-1.317882	-0.498126

C	-3.733611	-1.047038	0.909212
C	-3.809041	-0.258649	-1.407825
C	-3.809041	0.258649	1.407825
C	-3.714450	1.317882	0.498126
C	-3.733611	1.047038	-0.909212
C	-3.137136	2.191569	-1.615704
C	-3.044253	2.605853	0.660205
C	-2.605853	3.044253	-0.660205
C	-2.191569	3.137136	1.615704
C	-1.047038	3.733611	0.909212
C	-1.317882	3.714450	-0.498126
C	0.258649	3.809041	1.407825
C	-0.258649	3.809041	-1.407825
C	1.047038	3.733611	-0.909212
C	1.317882	3.714450	0.498126
C	2.191569	3.137136	-1.615704
C	2.605853	3.044253	0.660205
C	3.044253	2.605853	-0.660205
C	3.137136	2.191569	1.615704
H	-3.673947	0.425485	2.472858
H	-3.673947	-0.425485	-2.472858
H	-0.425485	-3.673947	2.472858
H	0.425485	-3.673947	-2.472858
H	3.673947	-0.425485	2.472858
H	3.673947	0.425485	-2.472858
H	0.425485	3.673947	2.472858
H	-0.425485	3.673947	-2.472858
C	-2.969756	4.005270	-3.688306
S	-2.928916	2.216558	-3.339930
H	-2.894150	4.097117	-4.774200
H	-2.138515	4.530704	-3.218130
H	-3.919386	4.417459	-3.342919
C	4.005270	2.969756	-3.688306
S	2.216558	2.928916	-3.339930
H	4.097117	2.894150	-4.774200
H	4.530704	2.138515	-3.218130
H	4.417459	3.919386	-3.342919
C	2.969756	-4.005270	-3.688306
S	2.928916	-2.216558	-3.339930
H	2.894150	-4.097117	-4.774200
H	2.138515	-4.530704	-3.218130
H	3.919386	-4.417459	-3.342919
C	-4.005270	-2.969756	-3.688306
S	-2.216558	-2.928916	-3.339930
H	-4.097117	-2.894150	-4.774200
H	-4.530704	-2.138515	-3.218130
H	-4.417459	-3.919386	-3.342919
C	-4.005270	2.969756	3.688306
S	-2.216558	2.928916	3.339930
H	-4.097117	2.894150	4.774200
H	-4.530704	2.138515	3.218130
H	-4.417459	3.919386	3.342919
C	2.969756	4.005270	3.688306
S	2.928916	2.216558	3.339930
H	2.894150	4.097117	4.774200
H	2.138515	4.530704	3.218130
H	3.919386	4.417459	3.342919
C	-2.969756	-4.005270	3.688306
S	-2.928916	-2.216558	3.339930
H	-2.894150	-4.097117	4.774200
H	-2.138515	-4.530704	3.218130
H	-3.919386	-4.417459	3.342919
C	4.005270	-2.969756	3.688306
S	2.216558	-2.928916	3.339930
H	4.097117	-2.894150	4.774200
H	4.530704	-2.138515	3.218130
H	4.417459	-3.919386	3.342919

Table S 88. Coordinates of the calculated structure of the triplet of 12_4 (n=4) (TPSS-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.709932	-1.043630	-0.926444
C	3.683560	-1.316342	0.502146
C	3.792599	0.263188	-1.417174
C	3.683560	1.316342	-0.502146
C	3.709932	1.043630	0.926444
C	3.792599	-0.263188	1.417174
C	3.130757	-2.174435	-1.628408
C	3.030521	-2.590639	0.662765
C	2.590639	-3.030521	-0.662765
C	2.174435	-3.130757	1.628408
C	1.316342	-3.683560	-0.502146
C	1.043630	-3.709932	0.926444
C	0.263188	-3.792599	-1.417174

C	-0.263188	-3.792599	1.417174
C	-1.043630	-3.709932	-0.926444
C	-1.316342	-3.683560	0.502146
C	-2.590639	-3.030521	0.662765
C	-2.174435	-3.130757	-1.628408
C	-3.030521	-2.590639	-0.662765
C	-3.130757	-2.174435	1.628408
C	-3.683560	-1.316342	-0.502146
C	-3.709932	-1.043630	0.926444
C	-3.792599	-0.263188	-1.417174
C	-3.792599	0.263188	1.417174
C	-3.683560	1.316342	0.502146
C	-3.709932	1.043630	-0.926444
C	-3.130757	2.174435	-1.628408
C	-3.030521	2.590639	0.662765
C	-2.590639	3.030521	-0.662765
C	-2.174435	3.130757	1.628408
C	-1.043630	3.709932	0.926444
C	-1.316342	3.683560	-0.502146
C	0.263188	3.792599	1.417174
C	-0.263188	3.792599	-1.417174
C	1.043630	3.709932	-0.926444
C	1.316342	3.683560	0.502146
C	2.174435	3.130757	-1.628408
C	2.590639	3.030521	0.662765
C	3.030521	2.590639	-0.662765
C	3.130757	2.174435	1.628408
H	-3.668659	0.438564	2.482229
H	-3.668659	-0.438564	-2.482229
H	-0.438564	-3.668659	2.482229
H	0.438564	-3.668659	-2.482229
H	3.668659	-0.438564	2.482229
H	3.668659	0.438564	-2.482229
H	0.438564	3.668659	2.482229
H	-0.438564	3.668659	-2.482229
C	-2.994905	3.985505	-3.702657
S	-2.880806	2.200348	-3.349139
H	-2.838745	4.086088	-4.779124
H	-2.230412	4.550539	-3.168199
H	-3.988595	4.348107	-3.434034
C	3.985505	2.994905	-3.702657
S	2.200348	2.880806	-3.349139
H	4.086088	2.838745	-4.779124
H	4.550539	2.230412	-3.168199
H	4.348107	3.988595	-3.434034
C	2.994905	-3.985505	-3.702657
S	2.880806	-2.200348	-3.349139
H	2.838745	-4.086088	-4.779124
H	2.230412	-4.550539	-3.168199
H	3.988595	-4.348107	-3.434034
C	-3.985505	-2.994905	-3.702657
S	-2.200348	-2.880806	-3.349139
H	-4.086088	-2.838745	-4.779124
H	-4.550539	-2.230412	-3.168199
H	-4.348107	-3.988595	-3.434034
C	-3.985505	2.994905	3.702657
S	-2.200348	2.880806	3.349139
H	-4.086088	2.838745	4.779124
H	-4.550539	2.230412	3.168199
H	-4.348107	3.988595	3.434034
C	2.994905	3.985505	3.702657
S	2.880806	2.200348	3.349139
H	2.838745	4.086088	4.779124
H	2.230412	4.550539	3.168199
H	3.988595	4.348107	3.434034
C	-2.994905	-3.985505	3.702657
S	-2.880806	-2.200348	3.349139
H	-2.838745	-4.086088	4.779124
H	-2.230412	-4.550539	3.168199
H	-3.988595	-4.348107	3.434034
C	3.985505	-2.994905	3.702657
S	2.200348	-2.880806	3.349139
H	4.086088	-2.838745	4.779124
H	4.550539	-2.230412	3.168199
H	4.348107	-3.988595	3.434034

Table S 89. Coordinates of the calculated structure of the open-shell singlet of 12_4 (n=4) (TDDFT, BP86-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.719220	-1.043342	-0.921395
C	3.707676	-1.323913	0.494155
C	3.802190	0.264929	-1.411424
C	3.707676	1.323913	-0.494155
C	3.719220	1.043342	0.921395

C	3.802190	-0.264929	1.411424
C	3.132107	-2.190338	-1.624967
C	3.063407	-2.617912	0.658712
C	2.617912	-3.063407	-0.658712
C	2.190338	-3.132107	1.624967
C	1.323913	-3.707676	-0.494155
C	1.043342	-3.719220	0.921395
C	0.264929	-3.802190	-1.411424
C	-0.264929	-3.802190	1.411424
C	-1.043342	-3.719220	-0.921395
C	-1.323913	-3.707676	0.494155
C	-2.617912	-3.063407	0.658712
C	-2.190338	-3.132107	-1.624967
C	-3.063407	-2.617912	-0.658712
C	-3.132107	-2.190338	1.624967
C	-3.707676	-1.323913	-0.494155
C	-3.719220	-1.043342	0.921395
C	-3.802190	-0.264929	-1.411424
C	-3.802190	0.264929	1.411424
C	-3.707676	1.323913	0.494155
C	-3.719220	1.043342	-0.921395
C	-3.132107	2.190338	-1.624967
C	-3.063407	2.617912	0.658712
C	-2.617912	3.063407	-0.658712
C	-2.190338	3.132107	1.624967
C	-1.043342	3.719220	0.921395
C	-1.323913	3.707676	-0.494155
C	0.264929	3.802190	1.411424
C	-0.264929	3.802190	-1.411424
C	1.043342	3.719220	-0.921395
C	1.323913	3.707676	0.494155
C	2.190338	3.132107	-1.624967
C	2.617912	3.063407	0.658712
C	3.063407	2.617912	-0.658712
C	3.132107	2.190338	1.624967
H	-3.666215	0.440572	2.479666
H	-3.666215	-0.440572	-2.479666
H	-0.440572	-3.666215	2.479666
H	0.440572	-3.666215	-2.479666
H	3.666215	-0.440572	2.479666
H	3.666215	0.440572	-2.479666
H	0.440572	3.666215	2.479666
H	-0.440572	3.666215	-2.479666
C	-2.960460	3.990490	-3.706993
S	-2.889734	2.209438	-3.339422
H	-2.823176	4.082463	-4.791247
H	-2.169760	4.545129	-3.190993
H	-3.941936	4.384595	-3.419127
C	3.990490	2.960460	-3.706993
S	2.209438	2.889734	-3.339422
H	4.082463	2.823176	-4.791247
H	4.545129	2.169760	-3.190993
H	4.384595	3.941936	-3.419127
C	2.960460	-3.990490	-3.706993
S	2.889734	-2.209438	-3.339422
H	2.823176	-4.082463	-4.791247
H	2.169760	-4.545129	-3.190993
H	3.941936	-4.384595	-3.419127
C	-3.990490	-2.960460	-3.706993
S	-2.209438	-2.889734	-3.339422
H	-4.082463	-2.823176	-4.791247
H	-4.545129	-2.169760	-3.190993
H	-4.384595	-3.941936	-3.419127
C	-3.990490	2.960460	3.706993
S	-2.209438	2.889734	3.339422
H	-4.082463	2.823176	4.791247
H	-4.545129	2.169760	3.190993
H	-4.384595	3.941936	3.419127
C	2.960460	3.990490	3.706993
S	2.889734	2.209438	3.339422
H	2.823176	4.082463	4.791247
H	2.169760	4.545129	3.190993
H	3.941936	4.384595	3.419127
C	-2.960460	-3.990490	3.706993
S	-2.889734	-2.209438	3.339422
H	-2.823176	-4.082463	4.791247
H	-2.169760	-4.545129	3.190993
H	-3.941936	-4.384595	3.419127
C	3.990490	-2.960460	3.706993
S	2.209438	-2.889734	3.339422
H	4.082463	-2.823176	4.791247
H	4.545129	-2.169760	3.190993
H	4.384595	-3.941936	3.419127

Table S 90. Coordinates of the calculated structure of 12_5 (n=5) (TPSS-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	-4.252581	-2.246185	1.614316
C	-4.729344	-1.049411	0.907067
C	-4.717741	-1.315096	-0.502836
C	-4.181234	-2.658107	-0.661260
C	-3.820082	-3.155189	0.661260
C	-4.785989	0.253386	1.410808
C	-4.717741	1.315096	0.502836
C	-4.729344	1.049411	-0.907067
C	-4.785989	-0.253386	-1.410808
C	-4.181234	2.658107	0.661260
C	-3.820082	3.155189	-0.661260
C	-4.252581	2.246185	-1.614316
C	-2.708593	4.080452	-0.502836
C	-2.459497	4.173587	0.907067
C	-3.450369	3.350336	1.614316
C	-1.237968	4.630046	1.410808
C	-0.207131	4.893226	0.502836
C	-0.463398	4.822159	-0.907067
C	-1.719936	4.473445	-1.410808
C	1.235938	4.797990	0.661260
C	1.820293	4.608121	-0.661260
C	0.822129	4.738555	-1.614316
C	3.043739	3.836954	-0.502836
C	3.209291	3.628830	0.907067
C	2.120136	4.316807	1.614316
C	4.020883	2.608140	1.410808
C	4.589727	1.709084	0.502836
C	4.442948	1.930847	-0.907067
C	3.723010	3.018127	-1.410808
C	4.760685	0.682402	-1.614316
C	4.945085	-0.307214	-0.661260
C	4.945085	0.307214	0.661260
C	4.589727	-1.709084	-0.502836
C	4.442948	-1.930847	0.907067
C	4.760685	-0.682402	1.614316
C	4.020883	-2.608140	-1.410808
C	3.209291	-3.628830	-0.907067
C	3.043739	-3.836954	0.502836
C	3.723010	-3.018127	1.410808
C	-3.450369	-3.350336	-1.614316
H	4.024182	2.406607	2.478106
H	3.532360	3.083542	-2.478106
H	-1.045279	4.570907	2.478106
H	-1.841063	4.312341	-2.478106
H	-4.670200	0.418369	2.478106
H	-4.670200	-0.418369	-2.478106
H	3.532360	-3.083542	2.478106
H	4.024182	-2.406607	-2.478106
C	-2.708593	-4.080452	0.502836
C	-2.459497	-4.173587	-0.907067
C	-1.719936	-4.473445	1.410808
C	-1.237968	-4.630046	-1.410808
C	-0.207131	-4.893226	-0.502836
C	-0.463398	-4.822159	0.907067
C	0.822129	-4.738555	1.614316
C	1.235938	-4.797990	-0.661260
C	1.820293	-4.608121	0.661260
C	2.120136	-4.316807	-1.614316
H	-1.841063	-4.312341	2.478106
H	-1.045279	-4.570907	-2.478106
C	5.972544	-0.675764	-3.693549
S	4.661004	0.542009	-3.344983
H	5.983512	-0.795978	-4.779276
H	5.771095	-1.637186	-3.221558
H	6.930973	-0.281572	-3.351434
C	1.202928	-5.889050	-3.693549
S	1.955810	-4.265388	-3.344983
H	1.091987	-5.936629	-4.779276
H	0.226310	-5.994556	-3.221558
H	1.873998	-6.678757	-3.351434
C	-5.229094	-2.963869	-3.693549
S	-3.452247	-3.178164	-3.344983
H	-5.308628	-2.873060	-4.779276
H	-5.631228	-2.067653	-3.221558
H	-5.772778	-3.846127	-3.351434
C	-4.434686	4.057278	-3.693549
S	-4.089416	2.301175	-3.344983
H	-4.372899	4.160980	-4.779276
H	-3.706600	4.716676	-3.221558
H	-5.441771	4.301720	-3.351434
C	2.488307	5.471405	-3.693549
S	0.924848	4.600368	-3.344983
H	2.606027	5.444688	-4.779276

H	3.340423	4.982719	-3.221558
H	2.409579	6.504736	-3.351434
C	5.972544	0.675764	3.693549
S	4.661004	-0.542009	3.344983
H	5.983512	0.795978	4.779276
H	5.771095	1.637186	3.221558
H	6.930973	0.281572	3.351434
C	2.488307	-5.471405	3.693549
S	0.924848	-4.600368	3.344983
H	2.606027	-5.444688	4.779276
H	3.340423	-4.982719	3.221558
H	2.409579	-6.504736	3.351434
C	-4.434686	-4.057278	3.693549
S	-4.089416	-2.301175	3.344983
H	-4.372899	-4.160980	4.779276
H	-3.706600	-4.716676	3.221558
H	-5.441771	-4.301720	3.351434
C	-5.229094	2.963869	3.693549
S	-3.452247	3.178164	3.344983
H	-5.308628	2.873060	4.779276
H	-5.631228	2.067653	3.221558
H	-5.772778	3.846127	3.351434
C	1.202928	5.889050	3.693549
S	1.955810	4.265388	3.344983
H	1.091987	5.936629	4.779276
H	0.226310	5.994556	3.221558
H	1.873998	6.678757	3.351434

Table S 91. Coordinates of the calculated structure of the triplet of 12_5 (n=5) (TPSS-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	-4.253431	-2.229389	1.617336
C	-4.722809	-1.047879	0.914260
C	-4.711103	-1.318553	-0.501876
C	-4.184150	-2.663108	-0.655033
C	-3.825740	-3.156417	0.655033
C	-4.779160	0.263012	1.410900
C	-4.711103	1.318553	0.501876
C	-4.722809	1.047879	-0.914260
C	-4.779160	-0.263012	-1.410900
C	-4.184150	2.663108	0.655033
C	-3.825740	3.156417	-0.655033
C	-4.253431	2.229389	-1.617336
C	-2.709829	4.073070	-0.501876
C	-2.456020	4.167846	0.914260
C	-3.434658	3.356335	1.617336
C	-1.226702	4.626527	1.410900
C	-0.201793	4.887981	0.501876
C	-0.462836	4.815470	-0.914260
C	-1.726981	4.463976	-1.410900
C	1.239793	4.802308	0.655033
C	1.819713	4.613881	-0.655033
C	0.805893	4.734173	-1.617336
C	3.036337	3.835849	-0.501876
C	3.204905	3.623749	0.914260
C	2.130696	4.303718	1.617336
C	4.021016	2.596339	1.410900
C	4.586389	1.702385	0.501876
C	4.436760	1.928246	-0.914260
C	3.711827	3.021901	-1.410900
C	4.751500	0.696490	-1.617336
C	4.950384	-0.304882	-0.655033
C	4.950384	0.304882	0.655033
C	4.586389	-1.702385	-0.501876
C	4.436760	-1.928246	0.914260
C	4.751500	-0.696490	1.617336
C	4.021016	-2.596339	-1.410900
C	3.204905	-3.623749	-0.914260
C	3.036337	-3.835849	0.501876
C	3.711827	-3.021901	1.410900
C	-3.434658	-3.356335	-1.617336
H	4.032457	2.395491	2.478706
H	3.524346	3.094847	-2.478706
H	-1.032150	4.575342	2.478706
H	-1.854292	4.308212	-2.478706
H	-4.670361	0.432226	2.478706
H	-4.670361	-0.432226	-2.478706
H	3.524346	-3.094847	2.478706
H	4.032457	-2.395491	-2.478706
C	-2.709829	-4.073070	0.501876
C	-2.456020	-4.167846	-0.914260
C	-1.726981	-4.463976	1.410900
C	-1.226702	-4.626527	-1.410900
C	-0.201793	-4.887981	-0.501876

C	-0.462836	-4.815470	0.914260
C	0.805893	-4.734173	1.617336
C	1.239793	-4.802308	-0.655033
C	1.819713	-4.613881	0.655033
C	2.130696	-4.303718	-1.617336
H	-1.854292	-4.308212	2.478706
H	-1.032150	-4.575342	-2.478706
C	5.969134	-0.654505	-3.694393
S	4.624564	0.527083	-3.342573
H	5.907378	-0.867930	-4.763895
H	5.847997	-1.578142	-3.128520
H	6.929758	-0.192382	-3.460309
C	1.222092	-5.879237	-3.694393
S	1.930354	-4.235345	-3.342573
H	1.000030	-5.886455	-4.763895
H	0.306229	-6.049448	-3.128520
H	1.958447	-6.650041	-3.460309
C	-5.213839	-2.979063	-3.694393
S	-3.431540	-3.144670	-3.342573
H	-5.289325	-2.770099	-4.763895
H	-5.658737	-2.160623	-3.128520
H	-5.719372	-3.917570	-3.460309
C	-4.444422	4.038075	-3.694393
S	-4.051163	2.291832	-3.342573
H	-4.269013	4.174440	-4.763895
H	-3.803520	4.714110	-3.128520
H	-5.493213	4.228850	-3.460309
C	2.467036	5.474730	-3.694393
S	0.927784	4.561100	-3.342573
H	2.650931	5.350045	-4.763895
H	3.308032	5.074103	-3.128520
H	2.324379	6.531143	-3.460309
C	5.969134	0.654505	3.694393
S	4.624564	-0.527083	3.342573
H	5.907378	0.867930	4.763895
H	5.847997	1.578142	3.128520
H	6.929758	0.192382	3.460309
C	2.467036	-5.474730	3.694393
S	0.927784	-4.561100	3.342573
H	2.650931	-5.350045	4.763895
H	3.308032	-5.074103	3.128520
H	2.324379	-6.531143	3.460309
C	-4.444422	-4.038075	3.694393
S	-4.051163	-2.291832	3.342573
H	-4.269013	-4.174440	4.763895
H	-3.803520	-4.714110	3.128520
H	-5.493213	-4.228850	3.460309
C	-5.213839	2.979063	3.694393
S	-3.431540	3.144670	3.342573
H	-5.289325	2.770099	4.763895
H	-5.658737	2.160623	3.128520
H	-5.719372	3.917570	3.460309
C	1.222092	5.879237	3.694393
S	1.930354	4.235345	3.342573
H	1.000030	5.886455	4.763895
H	0.306229	6.049448	3.128520
H	1.958447	6.650041	3.460309

Table S 92. Coordinates of the calculated structure of the open-shell singlet of 12_5 (n=5) (TDDFT, BP86-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	-4.239657	-2.231666	1.626574
C	-4.707027	-1.046577	0.924796
C	-4.695191	-1.317504	-0.504370
C	-4.179196	-2.654163	-0.663003
C	-3.815701	-3.154470	0.663003
C	-4.766470	0.260599	1.418758
C	-4.695191	1.317504	0.504370
C	-4.707027	1.046577	-0.924796
C	-4.766470	-0.260599	-1.418758
C	-4.179196	2.654163	0.663003
C	-3.815701	3.154470	-0.663003
C	-4.239657	2.231666	-1.626574
C	-2.703914	4.058261	-0.504370
C	-2.449905	4.153239	0.924796
C	-3.432567	3.342531	1.626574
C	-1.225076	4.613712	1.418758
C	-0.197874	4.872523	0.504370
C	-0.459197	4.800059	-0.924796
C	-1.720764	4.452653	-1.418758
C	1.232816	4.794833	0.663003
C	1.820963	4.603732	-0.663003
C	0.812315	4.721776	-1.626574
C	3.024080	3.825647	-0.504370

C	3.192903	3.613420	0.924796
C	2.118214	4.297464	1.626574
C	4.009331	2.590832	1.418758
C	4.572899	1.693881	0.504370
C	4.423228	1.920023	-0.924796
C	3.702979	3.012489	-1.418758
C	4.741695	0.686552	-1.626574
C	4.941118	-0.309207	-0.663003
C	4.941118	0.309207	0.663003
C	4.572899	-1.693881	-0.504370
C	4.423228	-1.920023	0.924796
C	4.741695	-0.686552	1.626574
C	4.009331	-2.590832	-1.418758
C	3.192903	-3.613420	-0.924796
C	3.024080	-3.825647	0.504370
C	3.702979	-3.012489	1.418758
C	-3.432567	-3.342531	-1.626574
H	4.019428	2.381654	2.489390
H	3.507159	3.086732	-2.489390
H	-1.023016	4.558675	2.489390
H	-1.851885	4.289359	-2.489390
H	-4.651686	0.435762	2.489390
H	-4.651686	-0.435762	-2.489390
H	3.507159	-3.086732	2.489390
H	4.019428	-2.381654	-2.489390
C	-2.703914	-4.058261	0.504370
C	-2.449905	-4.153239	-0.924796
C	-1.720764	-4.452653	1.418758
C	-1.225076	-4.613712	-1.418758
C	-0.197874	-4.872523	-0.504370
C	-0.459197	-4.800059	0.924796
C	0.812315	-4.721776	1.626574
C	1.232816	-4.794833	-0.663003
C	1.820963	-4.603732	0.663003
C	2.118214	-4.297464	-1.626574
H	-1.851885	-4.289359	2.489390
H	-1.023016	-4.558675	-2.489390
C	5.943689	-0.663159	-3.712231
S	4.599356	0.511032	-3.350679
H	5.919150	-0.824641	-4.796846
H	5.800926	-1.620655	-3.200185
H	6.905654	-0.224189	-3.423990
C	1.205999	-5.857712	-3.712231
S	1.907299	-4.216330	-3.350679
H	1.044838	-5.884274	-4.796846
H	0.251250	-6.017818	-3.200185
H	1.920748	-6.636946	-3.423990
C	-5.198341	-2.957106	-3.712231
S	-3.420580	-3.116867	-3.350679
H	-5.273405	-2.812041	-4.796846
H	-5.645645	-2.098561	-3.200185
H	-5.718567	-3.877669	-3.423990
C	-4.418750	4.030120	-3.712231
S	-4.021334	2.290000	-3.350679
H	-4.303981	4.146337	-4.796846
H	-3.740451	4.720836	-3.200185
H	-5.455017	4.240414	-3.423990
C	2.467403	5.447857	-3.712231
S	0.935259	4.532165	-3.350679
H	2.613398	5.374618	-4.796846
H	3.333919	5.016198	-3.200185
H	2.347181	6.498389	-3.423990
C	5.943689	0.663159	3.712231
S	4.599356	-0.511032	3.350679
H	5.919150	0.824641	4.796846
H	5.800926	1.620655	3.200185
H	6.905654	0.224189	3.423990
C	2.467403	-5.447857	3.712231
S	0.935259	-4.532165	3.350679
H	2.613398	-5.374618	4.796846
H	3.333919	-5.016198	3.200185
H	2.347181	-6.498389	3.423990
C	-4.418750	-4.030120	3.712231
S	-4.021334	-2.290000	3.350679
H	-4.303981	-4.146337	4.796846
H	-3.740451	-4.720836	3.200185
H	-5.455017	-4.240414	3.423990
C	-5.198341	2.957106	3.712231
S	-3.420580	3.116867	3.350679
H	-5.273405	2.812041	4.796846
H	-5.645645	2.098561	3.200185
H	-5.718567	3.877669	3.423990
C	1.205999	5.857712	3.712231
S	1.907299	4.216330	3.350679
H	1.044838	5.884274	4.796846
H	0.251250	6.017818	3.200185
H	1.920748	6.636946	3.423990

Table S 93. Coordinates of the calculated structure of 12_6 (n=6) (TPSS-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.324543	-2.276953	1.613233
C	-5.719260	-1.051041	0.905043
C	-5.711756	-1.313016	-0.505249
C	-5.265338	-2.687760	-0.661932
C	-4.960337	-3.216037	0.661932
C	-5.763183	0.250417	1.411782
C	-5.711756	1.313016	0.505249
C	-5.719260	1.051041	-0.905043
C	-5.763183	-0.250417	-1.411782
C	-5.265338	2.687760	0.661932
C	-4.960337	3.216037	-0.661932
C	-5.324543	2.276953	-1.613233
C	-3.992984	4.290018	-0.505249
C	-3.769858	4.427504	0.905043
C	-4.634171	3.472713	1.613233
C	-2.664724	5.116272	1.411782
C	-1.718773	5.603034	0.505249
C	-1.949402	5.478545	-0.905043
C	-3.098459	4.865855	-1.411782
C	-0.305001	5.903797	0.661932
C	0.305001	5.903797	-0.661932
C	-0.690373	5.749666	-1.613233
C	1.718773	5.603034	-0.505249
C	1.949402	5.478545	0.905043
C	0.690373	5.749666	1.613233
C	3.098459	4.865855	1.411782
C	3.992984	4.290018	0.505249
C	3.769858	4.427504	-0.905043
C	2.664724	5.116272	-1.411782
C	4.634171	3.472713	-1.613233
C	5.265338	2.687760	-0.661932
C	4.960337	3.216037	0.661932
C	5.711756	1.313016	-0.505249
C	5.719260	1.051041	0.905043
C	5.324543	2.276953	1.613233
C	5.763183	0.250417	-1.411782
C	5.719260	-1.051041	-0.905043
C	5.711756	-1.313016	0.505249
C	5.763183	-0.250417	1.411782
C	-4.634171	-3.472713	-1.613233
H	3.189501	4.696449	2.480650
H	2.472493	5.110413	-2.480650
H	-2.472493	5.110413	2.480650
H	-3.189501	4.696449	-2.480650
H	-5.661994	0.413965	2.480650
H	-5.661994	-0.413965	-2.480650
H	5.661994	-0.413965	2.480650
H	5.661994	0.413965	-2.480650
C	-3.992984	-4.290018	0.505249
C	-3.769858	-4.427504	-0.905043
C	-3.098459	-4.865855	1.411782
C	-2.664724	-5.116272	-1.411782
C	-1.718773	-5.603034	-0.505249
C	-1.949402	-5.478545	0.905043
C	-0.690373	-5.749666	1.613233
C	-0.305001	-5.903797	-0.661932
C	0.305001	-5.903797	0.661932
C	5.324543	-2.276953	-1.613233
H	-3.189501	-4.696449	2.480650
H	-2.472493	-5.110413	-2.480650
C	1.718773	-5.603034	0.505249
C	0.690373	-5.749666	-1.613233
C	1.949402	-5.478545	-0.905043
C	2.664724	-5.116272	1.411782
C	3.769858	-4.427504	0.905043
C	3.098459	-4.865855	-1.411782
C	3.992984	-4.290018	-0.505249
C	4.634171	-3.472713	1.613233
C	4.960337	-3.216037	-0.661932
C	5.265338	-2.687760	0.661932
H	2.472493	-5.110413	2.480650
H	3.189501	-4.696449	-2.480650
C	0.639961	7.000786	-3.690001
S	-0.565285	5.675591	-3.347801
H	0.756327	7.021578	-4.776018
H	1.604781	6.803901	-3.223205
H	0.238927	7.953178	-3.339026
C	6.382839	2.946171	-3.690001
S	4.632563	3.327347	-3.347801
H	6.459028	2.855790	-4.776018
H	6.694742	2.012169	-3.223205
H	7.007118	3.769672	-3.339026
C	5.742878	-4.054616	-3.690001

S	5.197848	-2.348244	-3.347801
H	5.702701	-4.165788	-4.776018
H	5.089960	-4.791732	-3.223205
H	6.768191	-4.183506	-3.339026
C	-0.639961	-7.000786	-3.690001
S	0.565285	-5.675591	-3.347801
H	-0.756327	-7.021578	-4.776018
H	-1.604781	-6.803901	-3.223205
H	-0.238927	-7.953178	-3.339026
C	-6.382839	-2.946171	-3.690001
S	-4.632563	-3.327347	-3.347801
H	-6.459028	-2.855790	-4.776018
H	-6.694742	-2.012169	-3.223205
H	-7.007118	-3.769672	-3.339026
C	-5.742878	4.054616	-3.690001
S	-5.197848	2.348244	-3.347801
H	-5.702701	4.165788	-4.776018
H	-5.089960	4.791732	-3.223205
H	-6.768191	4.183506	-3.339026
C	-0.639961	7.000786	3.690001
S	0.565285	5.675591	3.347801
H	-0.756327	7.021578	4.776018
H	-1.604781	6.803901	3.223205
H	-0.238927	7.953178	3.339026
C	5.742878	4.054616	3.690001

S	5.197848	2.348244	3.347801
H	5.702701	4.165788	4.776018
H	5.089960	4.791732	3.223205
H	6.768191	4.183506	3.339026
C	6.382839	-2.946171	3.690001
S	4.632563	-3.327347	3.347801
H	6.459028	-2.855790	4.776018
H	6.694742	-2.012169	3.223205
H	7.007118	-3.769672	3.339026
C	0.639961	-7.000786	3.690001
S	-0.565285	-5.675591	3.347801
H	0.756327	-7.021578	4.776018
H	1.604781	-6.803901	3.223205
H	0.238927	-7.953178	3.339026
C	-5.742878	-4.054616	3.690001
S	-5.197848	-2.348244	3.347801
H	-5.702701	-4.165788	4.776018
H	-5.089960	-4.791732	3.223205
H	-6.768191	-4.183506	3.339026
C	-6.382839	2.946171	3.690001
S	-4.632563	3.327347	3.347801
H	-6.459028	2.855790	4.776018
H	-6.694742	2.012169	3.223205
H	-7.007118	3.769672	3.339026

Table S 94. Coordinates of the calculated structure of the triplet of 12_6 (n=6) (TPSS-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.307160	-2.261875	1.621194
C	-5.694870	-1.048400	0.917559
C	-5.684689	-1.313066	-0.507445
C	-5.249120	-2.677328	-0.662729
C	-4.943194	-3.207207	0.662729
C	-5.742589	0.254589	1.418030
C	-5.684689	1.313066	0.507445
C	-5.694870	1.048400	-0.917559
C	-5.742589	-0.254589	-1.418030
C	-5.249120	2.677328	0.662729
C	-4.943194	3.207207	-0.662729
C	-5.307160	2.261875	-1.621194
C	-3.979493	4.266552	-0.507445
C	-3.755376	4.407703	0.917559
C	-4.612421	3.465197	1.621194

C	-2.650814	5.100522	1.418030
C	-1.705196	5.579618	0.507445
C	-1.939495	5.456102	-0.917559
C	-3.091775	4.845933	-1.418030
C	-0.305926	5.884535	0.662729
C	0.305926	5.884535	-0.662729
C	-0.694738	5.727073	-1.621194
C	1.705196	5.579618	-0.507445
C	1.939495	5.456102	0.917559
C	0.694738	5.727073	1.621194
C	3.091775	4.845933	1.418030
C	3.979493	4.266552	0.507445
C	3.755376	4.407703	-0.917559
C	2.650814	5.100522	-1.418030
C	4.612421	3.465197	-1.621194
C	5.249120	2.677328	-0.662729

C	4.943194	3.207207	0.662729
C	5.684689	1.313066	-0.507445
C	5.694870	1.048400	0.917559
C	5.307160	2.261875	1.621194
C	5.742589	0.254589	-1.418030
C	5.694870	-1.048400	-0.917559
C	5.684689	-1.313066	0.507445
C	5.742589	-0.254589	1.418030
C	-4.612421	-3.465197	-1.621194
H	3.191369	4.678581	2.486583
H	2.456086	5.103097	-2.486583
H	-2.456086	5.103097	2.486583
H	-3.191369	4.678581	-2.486583
H	-5.647454	0.424516	2.486583
H	-5.647454	-0.424516	-2.486583
H	5.647454	-0.424516	2.486583
H	5.647454	0.424516	-2.486583
C	-3.979493	-4.266552	0.507445
C	-3.755376	-4.407703	-0.917559
C	-3.091775	-4.845933	1.418030
C	-2.650814	-5.100522	-1.418030
C	-1.705196	-5.579618	-0.507445
C	-1.939495	-5.456102	0.917559
C	-0.694738	-5.727073	1.621194
C	-0.305926	-5.884535	-0.662729
C	0.305926	-5.884535	0.662729
C	5.307160	-2.261875	-1.621194
H	-3.191369	-4.678581	2.486583
H	-2.456086	-5.103097	-2.486583
C	1.705196	-5.579618	0.507445
C	0.694738	-5.727073	-1.621194
C	1.939495	-5.456102	-0.917559
C	2.650814	-5.100522	1.418030
C	3.755376	-4.407703	0.917559
C	3.091775	-4.845933	-1.418030
C	3.979493	-4.266552	-0.507445
C	4.612421	-3.465197	1.621194
C	4.943194	-3.207207	-0.662729
C	5.249120	-2.677328	0.662729
H	2.456086	-5.103097	2.486583
H	3.191369	-4.678581	-2.486583
C	0.613314	6.993135	-3.699467
S	-0.543529	5.625367	-3.353578
H	0.781622	6.974607	-4.778682
H	1.562219	6.859062	-3.179746
H	0.155167	7.940311	-3.409492
C	6.362889	2.965422	-3.699467
S	4.599946	3.283394	-3.353578
H	6.430998	2.810399	-4.778682
H	6.721231	2.076610	-3.179746
H	6.954095	3.835777	-3.409492
C	5.749575	-4.027713	-3.699467
S	5.143475	-2.341973	-3.353578
H	5.649376	-4.164208	-4.778682
H	5.159012	-4.782452	-3.179746
H	6.798927	-4.104534	-3.409492
C	-0.613314	-6.993135	-3.699467
S	0.543529	-5.625367	-3.353578
H	-0.781622	-6.974607	-4.778682
H	-1.562219	-6.859062	-3.179746
H	-0.155167	-7.940311	-3.409492
C	-6.362889	-2.965422	-3.699467
S	-4.599946	-3.283394	-3.353578
H	-6.430998	-2.810399	-4.778682
H	-6.721231	-2.076610	-3.179746
H	-6.954095	-3.835777	-3.409492
C	-5.749575	4.027713	-3.699467
S	-5.143475	2.341973	-3.353578
H	-5.649376	4.164208	-4.778682
H	-5.159012	4.782452	-3.179746
H	-6.798927	4.104534	-3.409492
C	-0.613314	6.993135	3.699467
S	0.543529	5.625367	3.353578
H	-0.781622	6.974607	4.778682
H	-1.562219	6.859062	3.179746
H	-0.155167	7.940311	3.409492
C	5.749575	4.027713	3.699467
S	5.143475	2.341973	3.353578
H	5.649376	4.164208	4.778682
H	5.159012	4.782452	3.179746
H	6.798927	4.104534	3.409492
C	6.362889	-2.965422	3.699467
S	4.599946	-3.283394	3.353578
H	6.430998	-2.810399	4.778682
H	6.721231	-2.076610	3.179746
H	6.954095	-3.835777	3.409492
C	0.613314	-6.993135	3.699467
S	-0.543529	-5.625367	3.353578

H	0.781622	-6.974607	4.778682
H	1.562219	-6.859062	3.179746
H	0.155167	-7.940311	3.409492
C	-5.749575	-4.027713	3.699467
S	-5.143475	-2.341973	3.353578
H	-5.649376	-4.164208	4.778682
H	-5.159012	-4.782452	3.179746
H	-6.798927	-4.104534	3.409492
C	-6.362889	2.965422	3.699467
S	-4.599946	3.283394	3.353578
H	-6.430998	2.810399	4.778682
H	-6.721231	2.076610	3.179746
H	-7.007118	3.769672	3.339026

Table S 95. Coordinates of the calculated structure of the open-shell singlet of 12_6 (n=6) (TDDFT, BP86-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-5.314221	-2.270036	1.623916
C	-5.703107	-1.049152	0.919015
C	-5.697782	-1.315506	-0.505067
C	-5.267349	-2.686832	-0.663402
C	-4.960539	-3.218243	0.663402
C	-5.749047	0.255753	1.417795
C	-5.697782	1.315506	0.505067
C	-5.703107	1.049152	-0.919015
C	-5.749047	-0.255753	-1.417795
C	-5.267349	2.686832	0.663402
C	-4.960539	3.218243	-0.663402
C	-5.314221	2.270036	-1.623916
C	-3.988152	4.276671	-0.505067
C	-3.760146	4.414459	0.919015
C	-4.623019	3.467232	1.623916
C	-2.653034	5.106697	1.417795
C	-1.709629	5.592177	0.505067
C	-1.942961	5.463611	-0.919015
C	-3.096012	4.850944	-1.417795
C	-0.306810	5.905074	0.663402
C	0.306810	5.905074	-0.663402
C	-0.691202	5.737268	-1.623916
C	1.709629	5.592177	-0.505067
C	1.942961	5.463611	0.919015
C	0.691202	5.737268	1.623916
C	3.096012	4.850944	1.417795
C	3.988152	4.276671	0.505067
C	3.760146	4.414459	-0.919015
C	2.653034	5.106697	-1.417795
C	4.623019	3.467232	-1.623916
C	5.267349	2.686832	-0.663402
C	4.960539	3.218243	0.663402
C	5.697782	1.315506	-0.505067
C	5.703107	1.049152	0.919015
C	5.314221	2.270036	1.623916
C	5.749047	0.255753	-1.417795
C	5.703107	-1.049152	-0.919015
C	5.697782	-1.315506	0.505067
C	5.749047	-0.255753	1.417795
C	-4.623019	-3.467232	-1.623916
H	3.193580	4.674933	2.489876
H	2.451821	5.103188	-2.489876
H	-2.451821	5.103188	2.489876
H	-3.193580	4.674933	-2.489876
H	-5.645401	0.428255	2.489876
H	-5.645401	-0.428255	-2.489876
H	5.645401	-0.428255	2.489876
H	5.645401	0.428255	-2.489876
C	-3.988152	-4.276671	0.505067
C	-3.760146	-4.414459	-0.919015
C	-3.096012	-4.850944	1.417795
C	-2.653034	-5.106697	-1.417795
C	-1.709629	-5.592177	-0.505067
C	-1.942961	-5.463611	0.919015
C	-0.691202	-5.737268	1.623916
C	-0.306810	-5.905074	-0.663402
C	0.306810	-5.905074	0.663402
C	5.314221	-2.270036	-1.623916
H	-3.193580	-4.674933	2.489876
H	-2.451821	-5.103188	-2.489876
C	1.709629	-5.592177	0.505067
C	0.691202	-5.737268	-1.623916
C	1.942961	-5.463611	-0.919015
C	2.653034	-5.106697	1.417795
C	3.760146	-4.414459	0.919015
C	3.096012	-4.850944	-1.417795
C	3.988152	-4.276671	-0.505067

C	4.623019	-3.467232	1.623916
C	4.960539	-3.218243	-0.663402
C	5.267349	-2.686832	0.663402
H	2.451821	-5.103188	2.489876
H	3.193580	-4.674933	-2.489876
C	0.636727	6.979647	-3.703247
S	-0.541423	5.635273	-3.353206
H	0.776820	6.981863	-4.791136
H	1.602920	6.817719	-3.214244
H	0.210033	7.936591	-3.381639
C	6.362915	2.938401	-3.703247
S	4.609578	3.286522	-3.353206
H	6.434881	2.818186	-4.791136
H	6.705778	2.020690	-3.214244
H	6.978306	3.786402	-3.381639
C	5.726188	-4.041245	-3.703247
S	5.151001	-2.348750	-3.353206
H	5.658061	-4.163677	-4.791136
H	5.102858	-4.797029	-3.214244
H	6.768273	-4.150190	-3.381639
C	-0.636727	-6.979647	-3.703247
S	0.541423	-5.635273	-3.353206
H	-0.776820	-6.981863	-4.791136
H	-1.602920	-6.817719	-3.214244
H	-0.210033	-7.936591	-3.381639
C	-6.362915	-2.938401	-3.703247
S	-4.609578	-3.286522	-3.353206
H	-6.434881	-2.818186	-4.791136
H	-6.705778	-2.020690	-3.214244
H	-6.978306	-3.786402	-3.381639
C	-5.726188	4.041245	-3.703247
S	-5.151001	2.348750	-3.353206
H	-5.658061	4.163677	-4.791136
H	-5.102858	4.797029	-3.214244
H	-6.768273	4.150190	-3.381639
C	-0.636727	6.979647	3.703247
S	0.541423	5.635273	3.353206
H	-0.776820	6.981863	4.791136
H	-1.602920	6.817719	3.214244
H	-0.210033	7.936591	3.381639
C	5.726188	4.041245	3.703247
S	5.151001	2.348750	3.353206
H	5.658061	4.163677	4.791136
H	5.102858	4.797029	3.214244
H	6.768273	4.150190	3.381639
C	6.362915	-2.938401	3.703247
S	4.609578	-3.286522	3.353206
H	6.434881	-2.818186	4.791136
H	6.705778	-2.020690	3.214244
H	6.978306	-3.786402	3.381639
C	0.636727	-6.979647	3.703247
S	-0.541423	-5.635273	3.353206
H	0.776820	-6.981863	4.791136
H	1.602920	-6.817719	3.214244
H	0.210033	-7.936591	3.381639
C	-5.726188	-4.041245	3.703247
S	-5.151001	-2.348750	3.353206
H	-5.658061	-4.163677	4.791136
H	-5.102858	-4.797029	3.214244
H	-6.768273	-4.150190	3.381639
C	-6.362915	2.938401	3.703247
S	-4.609578	3.286522	3.353206
H	-6.434881	2.818186	4.791136
H	-6.705778	2.020690	3.214244
H	-6.978306	3.786402	3.381639

Table S 96. Coordinates of the calculated structure of 12_7 (n=7) (TPSS-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.866108	-0.303913	-0.662576
C	6.603992	-1.724153	-0.507159
C	6.495535	-1.960466	0.903658
C	6.733859	-0.695457	1.612693
C	6.866108	0.303913	0.662576
C	6.178692	-2.699866	-1.412607
C	5.582654	-3.856084	-0.903658
C	5.465519	-4.088217	0.507159
C	5.963192	-3.147357	1.412607
C	4.742223	-4.831132	-1.612693
C	4.043340	-5.557626	-0.662576
C	4.518557	-5.178653	0.662576
C	2.769525	-6.238201	-0.507159
C	2.517146	-6.300744	0.903658
C	3.654762	-5.698353	1.612693

C	1.257287	-6.624556	1.412607
C	0.211398	-6.822076	0.507159
C	0.465920	-6.768923	-0.903658
C	1.741511	-6.514035	-1.412607
C	-0.820404	-6.719781	-1.612693
C	-1.824146	-6.626333	-0.662576
C	-1.231560	-6.761587	0.662576
C	-2.176445	-6.410273	1.612693
C	-3.356705	-5.896434	0.903658
C	-3.150451	-6.054756	-0.507159
C	-4.395381	-5.113329	1.412607
C	-5.201909	-4.418773	0.507159
C	-5.001661	-4.584625	-0.903658
C	-4.007063	-5.423002	-1.412607
C	-5.765250	-3.548297	-1.612693
C	-6.318012	-2.705277	-0.662576
C	-6.054287	-3.252909	0.662576
C	-6.368745	-2.295127	1.612693
C	-6.702889	-1.051989	0.903658
C	-6.698073	-1.311957	-0.507159
C	-6.738237	0.248338	1.412607
C	-6.698073	1.311957	0.507159
C	-6.702889	1.051989	-0.903658
C	-6.738237	-0.248338	-1.412607
C	-6.318012	2.705277	0.662576
C	-6.054287	3.252909	-0.662576
C	-6.368745	2.295127	-1.612693
C	-5.201909	4.418773	-0.507159
C	-5.001661	4.584625	0.903658
C	-5.765250	3.548297	1.612693
C	-4.007063	5.423002	1.412607
C	-3.150451	6.054756	0.507159
C	-3.356705	5.896434	-0.903658
C	-4.395381	5.113329	-1.412607
C	-2.176445	6.410273	-1.612693
C	-1.231560	6.761587	-0.662576
C	-1.824146	6.626333	0.662576
C	0.211398	6.822076	-0.507159
C	0.465920	6.768923	0.903658
C	-0.820404	6.719781	1.612693
C	1.741511	6.514035	1.412607
C	2.769525	6.238201	0.507159
C	2.517146	6.300744	-0.903658
C	1.257287	6.624556	-1.412607

C	6.733859	0.695457	-1.612693
H	1.879044	-6.388874	-2.482408
H	1.079069	-6.571463	2.482408
H	-3.823458	-5.452493	-2.482408
H	-4.464989	-4.940890	2.482408
H	-6.646818	-0.410274	-2.482408
H	-6.646818	0.410274	2.482408
H	6.166587	-2.514302	-2.482408
H	5.810565	-3.253590	2.482408
H	-4.464989	4.940890	-2.482408
H	-3.823458	5.452493	2.482408
H	1.079069	6.571463	-2.482408
H	1.879044	6.388874	2.482408
C	3.654762	5.698353	-1.612693
C	4.043340	5.557626	0.662576
C	4.518557	5.178653	-0.662576
C	5.465519	4.088217	-0.507159
C	4.742223	4.831132	1.612693
C	5.582654	3.856084	0.903658
C	5.963192	3.147357	-1.412607
C	6.178692	2.699866	1.412607
C	6.495535	1.960466	-0.903658
C	6.603992	1.724153	0.507159
H	5.810565	3.253590	-2.482408
H	6.166587	2.514302	2.482408
C	5.475230	5.877602	-3.690402
S	3.707893	5.583449	-3.349656
H	5.577393	5.834872	-4.777218
H	6.110326	5.118584	-3.234345
H	5.753089	6.868785	-3.328055
C	8.009045	-0.616082	-3.690402
S	6.677150	0.582276	-3.349656
H	8.039335	-0.722598	-4.777218
H	7.811596	-1.585861	-3.234345
H	8.957224	-0.215329	-3.328055
C	4.511885	-6.645844	-3.690402
S	4.618377	-4.857363	-3.349656
H	4.447493	-6.735938	-4.777218
H	3.630575	-7.096119	-3.234345
H	5.416388	-7.137295	-3.328055
C	-2.382816	-7.671150	-3.690402
S	-0.918128	-6.639308	-3.349656
H	-2.493402	-7.676979	-4.777218
H	-3.284343	-7.262856	-3.234345

H	-2.203100	-8.684733	-3.328055
C	-7.483208	-2.919923	-3.690402
S	-5.763264	-3.421719	-3.349656
H	-7.556714	-2.837098	-4.777218
H	-7.726084	-1.960513	-3.234345
H	-8.163608	-3.692390	-3.328055
C	-6.948592	4.030065	-3.690402
S	-6.268544	2.372494	-3.349656
H	-6.929667	4.139175	-4.777218
H	-6.349926	4.818135	-3.234345
H	-7.976753	4.080398	-3.328055
C	-1.181544	7.945332	-3.690402
S	-2.053483	6.380171	-3.349656
H	-1.084439	7.998565	-4.777218
H	-0.192144	7.968630	-3.234345
H	-1.783240	8.780563	-3.328055
C	4.511885	6.645844	3.690402
S	4.618377	4.857363	3.349656
H	4.447493	6.735938	4.777218
H	3.630575	7.096119	3.234345
H	5.416388	7.137295	3.328055
C	8.009045	0.616082	3.690402
S	6.677150	-0.582276	3.349656
H	8.039335	0.722598	4.777218
H	7.811596	1.585861	3.234345
H	8.957224	0.215329	3.328055
C	5.475230	-5.877602	3.690402
S	3.707893	-5.583449	3.349656
H	5.577393	-5.834872	4.777218
H	6.110326	-5.118584	3.234345
H	5.753089	-6.868785	3.328055
C	-1.181544	-7.945332	3.690402
S	-2.053483	-6.380171	3.349656
H	-1.084439	-7.998565	4.777218
H	-0.192144	-7.968630	3.234345
H	-1.783240	-8.780563	3.328055
C	-6.948592	-4.030065	3.690402
S	-6.268544	-2.372494	3.349656
H	-6.929667	-4.139175	4.777218
H	-6.349926	-4.818135	3.234345
H	-7.976753	-4.080398	3.328055
C	-7.483208	2.919923	3.690402
S	-5.763264	3.421719	3.349656
H	-7.556714	2.837098	4.777218
H	-7.726084	1.960513	3.234345
H	-8.163608	3.692390	3.328055
C	-2.382816	7.671150	3.690402
S	-0.918128	6.639308	3.349656
H	-2.493402	7.676979	4.777218
H	-3.284343	7.262856	3.234345
H	-2.203100	8.684733	3.328055

Table S 97. Coordinates of the calculated structure of the triplet of 12_7 (n=7) (TPSS-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.869198	-0.302203	-0.658047
C	6.600137	-1.719504	-0.506617
C	6.489516	-1.958814	0.908822
C	6.725560	-0.705834	1.614573
C	6.869198	0.302203	0.658047
C	6.176841	-2.691397	-1.412854
C	5.577609	-3.852407	-0.908822
C	5.459481	-4.088102	0.506617
C	5.955417	-3.151190	1.412854
C	4.745161	-4.818174	-1.614573
C	4.046603	-5.558976	-0.658047
C	4.519147	-5.182135	0.658047
C	2.770756	-6.232288	-0.506617
C	2.514685	-6.295008	0.908822
C	3.641474	-5.698335	1.614573
C	1.249442	-6.620867	1.412854
C	0.207724	-6.817284	0.506617
C	0.465649	-6.762687	-0.908822
C	1.746978	-6.507308	-1.412854
C	-0.808440	-6.713999	-1.614573
C	-1.823167	-6.629726	-0.658047
C	-1.233914	-6.764219	0.658047
C	-2.184715	-6.399873	1.614573
C	-3.353755	-5.890933	0.908822
C	-3.145061	-6.052032	-0.506617
C	-4.397388	-5.104896	1.412854
C	-5.200454	-4.412912	0.506617
C	-4.996954	-4.580526	-0.908822
C	-3.998395	-5.423082	-1.412854

C	-5.753270	-3.554046	-1.614573
C	-6.320054	-2.708158	-0.658047
C	-6.057812	-3.252709	0.658047
C	-6.365770	-2.282176	1.614573
C	-6.696749	-1.050865	0.908822
C	-6.692583	-1.314473	-0.506617
C	-6.732895	0.255166	1.412854
C	-6.692583	1.314473	0.506617
C	-6.696749	1.050865	-0.908822
C	-6.732895	-0.255166	-1.412854
C	-6.320054	2.708158	0.658047
C	-6.057812	3.252709	-0.658047
C	-6.365770	2.282176	-1.614573
C	-5.200454	4.412912	-0.506617
C	-4.996954	4.580526	0.908822
C	-5.753270	3.554046	1.614573
C	-3.998395	5.423082	1.412854
C	-3.145061	6.052032	0.506617
C	-3.353755	5.890933	-0.908822
C	-4.397388	5.104896	-1.412854
C	-2.184715	6.399873	-1.614573
C	-1.233914	6.764219	-0.658047
C	-1.823167	6.629726	0.658047
C	0.207724	6.817284	-0.506617
C	0.465649	6.762687	0.908822
C	-0.808440	6.713999	1.614573
C	1.746978	6.507308	1.412854
C	2.770756	6.232288	0.506617
C	2.514685	6.295008	-0.908822
C	1.249442	6.620867	-1.412854
C	6.725560	0.705834	-1.614573
H	1.888534	-6.386554	-2.483005
H	1.069512	-6.573491	2.483005
H	-3.815728	-5.458466	-2.483005
H	-4.472532	-4.934683	2.483005
H	-6.646668	-0.420042	-2.483005
H	-6.646668	0.420042	2.483005
H	6.170691	-2.505436	-2.483005
H	5.806192	-3.262326	2.483005
H	-4.472532	4.934683	-2.483005
H	-3.815728	5.458466	2.483005
H	1.069512	6.573491	-2.483005
H	1.888534	6.386554	2.483005
C	3.641474	5.698335	-1.614573
C	4.046603	5.558976	0.658047
C	4.519147	5.182135	-0.658047
C	5.459481	4.088102	-0.506617
C	4.745161	4.818174	1.614573
C	5.577609	3.852407	0.908822
C	5.955417	3.151190	-1.412854
C	6.176841	2.691397	1.412854
C	6.489516	1.958814	-0.908822
C	6.600137	1.719504	0.506617
H	5.806192	3.262326	-2.483005
H	6.170691	2.505436	2.483005
C	5.455336	5.881009	-3.694289
S	3.695299	5.547120	-3.347790
H	5.579279	5.740532	-4.770477
H	6.108357	5.192970	-3.157864
H	5.689630	6.911756	-3.422674
C	7.999304	-0.598404	-3.694289
S	6.640895	0.569472	-3.347790
H	7.966752	-0.782893	-4.770477
H	7.868525	-1.537942	-3.157864
H	8.951254	-0.138923	-3.422674
C	4.519633	-6.627207	-3.694289
S	4.585761	-4.837001	-3.347790
H	4.355098	-6.716783	-4.770477
H	3.703534	-7.110752	-3.157864
H	5.472402	-7.084989	-3.422674
C	-2.363414	-7.665587	-3.694289
S	-0.922544	-6.601113	-3.347790
H	-2.536033	-7.592799	-4.770477
H	-3.250294	-7.329021	-3.157864
H	-2.127281	-8.695915	-3.422674
C	-7.466762	-2.931624	-3.694289
S	-5.736155	-3.394453	-3.347790
H	-7.517480	-2.751282	-4.770477
H	-7.756585	-2.028387	-3.157864
H	-8.125078	-3.758639	-3.422674
C	-6.947486	4.009912	-3.694289
S	-6.230324	2.368300	-3.347790
H	-6.838111	4.162006	-4.770477
H	-6.422008	4.799663	-3.157864
H	-8.004525	4.008969	-3.422674
C	-1.196612	7.931902	-3.694289
S	-2.032932	6.347674	-3.347790
H	-1.009505	7.941219	-4.770477

H	-0.251529	8.013469	-3.157864
H	-1.856402	8.757741	-3.422674
C	4.519633	6.627207	3.694289
S	4.585761	4.837001	3.347790
H	4.355098	6.716783	4.770477
H	3.703534	7.110752	3.157864
H	5.472402	7.084989	3.422674
C	7.999304	0.598404	3.694289
S	6.640895	-0.569472	3.347790
H	7.966752	0.782893	4.770477
H	7.868525	1.537942	3.157864
H	8.951254	0.138923	3.422674
C	5.455336	-5.881009	3.694289
S	3.695299	-5.547120	3.347790
H	5.579279	-5.740532	4.770477
H	6.108357	-5.192970	3.157864
H	5.689630	-6.911756	3.422674
C	-1.196612	-7.931902	3.694289
S	-2.032932	-6.347674	3.347790
H	-1.009505	-7.941219	4.770477
H	-0.251529	-8.013469	3.157864
H	-1.856402	-8.757741	3.422674
C	-6.947486	-4.009912	3.694289
S	-6.230324	-2.368300	3.347790
H	-6.838111	-4.162006	4.770477
H	-6.422008	-4.799663	3.157864
H	-8.004525	-4.008969	3.422674
C	-7.466762	2.931624	3.694289
S	-5.736155	3.394453	3.347790
H	-7.517480	2.751282	4.770477
H	-7.756585	2.028387	3.157864
H	-8.125078	3.758639	3.422674
C	-2.363414	7.665587	3.694289
S	-0.922544	6.601113	3.347790
H	-2.536033	7.592799	4.770477
H	-3.250294	7.329021	3.157864
H	-2.127281	8.695915	3.422674

Table S 98. Coordinates of the calculated structure of the open-shell singlet of 12_7 (n=7) (TDDFT, BP86-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.860494	-0.305731	-0.663596
C	6.587625	-1.713311	-0.508196
C	6.476306	-1.953493	0.917998
C	6.714975	-0.699038	1.622082
C	6.860494	0.305731	0.663596
C	6.164107	-2.686260	-1.418885
C	5.565213	-3.845397	-0.917998
C	5.446838	-4.082180	0.508196
C	5.943461	-3.144437	1.418885
C	4.733248	-4.814136	-1.622082
C	4.038418	-5.554370	-0.663596
C	4.516478	-5.173130	0.663596
C	2.767796	-6.218645	-0.508196
C	2.510608	-6.281363	0.917998
C	3.640188	-5.685822	1.622082
C	1.247268	-6.607309	1.418885
C	0.204471	-6.803707	0.508196
C	0.463401	-6.748625	-0.917998
C	1.743055	-6.494149	-1.418885
C	-0.812711	-6.702167	-1.622082
C	-1.824669	-6.620456	-0.663596
C	-1.228538	-6.756519	0.663596
C	-2.175734	-6.391066	1.622082
C	-3.345628	-5.879238	0.917998
C	-3.136239	-6.041212	-0.508196
C	-4.388144	-5.094743	1.418885
C	-5.191867	-4.401903	0.508196
C	-4.987361	-4.570000	-0.917998
C	-3.990553	-5.411811	-1.418885
C	-5.746682	-3.543330	-1.622082
C	-6.313743	-2.701203	-0.663596
C	-6.048440	-3.252111	0.663596
C	-6.353284	-2.283707	1.622082
C	-6.682539	-1.049928	0.917998
C	-6.678623	-1.314623	-0.508196
C	-6.719193	0.254269	1.418885
C	-6.678623	1.314623	0.508196
C	-6.682539	1.049928	-0.917998
C	-6.719193	-0.254269	-1.418885
C	-6.313743	2.701203	0.663596
C	-6.048440	3.252111	-0.663596
C	-6.353284	2.283707	-1.622082
C	-5.191867	4.401903	-0.508196

C	-4.987361	4.570000	0.917998
C	-5.746682	3.543330	1.622082
C	-3.990553	5.411811	1.418885
C	-3.136239	6.041212	0.508196
C	-3.345628	5.879238	-0.917998
C	-4.388144	5.094743	-1.418885
C	-2.175734	6.391066	-1.622082
C	-1.228538	6.756519	-0.663596
C	-1.824669	6.620456	0.663596
C	0.204471	6.803707	-0.508196
C	0.463401	6.748625	0.917998
C	-0.812711	6.702167	1.622082
C	1.743055	6.494149	1.418885
C	2.767796	6.218645	0.508196
C	2.510608	6.281363	-0.917998
C	1.247268	6.607309	-1.418885
C	6.714975	0.699038	-1.622082
H	1.888355	-6.365499	-2.492196
H	1.060537	-6.554443	2.492196
H	-3.799377	-5.445199	-2.492196
H	-4.463236	-4.915790	2.492196
H	-6.626101	-0.424553	-2.492196
H	-6.626101	0.424553	2.492196
H	6.154118	-2.492448	-2.492196
H	5.785704	-3.257467	2.492196
H	-4.463236	4.915790	-2.492196
H	-3.799377	5.445199	2.492196
H	1.060537	6.554443	-2.492196
H	1.888355	6.365499	2.492196
C	3.640188	5.685822	-1.622082
C	4.038418	5.554370	0.663596
C	4.516478	5.173130	-0.663596
C	5.446838	4.082180	-0.508196
C	4.733248	4.814136	1.622082
C	5.565213	3.845397	0.917998
C	5.943461	3.144437	-1.418885
C	6.164107	2.686260	1.418885
C	6.476306	1.953493	-0.917998
C	6.587625	1.713311	0.508196
H	5.785704	3.257467	-2.492196
H	6.154118	2.492448	2.492196
C	5.454605	5.858221	-3.698957
S	3.696665	5.528031	-3.354570
H	5.570292	5.769763	-4.786114
H	6.113515	5.136516	-3.205185
H	5.708448	6.875636	-3.380343
C	7.981033	-0.612041	-3.698957
S	6.626821	0.556502	-3.354570
H	7.984003	-0.757641	-4.786114
H	7.827604	-1.577173	-3.205185
H	8.934748	-0.176156	-3.380343
C	4.497580	-6.621424	-3.698957
S	4.566846	-4.834084	-3.354570
H	4.385597	-6.714526	-4.786114
H	3.647348	-7.103219	-3.205185
H	5.433000	-7.095298	-3.380343
C	-2.372642	-7.644740	-3.698957
S	-0.932058	-6.584506	-3.354570
H	-2.515253	-7.615236	-4.786114
H	-3.279436	-7.280396	-3.205185
H	-2.159908	-8.671536	-3.380343
C	-7.456216	-2.911411	-3.698957
S	-5.729103	-3.376661	-3.354570
H	-7.522066	-2.781518	-4.786114
H	-7.736737	-1.975286	-3.205185
H	-8.126361	-3.717931	-3.380343
C	-6.925107	4.014270	-3.698957
S	-6.212017	2.373879	-3.354570
H	-6.864610	4.146740	-4.786114
H	-6.368118	4.817254	-3.205185
H	-7.973498	4.035353	-3.380343
C	-1.179251	7.917123	-3.698957
S	-2.017155	6.336840	-3.354570
H	-1.037962	7.952418	-4.786114
H	-0.204176	7.982304	-3.205185
H	-1.816429	8.749933	-3.380343
C	4.497580	6.621424	3.698957
S	4.566846	4.834084	3.354570
H	4.385597	6.714526	4.786114
H	3.647348	7.103219	3.205185
H	5.433000	7.095298	3.380343
C	7.981033	0.612041	3.698957
S	6.626821	-0.556502	3.354570
H	7.984003	0.757641	4.786114
H	7.827604	1.577173	3.205185
H	8.934748	0.176156	3.380343
C	5.454605	-5.858221	3.698957
S	3.696665	-5.528031	3.354570

H	5.570292	-5.769763	4.786114
H	6.113515	-5.136516	3.205185
H	5.708448	-6.875636	3.380343
C	-1.179251	-7.917123	3.698957
S	-2.017155	-6.336840	3.354570
H	-1.037962	-7.952418	4.786114
H	-0.204176	-7.982304	3.205185
H	-1.816429	-8.749933	3.380343
C	-6.925107	-4.014270	3.698957
S	-6.212017	-2.373879	3.354570
H	-6.864610	-4.146740	4.786114
H	-6.368118	-4.817254	3.205185
H	-7.973498	-4.035353	3.380343
C	-7.456216	2.911411	3.698957
S	-5.729103	3.376661	3.354570
H	-7.522066	2.781518	4.786114
H	-7.736737	1.975286	3.205185
H	-8.126361	3.717931	3.380343
C	-2.372642	7.644740	3.698957
S	-0.932058	6.584506	3.354570
H	-2.515253	7.615236	4.786114
H	-3.279436	7.280396	3.205185
H	-2.159908	8.671536	3.380343

Table S 99. Coordinates of the calculated structure of 12_8 (n=8) (TPSS-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.713131	0.247036	1.412983
C	-7.680745	1.311090	0.508227
C	-7.683686	1.052617	-0.902660
C	-7.713131	-0.247036	-1.412983
H	-7.630027	-0.407957	-2.483529
C	-7.680745	-1.311090	-0.508227
C	-7.683686	-1.052617	0.902660
C	-7.395313	-2.306944	1.612271
C	-7.118956	-3.276809	0.662983
C	-7.350916	-2.716808	-0.662983
C	-6.860532	-3.598020	-1.612271
C	-6.358188	-4.504026	0.508227
C	-5.628688	-5.279326	1.412983
H	-5.683713	-5.106775	2.483529
C	-6.177499	-4.688874	-0.902660
C	-4.688874	-6.177499	0.902660
C	-4.504026	-6.358188	-0.508227
C	-5.279326	-5.628688	-1.412983
C	-3.598020	-6.860532	1.612271
C	-2.716808	-7.350916	0.662983
C	-3.276809	-7.118956	-0.662983
C	-2.306944	-7.395313	-1.612271
C	-1.052617	-7.683686	-0.902660
C	-1.311090	-7.680745	0.508227
C	-0.247036	-7.713131	1.412983
C	0.247036	-7.713131	-1.412983
C	1.311090	-7.680745	-0.508227
C	1.052617	-7.683686	0.902660
C	2.306944	-7.395313	1.612271
C	3.276809	-7.118956	0.662983
C	2.716808	-7.350916	-0.662983
C	3.598020	-6.860532	-1.612271
C	4.688874	-6.177499	-0.902660
C	4.504026	-6.358188	0.508227
C	5.279326	-5.628688	1.412983
C	5.628688	-5.279326	-1.412983
C	6.358188	-4.504026	-0.508227
C	6.177499	-4.688874	0.902660
C	6.860532	-3.598020	1.612271
C	7.118956	-3.276809	-0.662983
C	7.350916	-2.716808	0.662983
C	7.395313	-2.306944	-1.612271
C	7.683686	-1.052617	-0.902660
C	7.680745	-1.311090	0.508227
C	7.713131	-0.247036	1.412983
C	7.713131	0.247036	-1.412983
C	7.680745	1.311090	-0.508227
C	7.683686	1.052617	0.902660
C	7.350916	2.716808	-0.662983
C	7.395313	2.306944	1.612271
C	6.860532	3.598020	-1.612271
C	7.118956	3.276809	0.662983
C	6.177499	4.688874	-0.902660
C	6.358188	4.504026	0.508227
C	5.279326	5.628688	-1.412983
C	5.628688	5.279326	1.412983
C	4.688874	6.177499	0.902660

C	4.504026	6.358188	-0.508227
C	3.276809	7.118956	-0.662983
C	3.598020	6.860532	1.612271
C	2.716808	7.350916	0.662983
C	2.306944	7.395313	-1.612271
C	1.052617	7.683686	-0.902660
C	1.311090	7.680745	0.508227
C	0.247036	7.713131	1.412983
C	-0.247036	7.713131	-1.412983
C	-1.311090	7.680745	-0.508227
C	-1.052617	7.683686	0.902660
C	-2.306944	7.395313	1.612271
C	-7.350916	2.716808	0.662983
C	-7.395313	2.306944	-1.612271
C	-7.118956	3.276809	-0.662983
H	-7.630027	0.407957	2.483529
H	-5.106775	-5.683713	-2.483529
H	-0.407957	-7.630027	2.483529
H	0.407957	-7.630027	-2.483529
H	5.683713	-5.106775	-2.483529
H	5.106775	-5.683713	2.483529
H	7.630027	0.407957	-2.483529
H	7.630027	-0.407957	2.483529
H	5.106775	5.683713	-2.483529
H	5.683713	5.106775	2.483529
H	-0.407957	7.630027	-2.483529
H	0.407957	7.630027	2.483529
C	-2.716808	7.350916	-0.662983
C	-3.276809	7.118956	0.662983
C	-3.598020	6.860532	-1.612271
C	-4.504026	6.358188	0.508227
C	-4.688874	6.177499	-0.902660
C	-5.279326	5.628688	1.412983
C	-5.628688	5.279326	-1.412983
C	-6.177499	4.688874	0.902660
C	-6.358188	4.504026	-0.508227
H	-5.106775	5.683713	2.483529
H	-5.683713	5.106775	-2.483529
C	-6.860532	3.598020	1.612271
C	8.555578	2.896373	-3.686844
S	6.861446	3.483056	-3.350883
C	8.097752	-4.001663	-3.686844
S	7.314668	-2.388882	-3.350883
C	2.896373	-8.555578	-3.686844

S	3.483056	-6.861446	-3.350883
C	-4.001663	-8.097752	-3.686844
S	-2.388882	-7.314668	-3.350883
C	-8.555578	-2.896373	-3.686844
S	-6.861446	-3.483056	-3.350883
C	-8.097752	4.001663	-3.686844
S	-7.314668	2.388882	-3.350883
C	-2.896373	8.555578	-3.686844
S	-3.483056	6.861446	-3.350883
C	4.001663	8.097752	-3.686844
S	2.388882	7.314668	-3.350883
C	8.555578	-2.896373	3.686844
S	6.861446	-3.483056	3.350883
C	4.001663	-8.097752	3.686844
S	2.388882	-7.314668	3.350883
C	-2.896373	-8.555578	3.686844
S	-3.483056	-6.861446	3.350883
C	-8.097752	-4.001663	3.686844
S	-7.314668	-2.388882	3.350883
C	-8.555578	2.896373	3.686844
S	-6.861446	3.483056	3.350883
C	-4.001663	8.097752	3.686844
S	-2.388882	7.314668	3.350883
C	2.896373	8.555578	3.686844
S	3.483056	6.861446	3.350883
C	8.097752	4.001663	3.686844
S	7.314668	2.388882	3.350883
H	-3.987635	9.125973	3.321319
H	-4.824605	7.547643	3.231342
H	-4.113316	8.089161	4.773549
H	3.633353	9.272721	3.321319
H	2.811347	8.628454	4.773549
H	1.925479	8.748500	3.231342
H	8.748500	-1.925479	3.231342
H	9.272721	-3.633353	3.321319
H	8.628454	-2.811347	4.773549
H	-8.628454	2.811347	4.773549
H	-8.748500	1.925479	3.231342
H	-9.272721	3.633353	3.321319
H	3.987635	-9.125973	3.321319
H	4.113316	-8.089161	4.773549
H	4.824605	-7.547643	3.231342
H	7.547643	4.824605	3.231342
H	9.125973	3.987635	3.321319

H	8.089161	4.113316	4.773549
H	-3.633353	-9.272721	3.321319
H	-1.925479	-8.748500	3.231342
H	-2.811347	-8.628454	4.773549
H	-8.089161	-4.113316	4.773549
H	-7.547643	-4.824605	3.231342
H	-9.125973	-3.987635	3.321319
H	2.811347	-8.628454	-4.773549
H	3.633353	-9.272721	-3.321319
H	1.925479	-8.748500	-3.231342
H	-4.824605	-7.547643	-3.231342
H	-4.113316	-8.089161	-4.773549
H	-3.987635	-9.125973	-3.321319
H	7.547643	-4.824605	-3.231342
H	9.125973	-3.987635	-3.321319
H	8.089161	-4.113316	-4.773549

H	4.113316	8.089161	-4.773549
H	3.987635	9.125973	-3.321319
H	4.824605	7.547643	-3.231342
H	-8.628454	-2.811347	-4.773549
H	-9.272721	-3.633353	-3.321319
H	-8.748500	-1.925479	-3.231342
H	-8.089161	4.113316	-4.773549
H	-7.547643	4.824605	-3.231342
H	-9.125973	3.987635	-3.321319
H	-3.633353	9.272721	-3.321319
H	-2.811347	8.628454	-4.773549
H	-1.925479	8.748500	-3.231342
H	8.748500	1.925479	-3.231342
H	8.628454	2.811347	-4.773549
H	9.272721	3.633353	-3.321319

Table S 100. Coordinates of the calculated structure of the triplet of 12_8 (n=8) (TPSS-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.708268	0.252978	1.413246
C	-7.675656	1.313319	0.507820
C	-7.677861	1.051650	-0.907152
C	-7.708268	-0.252978	-1.413246
H	-7.629778	-0.416440	-2.484075
C	-7.675656	-1.313319	-0.507820
C	-7.677861	-1.051650	0.907152
C	-7.391677	-2.295447	1.613847
C	-7.121634	-3.276277	0.659009
C	-7.352434	-2.719078	-0.659009
C	-6.849831	-3.603579	-1.613847
C	-6.356165	-4.498851	0.507820
C	-5.629451	-5.271686	1.413246
H	-5.689535	-5.100600	2.484075
C	-6.172697	-4.685439	-0.907152
C	-4.685439	-6.172697	0.907152
C	-4.498851	-6.356165	-0.507820
C	-5.271686	-5.629451	-1.413246
C	-3.603579	-6.849831	1.613847
C	-2.719078	-7.352434	0.659009
C	-3.276277	-7.121634	-0.659009
C	-2.295447	-7.391677	-1.613847
C	-1.051650	-7.677861	-0.907152
C	-1.313319	-7.675656	0.507820

C	-0.252978	-7.708268	1.413246
C	0.252978	-7.708268	-1.413246
C	1.313319	-7.675656	-0.507820
C	1.051650	-7.677861	0.907152
C	2.295447	-7.391677	1.613847
C	3.276277	-7.121634	0.659009
C	2.719078	-7.352434	-0.659009
C	3.603579	-6.849831	-1.613847
C	4.685439	-6.172697	-0.907152
C	4.498851	-6.356165	0.507820
C	5.271686	-5.629451	1.413246
C	5.629451	-5.271686	-1.413246
C	6.356165	-4.498851	-0.507820
C	6.172697	-4.685439	0.907152
C	6.849831	-3.603579	1.613847
C	7.121634	-3.276277	-0.659009
C	7.352434	-2.719078	0.659009
C	7.391677	-2.295447	-1.613847
C	7.677861	-1.051650	-0.907152
C	7.675656	-1.313319	0.507820
C	7.708268	-0.252978	1.413246
C	7.708268	0.252978	-1.413246
C	7.675656	1.313319	-0.507820
C	7.677861	1.051650	0.907152
C	7.352434	2.719078	-0.659009

C	7.391677	2.295447	1.613847
C	6.849831	3.603579	-1.613847
C	7.121634	3.276277	0.659009
C	6.172697	4.685439	-0.907152
C	6.356165	4.498851	0.507820
C	5.271686	5.629451	-1.413246
C	5.629451	5.271686	1.413246
C	4.685439	6.172697	0.907152
C	4.498851	6.356165	-0.507820
C	3.276277	7.121634	-0.659009
C	3.603579	6.849831	1.613847
C	2.719078	7.352434	0.659009
C	2.295447	7.391677	-1.613847
C	1.051650	7.677861	-0.907152
C	1.313319	7.675656	0.507820
C	0.252978	7.708268	1.413246
C	-0.252978	7.708268	-1.413246
C	-1.313319	7.675656	-0.507820
C	-1.051650	7.677861	0.907152
C	-2.295447	7.391677	1.613847
C	-7.352434	2.719078	0.659009
C	-7.391677	2.295447	-1.613847
C	-7.121634	3.276277	-0.659009
H	-7.629778	0.416440	2.484075
H	-5.100600	-5.689535	-2.484075
H	-0.416440	-7.629778	2.484075
H	0.416440	-7.629778	-2.484075
H	5.689535	-5.100600	-2.484075
H	5.100600	-5.689535	2.484075
H	7.629778	0.416440	-2.484075
H	7.629778	-0.416440	2.484075
H	5.100600	5.689535	-2.484075
H	5.689535	5.100600	2.484075
H	-0.416440	7.629778	-2.484075
H	0.416440	7.629778	2.484075
C	-2.719078	7.352434	-0.659009
C	-3.276277	7.121634	0.659009
C	-3.603579	6.849831	-1.613847
C	-4.498851	6.356165	0.507820
C	-4.685439	6.172697	-0.907152
C	-5.271686	5.629451	1.413246
C	-5.629451	5.271686	-1.413246
C	-6.172697	4.685439	0.907152
C	-6.356165	4.498851	-0.507820

H	-5.100600	5.689535	2.484075
H	-5.689535	5.100600	-2.484075
C	-6.849831	3.603579	1.613847
C	8.539199	2.907230	-3.691851
S	6.834060	3.459736	-3.349369
C	8.093848	-3.982403	-3.691851
S	7.278813	-2.386008	-3.349369
C	2.907230	-8.539199	-3.691851
S	3.459736	-6.834060	-3.349369
C	-3.982403	-8.093848	-3.691851
S	-2.386008	-7.278813	-3.349369
C	-8.539199	-2.907230	-3.691851
S	-6.834060	-3.459736	-3.349369
C	-8.093848	3.982403	-3.691851
S	-7.278813	2.386008	-3.349369
C	-2.907230	8.539199	-3.691851
S	-3.459736	6.834060	-3.349369
C	3.982403	8.093848	-3.691851
S	2.386008	7.278813	-3.349369
C	8.539199	-2.907230	3.691851
S	6.834060	-3.459736	3.349369
C	3.982403	-8.093848	3.691851
S	2.386008	-7.278813	3.349369
C	-2.907230	-8.539199	3.691851
S	-3.459736	-6.834060	3.349369
C	-8.093848	-3.982403	3.691851
S	-7.278813	-2.386008	3.349369
C	-8.539199	2.907230	3.691851
S	-6.834060	3.459736	3.349369
C	-3.982403	8.093848	3.691851
S	-2.386008	7.278813	3.349369
C	2.907230	8.539199	3.691851
S	3.459736	6.834060	3.349369
C	8.093848	3.982403	3.691851
S	7.278813	2.386008	3.349369
H	-3.920217	9.146640	3.410906
H	-4.802722	7.610870	3.161465
H	-4.138429	8.003004	4.769213
H	3.695639	9.239663	3.410906
H	2.732668	8.585290	4.769213
H	1.985661	8.777735	3.161465
H	8.777735	-1.985661	3.161465
H	9.239663	-3.695639	3.410906
H	8.585290	-2.732668	4.769213

H	-8.585290	2.732668	4.769213
H	-8.777735	1.985661	3.161465
H	-9.239663	3.695639	3.410906
H	3.920217	-9.146640	3.410906
H	4.138429	-8.003004	4.769213
H	4.802722	-7.610870	3.161465
H	7.610870	4.802722	3.161465
H	9.146640	3.920217	3.410906
H	8.003004	4.138429	4.769213
H	-3.695639	-9.239663	3.410906
H	-1.985661	-8.777735	3.161465
H	-2.732668	-8.585290	4.769213
H	-8.003004	-4.138429	4.769213
H	-7.610870	-4.802722	3.161465
H	-9.146640	-3.920217	3.410906
H	2.732668	-8.585290	-4.769213
H	3.695639	-9.239663	-3.410906
H	1.985661	-8.777735	-3.161465
H	-4.802722	-7.610870	-3.161465
H	-4.138429	-8.003004	-4.769213
H	-3.920217	-9.146640	-3.410906
H	7.610870	-4.802722	-3.161465
H	9.146640	-3.920217	-3.410906
H	8.003004	-4.138429	-4.769213
H	4.138429	8.003004	-4.769213
H	3.920217	9.146640	-3.410906
H	4.802722	7.610870	-3.161465
H	-8.585290	-2.732668	-4.769213
H	-9.239663	-3.695639	-3.410906
H	-8.777735	-1.985661	-3.161465
H	-8.003004	4.138429	-4.769213
H	-7.610870	4.802722	-3.161465
H	-9.146640	3.920217	-3.410906
H	-3.695639	9.239663	-3.410906
H	-2.732668	8.585290	-4.769213
H	-1.985661	8.777735	-3.161465
H	8.777735	1.985661	-3.161465
H	8.585290	2.732668	-4.769213
H	9.239663	3.695639	-3.410906

Table S 101. Coordinates of the calculated structure of the open-shell singlet of 12_8 (n=8) (TDDFT, BP86-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.698696	0.251687	1.418145
C	-7.667287	1.313529	0.508373
C	-7.668514	1.051179	-0.914724
C	-7.698696	-0.251687	-1.418145
H	-7.611991	-0.420185	-2.492100
C	-7.667287	-1.313529	-0.508373
C	-7.668514	-1.051179	0.914724
C	-7.383344	-2.300292	1.620852
C	-7.116331	-3.277552	0.664092
C	-7.349585	-2.714427	-0.664092
C	-6.847364	-3.594261	-1.620852
C	-6.350396	-4.492786	0.508373
C	-5.621770	-5.265830	1.418145
H	-5.679606	-5.085375	2.492100
C	-6.165754	-4.679163	-0.914724
C	-4.679163	-6.165754	0.914724
C	-4.492786	-6.350396	-0.508373
C	-5.265830	-5.621770	-1.418145
C	-3.594261	-6.847364	1.620852
C	-2.714427	-7.349585	0.664092
C	-3.277552	-7.116331	-0.664092
C	-2.300292	-7.383344	-1.620852
C	-1.051179	-7.668514	-0.914724
C	-1.313529	-7.667287	0.508373
C	-0.251687	-7.698696	1.418145
C	0.251687	-7.698696	-1.418145
C	1.313529	-7.667287	-0.508373
C	1.051179	-7.668514	0.914724
C	2.300292	-7.383344	1.620852
C	3.277552	-7.116331	0.664092
C	2.714427	-7.349585	-0.664092
C	3.594261	-6.847364	-1.620852
C	4.679163	-6.165754	-0.914724
C	4.492786	-6.350396	0.508373
C	5.265830	-5.621770	1.418145
C	5.621770	-5.265830	-1.418145
C	6.350396	-4.492786	-0.508373
C	6.165754	-4.679163	0.914724
C	6.847364	-3.594261	1.620852
C	7.116331	-3.277552	-0.664092
C	7.349585	-2.714427	0.664092

C	7.383344	-2.300292	-1.620852
C	7.668514	-1.051179	-0.914724
C	7.667287	-1.313529	0.508373
C	7.698696	-0.251687	1.418145
C	7.698696	0.251687	-1.418145
C	7.667287	1.313529	-0.508373
C	7.668514	1.051179	0.914724
C	7.349585	2.714427	-0.664092
C	7.383344	2.300292	1.620852
C	6.847364	3.594261	-1.620852
C	7.116331	3.277552	0.664092
C	6.165754	4.679163	-0.914724
C	6.350396	4.492786	0.508373
C	5.265830	5.621770	-1.418145
C	5.621770	5.265830	1.418145
C	4.679163	6.165754	0.914724
C	4.492786	6.350396	-0.508373
C	3.277552	7.116331	-0.664092
C	3.594261	6.847364	1.620852
C	2.714427	7.349585	0.664092
C	2.300292	7.383344	-1.620852
C	1.051179	7.668514	-0.914724
C	1.313529	7.667287	0.508373
C	0.251687	7.698696	1.418145
C	-0.251687	7.698696	-1.418145
C	-1.313529	7.667287	-0.508373
C	-1.051179	7.668514	0.914724
C	-2.300292	7.383344	1.620852
C	-7.349585	2.714427	0.664092
C	-7.383344	2.300292	-1.620852
C	-7.116331	3.277552	-0.664092
H	-7.611991	0.420185	2.492100
H	-5.085375	-5.679606	-2.492100
H	-0.420185	-7.611991	2.492100
H	0.420185	-7.611991	-2.492100
H	5.679606	-5.085375	-2.492100
H	5.085375	-5.679606	2.492100
H	7.611991	0.420185	-2.492100
H	7.611991	-0.420185	2.492100
H	5.085375	5.679606	-2.492100
H	5.679606	5.085375	2.492100
H	-0.420185	7.611991	-2.492100
H	0.420185	7.611991	2.492100
C	-2.714427	7.349585	-0.664092

C	-3.277552	7.116331	0.664092
C	-3.594261	6.847364	-1.620852
C	-4.492786	6.350396	0.508373
C	-4.679163	6.165754	-0.914724
C	-5.265830	5.621770	1.418145
C	-5.621770	5.265830	-1.418145
C	-6.165754	4.679163	0.914724
C	-6.350396	4.492786	-0.508373
H	-5.085375	5.679606	2.492100
H	-5.679606	5.085375	-2.492100
C	-6.847364	3.594261	1.620852
C	8.534871	2.885821	-3.693863
S	6.835919	3.449776	-3.355477
C	8.075649	-3.994482	-3.693863
S	7.273085	-2.394365	-3.355477
C	2.885821	-8.534871	-3.693863
S	3.449776	-6.835919	-3.355477
C	-3.994482	-8.075649	-3.693863
S	-2.394365	-7.273085	-3.355477
C	-8.534871	-2.885821	-3.693863
S	-6.835919	-3.449776	-3.355477
C	-8.075649	3.994482	-3.693863
S	-7.273085	2.394365	-3.355477
C	-2.885821	8.534871	-3.693863
S	-3.449776	6.835919	-3.355477
C	3.994482	8.075649	-3.693863
S	2.394365	7.273085	-3.355477
C	8.534871	-2.885821	3.693863
S	6.835919	-3.449776	3.355477
C	3.994482	-8.075649	3.693863
S	2.394365	-7.273085	3.355477
C	-2.885821	-8.534871	3.693863
S	-3.449776	-6.835919	3.355477
C	-8.075649	-3.994482	3.693863
S	-7.273085	-2.394365	3.355477
C	-8.534871	2.885821	3.693863
S	-6.835919	3.449776	3.355477
C	-3.994482	8.075649	3.693863
S	-2.394365	7.273085	3.355477
C	2.885821	8.534871	3.693863
S	3.449776	6.835919	3.355477
C	8.075649	3.994482	3.693863
S	7.273085	2.394365	3.355477
H	-3.962796	9.117748	3.355943

H	-4.828011	7.552304	3.214385
H	-4.123654	8.041892	4.782599
H	3.645102	9.249341	3.355943
H	2.770613	8.602340	4.782599
H	1.926366	8.754205	3.214385
H	8.754205	-1.926366	3.214385
H	9.249341	-3.645102	3.355943
H	8.602340	-2.770613	4.782599
H	-8.602340	2.770613	4.782599
H	-8.754205	1.926366	3.214385
H	-9.249341	3.645102	3.355943
H	3.962796	-9.117748	3.355943
H	4.123654	-8.041892	4.782599
H	4.828011	-7.552304	3.214385
H	7.552304	4.828011	3.214385
H	9.117748	3.962796	3.355943
H	8.041892	4.123654	4.782599
H	-3.645102	-9.249341	3.355943
H	-1.926366	-8.754205	3.214385
H	-2.770613	-8.602340	4.782599
H	-8.041892	-4.123654	4.782599
H	-7.552304	-4.828011	3.214385
H	-9.117748	-3.962796	3.355943
H	2.770613	-8.602340	-4.782599

H	3.645102	-9.249341	-3.355943
H	1.926366	-8.754205	-3.214385
H	-4.828011	-7.552304	-3.214385
H	-4.123654	-8.041892	-4.782599
H	-3.962796	-9.117748	-3.355943
H	7.552304	-4.828011	-3.214385
H	9.117748	-3.962796	-3.355943
H	8.041892	-4.123654	-4.782599
H	4.123654	8.041892	-4.782599
H	3.962796	9.117748	-3.355943
H	4.828011	7.552304	-3.214385
H	-8.602340	-2.770613	-4.782599
H	-9.249341	-3.645102	-3.355943
H	-8.754205	-1.926366	-3.214385
H	-8.041892	4.123654	-4.782599
H	-7.552304	4.828011	-3.214385
H	-9.117748	3.962796	-3.355943
H	-3.645102	9.249341	-3.355943
H	-2.770613	8.602340	-4.782599
H	-1.926366	8.754205	-3.214385
H	8.754205	1.926366	-3.214385
H	8.602340	2.770613	-4.782599
H	9.249341	3.645102	-3.355943

4.7 Calculated coordinates of phenyl-substituted cyclacenes 13_n

Below can be found coordinates for the calculated structures of phenyl-substituted $[5.5.6]_n$cyclacenes $\mathbf{13_n}$ as singlets and triplets at the TPSS-D3/def2-TZVP level of theory and of the open-shell singlets calculated using TDDFT at the BP86-D3/def2-TZVP level of theory, optimized in point group D_n.

Table S 102. Coordinates of the calculated structure of 13_3 (n=3) (TPSS-D3/def2-TZVP) in C_1 geometry.

	x	y	z
C	-2.879098	1.407968	-0.785793
C	-2.762055	1.260136	0.695465
C	-1.753251	2.153285	1.173483
C	-1.122432	2.738014	-0.013056
C	-1.712393	2.070956	-1.169801
C	-2.990704	0.043281	1.353741
C	-2.063193	-0.359508	2.329776
C	-1.146907	0.578980	2.898566
C	-1.069346	1.875665	2.369516
C	-1.381250	-1.656460	2.340128
C	-0.040203	-1.429224	2.874122
C	0.030958	-0.155612	3.443882
C	0.879814	-2.197111	2.025421
C	0.069868	-2.921573	1.094254
C	-1.351697	-2.646642	1.372177
C	0.546607	-3.257573	-0.176906
C	1.689671	-2.579537	-0.639434
C	2.533930	-1.892519	0.292862
C	2.178036	-1.812034	1.648161
C	1.738884	-1.810169	-1.887106
C	2.549735	-0.630249	-1.612432
C	3.256721	-0.802933	-0.419696
C	1.858320	0.506295	-2.225713
C	0.724120	-0.032997	-2.910218
C	0.806385	-1.520721	-2.886792
C	-0.489145	0.668789	-2.912267
C	-0.614801	1.813354	-2.104398
C	0.552660	2.415533	-1.531653
C	1.800276	1.799323	-1.674882
C	0.156726	3.194677	-0.323810
H	-1.389392	0.160935	-3.235824
H	2.630132	2.137209	-1.067773
H	-0.127040	-3.731655	-0.882141
H	2.730298	-1.150662	2.302849
H	-3.608917	-0.712633	0.885377
H	-0.239948	2.514219	2.643723
C	3.082921	5.228453	0.939020
C	2.552936	5.761009	2.114868
C	1.220472	5.497004	2.446886
C	0.444920	4.682794	1.633375
C	0.981791	4.079427	0.472441
C	2.309224	4.409742	0.123119
H	4.106177	5.453997	0.652304
H	3.160921	6.396999	2.751675
H	0.782244	5.942267	3.335879
H	-0.601603	4.522255	1.872061
H	2.731671	4.039636	-0.802566
C	-6.019629	-0.337439	-1.925436
C	-5.876800	-0.285275	-3.312472
C	-4.769462	0.366564	-3.865026
C	-3.807119	0.932724	-3.040395
C	-3.901154	0.834231	-1.633391
C	-5.050659	0.215846	-1.096369
H	-6.890188	-0.815002	-1.485355
H	-6.631827	-0.724152	-3.958335
H	-4.669572	0.449773	-4.943792
H	-2.984342	1.488957	-3.476756
H	-5.190521	0.187382	-0.022231
C	2.315332	2.202143	5.326228
C	3.370424	1.347797	5.648717
C	3.289554	-0.003978	5.300882
C	2.185606	-0.481844	4.608722
C	1.137281	0.380222	4.211591
C	1.209809	1.726813	4.628857
H	2.351301	3.247009	5.620996
H	4.233615	1.723505	6.190379
H	4.083160	-0.688762	5.586777
H	2.104714	-1.540869	4.384878
H	0.389640	2.402599	4.423786
C	-0.710535	-4.761249	-4.030346
C	-1.684606	-4.322710	-4.932255

C	-1.799639	-2.958905	-5.208126
C	-0.983234	-2.037776	-4.561182
C	-0.031978	-2.455863	-3.603855
C	0.113342	-3.846109	-3.390212
H	-0.586148	-5.822988	-3.837958
H	-2.328627	-5.039345	-5.433290
H	-2.527825	-2.610475	-5.935304
H	-1.063833	-0.987475	-4.814154
H	0.900421	-4.197260	-2.730817
C	5.903401	0.705169	1.817905
C	6.351638	1.763560	1.026378
C	5.825194	1.930690	-0.258112
C	4.839054	1.073730	-0.726186
C	4.322872	0.036308	0.084577
C	4.913308	-0.153444	1.353031
H	6.329348	0.544640	2.804198
H	7.122180	2.434804	1.394190
H	6.198122	2.723510	-0.900657
H	4.469660	1.178948	-1.741276
H	4.609342	-0.989095	1.970626
C	-3.602017	-3.040901	-1.636779
C	-4.732852	-3.618136	-1.058613
C	-4.752439	-3.881349	0.312000
C	-3.643712	-3.579506	1.100369
C	-2.488055	-3.025280	0.525593
C	-2.488838	-2.749387	-0.854799
H	-3.588382	-2.797016	-2.694142
H	-5.601039	-3.845241	-1.670551
H	-5.634355	-4.320398	0.770236
H	-3.656448	-3.777216	2.168234
H	-1.635524	-2.254867	-1.303854

Table S 103. Coordinates of the calculated structure of the triplet of 13_3 (n=3) (TPSS-D3/def2-TZVP) in C_1 geometry.

	x	y	z
C	-2.912633	1.411923	-0.750237
C	-2.765938	1.250940	0.701880
C	-1.739077	2.145107	1.182776
C	-1.136403	2.753843	0.022554
C	-1.742051	2.101671	-1.148382
C	-2.982955	0.024737	1.359810
C	-2.033821	-0.382729	2.303041
C	-1.104785	0.557290	2.886723
C	-1.032279	1.851192	2.370113
C	-1.356890	-1.677932	2.305237
C	-0.016842	-1.453438	2.833714
C	0.064365	-0.178222	3.418201
C	0.896932	-2.195580	1.960714
C	0.070390	-2.912855	1.016085
C	-1.337410	-2.657074	1.313846
C	0.542544	-3.223025	-0.258268
C	1.696108	-2.545024	-0.709949
C	2.555484	-1.871931	0.239428
C	2.195685	-1.822650	1.601934
C	1.745020	-1.778494	-1.934779
C	2.566885	-0.596619	-1.646100
C	3.277811	-0.791089	-0.434599
C	1.836769	0.520915	-2.167854
C	0.669905	-0.022977	-2.875924
C	0.778558	-1.474174	-2.927825
C	-0.532799	0.688328	-2.878083
C	-0.651884	1.805736	-2.029880
C	0.550508	2.421366	-1.446154
C	1.796001	1.817645	-1.623783
C	0.167709	3.209724	-0.283088
H	-1.435604	0.197695	-3.218901
H	2.638270	2.154170	-1.033930
H	-0.125133	-3.691966	-0.972402
H	2.754223	-1.181560	2.271111
H	-3.605996	-0.728000	0.892872
H	-0.204992	2.493056	2.642970
C	3.087513	5.223761	1.023082
C	2.546494	5.754325	2.195649
C	1.209561	5.494684	2.509833
C	0.440401	4.685588	1.684325
C	0.987182	4.085828	0.525851
C	2.320474	4.414038	0.193401
H	4.115073	5.445741	0.749259
H	3.150083	6.384223	2.842438
H	0.762437	5.936117	3.396307
H	-0.608031	4.524453	1.914657
H	2.752806	4.051470	-0.730784

C	-6.036715	-0.357020	-1.892435
C	-5.900807	-0.291307	-3.280672
C	-4.805368	0.381083	-3.830650
C	-3.846049	0.951242	-3.004392
C	-3.932131	0.840132	-1.597019
C	-5.074506	0.203389	-1.062250
H	-6.899515	-0.849361	-1.453254
H	-6.652680	-0.734465	-3.927156
H	-4.710401	0.476016	-4.908931
H	-3.032540	1.521574	-3.440363
H	-5.213905	0.167987	0.011854
C	2.368121	2.152065	5.311535
C	3.422596	1.291142	5.620458
C	3.333516	-0.056342	5.260079
C	2.224130	-0.523207	4.568177
C	1.175583	0.345406	4.185393
C	1.256560	1.687732	4.617245
H	2.409168	3.193935	5.616304
H	4.290132	1.658494	6.160824
H	4.125805	-0.747508	5.534379
H	2.138609	-1.579915	4.335125
H	0.437243	2.369151	4.427118
C	-4.755286	-3.897895	0.321311
C	-4.759796	-3.653253	-1.052968
C	-3.640946	-3.078767	-1.656483
C	-2.516540	-2.772046	-0.896486
C	-2.488248	-3.033880	0.486516
C	-3.633758	-3.584317	1.086423
H	-5.627833	-4.333667	0.800258
H	-5.637361	-3.891082	-1.647234
H	-3.645371	-2.846726	-2.716599
H	-1.674905	-2.276944	-1.366740
H	-3.627004	-3.771767	2.156267
C	-0.687852	-4.720443	-4.117932
C	-1.692402	-4.285906	-4.987064
C	-1.845470	-2.918293	-5.225822
C	-1.036147	-1.992967	-4.577010
C	-0.054225	-2.409049	-3.648868
C	0.126689	-3.800554	-3.471713
H	-0.533443	-5.782905	-3.952851
H	-2.330504	-5.005642	-5.491007
H	-2.597701	-2.569818	-5.928195
H	-1.145695	-0.940438	-4.809343
H	0.931598	-4.149293	-2.832462
C	5.910706	0.701810	1.827005
C	6.349012	1.779858	1.054929
C	5.821772	1.962177	-0.226551
C	4.843261	1.103805	-0.709542
C	4.336552	0.045528	0.081556
C	4.932419	-0.160292	1.346762
H	6.337924	0.528194	2.810574
H	7.111881	2.452696	1.435358
H	6.186267	2.769450	-0.855940
H	4.473941	1.224241	-1.723098
H	4.641953	-1.012264	1.948693

Table S 104. Coordinates of the calculated structure of 13_4 (n=4) (TPSS-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.668995	-1.034846	-0.961257
C	3.660944	-1.310985	0.486864
C	3.821633	0.277571	-1.417395
C	3.660944	1.310985	-0.486864
C	3.668995	1.034846	0.961257
C	3.821633	-0.277571	1.417395
C	3.088858	-2.151175	-1.660257
C	3.008036	-2.567058	0.662235
C	2.567058	-3.008036	-0.662235
C	2.151175	-3.088858	1.660257
C	1.310985	-3.660944	-0.486864
C	1.034846	-3.668995	0.961257
C	0.277571	-3.821633	-1.417395
C	-0.277571	-3.821633	1.417395
C	-1.034846	-3.668995	-0.961257
C	-1.310985	-3.660944	0.486864
C	-2.567058	-3.008036	0.662235
C	-2.151175	-3.088858	-1.660257
C	-3.008036	-2.567058	-0.662235
C	-3.088858	-2.151175	1.660257
C	-3.660944	-1.310985	-0.486864
C	-3.668995	-1.034846	0.961257
C	-3.821633	-0.277571	-1.417395
C	-3.821633	0.277571	1.417395
C	-3.660944	1.310985	0.486864

C	-3.668995	1.034846	-0.961257
C	-3.088858	2.151175	-1.660257
C	-3.008036	2.567058	0.662235
C	-2.567058	3.008036	-0.662235
C	-2.151175	3.088858	1.660257
C	-1.034846	3.668995	0.961257
C	-1.310985	3.660944	-0.486864
C	0.277571	3.821633	1.417395
C	-0.277571	3.821633	-1.417395
C	1.034846	3.668995	-0.961257
C	1.310985	3.660944	0.486864
C	2.151175	3.088858	-1.660257
C	2.567058	3.008036	0.662235
C	3.008036	2.567058	-0.662235
C	3.088858	2.151175	1.660257
H	-3.812991	0.504293	2.475931
H	-3.812991	-0.504293	-2.475931
H	-0.504293	-3.812991	2.475931
H	0.504293	-3.812991	-2.475931
H	3.812991	-0.504293	2.475931
H	3.812991	0.504293	-2.475931
H	0.504293	3.812991	2.475931
H	-0.504293	3.812991	-2.475931
C	-2.216118	1.507396	-5.299207
C	-2.282222	2.802010	-5.815157
C	-2.612865	3.862062	-4.967971
C	-2.884795	3.623311	-3.625563
C	-2.833303	2.319798	-3.088891
C	-2.483367	1.264320	-3.954166
H	-1.942979	0.674617	-5.939902
H	-2.072299	2.985699	-6.865036
H	-2.663282	4.875558	-5.355826
H	-3.152761	4.445291	-2.967677
H	-2.370170	0.256653	-3.572964
C	3.862062	2.612865	-4.967971
C	2.802010	2.282222	-5.815157
C	1.507396	2.216118	-5.299207
C	1.264320	2.483367	-3.954166
C	2.319798	2.833303	-3.088891
C	3.623311	2.884795	-3.625563
H	4.875558	2.663282	-5.355826
H	2.985699	2.072299	-6.865036
H	0.674617	1.942979	-5.939902
H	0.256653	2.370170	-3.572964

H	4.445291	3.152761	-2.967677
C	2.216118	-1.507396	-5.299207
C	2.282222	-2.802010	-5.815157
C	2.612865	-3.862062	-4.967971
C	2.884795	-3.623311	-3.625563
C	2.833303	-2.319798	-3.088891
C	2.483367	-1.264320	-3.954166
H	1.942979	-0.674617	-5.939902
H	2.072299	-2.985699	-6.865036
H	2.663282	-4.875558	-5.355826
H	3.152761	-4.445291	-2.967677
H	2.370170	-0.256653	-3.572964
C	-1.507396	-2.216118	-5.299207
C	-2.802010	-2.282222	-5.815157
C	-3.862062	-2.612865	-4.967971
C	-3.623311	-2.884795	-3.625563
C	-2.319798	-2.833303	-3.088891
C	-1.264320	-2.483367	-3.954166
H	-0.674617	-1.942979	-5.939902
H	-2.985699	-2.072299	-6.865036
H	-4.875558	-2.663282	-5.355826
H	-4.445291	-3.152761	-2.967677
H	-0.256653	-2.370170	-3.572964
C	-1.507396	2.216118	5.299207
C	-2.802010	2.282222	5.815157
C	-3.862062	2.612865	4.967971
C	-3.623311	2.884795	3.625563
C	-2.319798	2.833303	3.088891
C	-1.264320	2.483367	3.954166
H	-0.674617	1.942979	5.939902
H	-2.985699	2.072299	6.865036
H	-4.875558	2.663282	5.355826
H	-4.445291	3.152761	2.967677
H	-0.256653	2.370170	3.572964
C	2.612865	3.862062	4.967971
C	2.282222	2.802010	5.815157
C	2.216118	1.507396	5.299207
C	2.483367	1.264320	3.954166
C	2.833303	2.319798	3.088891
C	2.884795	3.623311	3.625563
H	2.663282	4.875558	5.355826
H	2.072299	2.985699	6.865036
H	1.942979	0.674617	5.939902
H	2.370170	0.256653	3.572964

H	3.152761	4.445291	2.967677
C	3.862062	-2.612865	4.967971
C	2.802010	-2.282222	5.815157
C	1.507396	-2.216118	5.299207
C	1.264320	-2.483367	3.954166
C	2.319798	-2.833303	3.088891
C	3.623311	-2.884795	3.625563
H	4.875558	-2.663282	5.355826
H	2.985699	-2.072299	6.865036
H	0.674617	-1.942979	5.939902
H	0.256653	-2.370170	3.572964
H	4.445291	-3.152761	2.967677
C	-2.612865	-3.862062	4.967971
C	-2.282222	-2.802010	5.815157
C	-2.216118	-1.507396	5.299207
C	-2.483367	-1.264320	3.954166
C	-2.833303	-2.319798	3.088891
C	-2.884795	-3.623311	3.625563
H	-2.663282	-4.875558	5.355826
H	-2.072299	-2.985699	6.865036
H	-1.942979	-0.674617	5.939902
H	-2.370170	-0.256653	3.572964
H	-3.152761	-4.445291	2.967677

Table S 105. Coordinates of the calculated structure of the Triplet of 13_4 (n=4) (TPSS-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.691468	-1.037728	-0.944011
C	3.690433	-1.312435	0.481703
C	3.839898	0.274730	-1.408636
C	3.690433	1.312435	-0.481703
C	3.691468	1.037728	0.944011
C	3.839898	-0.274730	1.408636
C	3.088656	-2.164798	-1.646785
C	3.022278	-2.583286	0.659080
C	2.583286	-3.022278	-0.659080
C	2.164798	-3.088656	1.646785
C	1.312435	-3.690433	-0.481703
C	1.037728	-3.691468	0.944011
C	0.274730	-3.839898	-1.408636
C	-0.274730	-3.839898	1.408636
C	-1.037728	-3.691468	-0.944011
C	-1.312435	-3.690433	0.481703
C	-2.583286	-3.022278	0.659080
C	-2.164798	-3.088656	-1.646785
C	-3.022278	-2.583286	-0.659080
C	-3.088656	-2.164798	1.646785
C	-3.690433	-1.312435	-0.481703
C	-3.691468	-1.037728	0.944011
C	-3.839898	-0.274730	-1.408636
C	-3.839898	0.274730	1.408636
C	-3.690433	1.312435	0.481703
C	-3.691468	1.037728	-0.944011
C	-3.088656	2.164798	-1.646785
C	-3.022278	2.583286	0.659080
C	-2.583286	3.022278	-0.659080
C	-2.164798	3.088656	1.646785
C	-1.037728	3.691468	0.944011
C	-1.312435	3.690433	-0.481703
C	0.274730	3.839898	1.408636
C	-0.274730	3.839898	-1.408636
C	1.037728	3.691468	-0.944011
C	1.312435	3.690433	0.481703
C	2.164798	3.088656	-1.646785
C	2.583286	3.022278	0.659080
C	3.022278	2.583286	-0.659080
C	3.088656	2.164798	1.646785
H	-3.826550	0.494826	2.468567
H	-3.826550	-0.494826	-2.468567
H	-0.494826	-3.826550	2.468567
H	0.494826	-3.826550	-2.468567
H	3.826550	-0.494826	2.468567
H	3.826550	0.494826	-2.468567
H	0.494826	3.826550	2.468567
H	-0.494826	3.826550	-2.468567
C	-2.207690	1.495043	-5.278557
C	-2.276383	2.785912	-5.803732
C	-2.608139	3.851947	-4.964747
C	-2.880791	3.622423	-3.620825
C	-2.827790	2.322555	-3.075407
C	-2.475530	1.261059	-3.932202
H	-1.933502	0.658287	-5.913536
H	-2.068156	2.961910	-6.855303
H	-2.660307	4.862346	-5.360255

H	-3.153212	4.447201	-2.968486
H	-2.361556	0.256666	-3.542838
C	3.851947	2.608139	-4.964747
C	2.785912	2.276383	-5.803732
C	1.495043	2.207690	-5.278557
C	1.261059	2.475530	-3.932202
C	2.322555	2.827790	-3.075407
C	3.622423	2.880791	-3.620825
H	4.862346	2.660307	-5.360255
H	2.961910	2.068156	-6.855303
H	0.658287	1.933502	-5.913536
H	0.256666	2.361556	-3.542838
H	4.447201	3.153212	-2.968486
C	2.207690	-1.495043	-5.278557
C	2.276383	-2.785912	-5.803732
C	2.608139	-3.851947	-4.964747
C	2.880791	-3.622423	-3.620825
C	2.827790	-2.322555	-3.075407
C	2.475530	-1.261059	-3.932202
H	1.933502	-0.658287	-5.913536
H	2.068156	-2.961910	-6.855303
H	2.660307	-4.862346	-5.360255
H	3.153212	-4.447201	-2.968486
H	2.361556	-0.256666	-3.542838
C	-1.495043	-2.207690	-5.278557
C	-2.785912	-2.276383	-5.803732
C	-3.851947	-2.608139	-4.964747
C	-3.622423	-2.880791	-3.620825
C	-2.322555	-2.827790	-3.075407
C	-1.261059	-2.475530	-3.932202
H	-0.658287	-1.933502	-5.913536
H	-2.961910	-2.068156	-6.855303
H	-4.862346	-2.660307	-5.360255
H	-4.447201	-3.153212	-2.968486
H	-0.256666	-2.361556	-3.542838
C	-1.495043	2.207690	5.278557
C	-2.785912	2.276383	5.803732
C	-3.851947	2.608139	4.964747
C	-3.622423	2.880791	3.620825
C	-2.322555	2.827790	3.075407
C	-1.261059	2.475530	3.932202
H	-0.658287	1.933502	5.913536
H	-2.961910	2.068156	6.855303
H	-4.862346	2.660307	5.360255
H	-4.447201	3.153212	2.968486
H	-0.256666	2.361556	3.542838
C	2.608139	3.851947	4.964747
C	2.276383	2.785912	5.803732
C	2.207690	1.495043	5.278557
C	2.475530	1.261059	3.932202
C	2.827790	2.322555	3.075407
C	2.880791	3.622423	3.620825
H	2.660307	4.862346	5.360255
H	2.068156	2.961910	6.855303
H	1.933502	0.658287	5.913536
H	2.361556	0.256666	3.542838
H	3.153212	4.447201	2.968486
C	3.851947	-2.608139	4.964747
C	2.785912	-2.276383	5.803732
C	1.495043	-2.207690	5.278557
C	1.261059	-2.475530	3.932202
C	2.322555	-2.827790	3.075407
C	3.622423	-2.880791	3.620825
H	4.862346	-2.660307	5.360255
H	2.961910	-2.068156	6.855303
H	0.658287	-1.933502	5.913536
H	0.256666	-2.361556	3.542838
H	4.447201	-3.153212	2.968486
C	-2.608139	-3.851947	4.964747
C	-2.276383	-2.785912	5.803732
C	-2.207690	-1.495043	5.278557
C	-2.475530	-1.261059	3.932202
C	-2.827790	-2.322555	3.075407
C	-2.880791	-3.622423	3.620825
H	-2.660307	-4.862346	5.360255
H	-2.068156	-2.961910	6.855303
H	-1.933502	-0.658287	5.913536
H	-2.361556	-0.256666	3.542838
H	-3.152761	-4.445291	2.967677

Table S 106. Coordinates of the calculated structure of the open-shell singlet of 13_4 (n=4) (TDDFT, BP86-D3/def2-TZVP) in D_4 geometry.

	x	y	z
C	3.657567	-1.031589	-0.963206

C	3.663159	-1.314118	0.479749
C	3.817730	0.280260	-1.416936
C	3.663159	1.314118	-0.479749
C	3.657567	1.031589	0.963206
C	3.817730	-0.280260	1.416936
C	3.075797	-2.157755	-1.666777
C	3.028345	-2.582395	0.660287
C	2.582395	-3.028345	-0.660287
C	2.157755	-3.075797	1.666777
C	1.314118	-3.663159	-0.479749
C	1.031589	-3.657567	0.963206
C	0.280260	-3.817730	-1.416936
C	-0.280260	-3.817730	1.416936
C	-1.031589	-3.657567	-0.963206
C	-1.314118	-3.663159	0.479749
C	-2.582395	-3.028345	0.660287
C	-2.157755	-3.075797	-1.666777
C	-3.028345	-2.582395	-0.660287
C	-3.075797	-2.157755	1.666777
C	-3.663159	-1.314118	-0.479749
C	-3.657567	-1.031589	0.963206
C	-3.817730	-0.280260	-1.416936
C	-3.817730	0.280260	1.416936
C	-3.663159	1.314118	0.479749
C	-3.657567	1.031589	-0.963206
C	-3.075797	2.157755	-1.666777
C	-3.028345	2.582395	0.660287
C	-2.582395	3.028345	-0.660287
C	-2.157755	3.075797	1.666777
C	-1.031589	3.657567	0.963206
C	-1.314118	3.663159	-0.479749
C	0.280260	3.817730	1.416936
C	-0.280260	3.817730	-1.416936
C	1.031589	3.657567	-0.963206
C	1.314118	3.663159	0.479749
C	2.157755	3.075797	-1.666777
C	2.582395	3.028345	0.660287
C	3.028345	2.582395	-0.660287
C	3.075797	2.157755	1.666777
H	-3.815379	0.512440	2.478431
H	-3.815379	-0.512440	-2.478431
H	-0.512440	-3.815379	2.478431
H	0.512440	-3.815379	-2.478431
H	3.815379	-0.512440	2.478431
H	3.815379	0.512440	-2.478431
H	0.512440	3.815379	2.478431
H	-0.512440	3.815379	-2.478431
C	-2.158464	1.449428	-5.279401
C	-2.179953	2.741013	-5.813069
C	-2.488414	3.821946	-4.980044
C	-2.790640	3.607079	-3.639350
C	-2.789215	2.305664	-3.084209
C	-2.452857	1.228581	-3.936332
H	-1.898166	0.596640	-5.906392
H	-1.951427	2.906736	-6.866361
H	-2.502823	4.836012	-5.381205
H	-3.052590	4.447173	-2.994712
H	-2.363885	0.218806	-3.541789
C	3.821946	2.488414	-4.980044
C	2.741013	2.179953	-5.813069
C	1.449428	2.158464	-5.279401
C	1.228581	2.452857	-3.936332
C	2.305664	2.789215	-3.084209
C	3.607079	2.790640	-3.639350
H	4.836012	2.502823	-5.381205
H	2.906736	1.951427	-6.866361
H	0.596640	1.898166	-5.906392
H	0.218806	2.363885	-3.541789
H	4.447173	3.052590	-2.994712
C	2.158464	-1.449428	-5.279401
C	2.179953	-2.741013	-5.813069
C	2.488414	-3.821946	-4.980044
C	2.790640	-3.607079	-3.639350
C	2.789215	-2.305664	-3.084209
C	2.452857	-1.228581	-3.936332
H	1.898166	-0.596640	-5.906392
H	1.951427	-2.906736	-6.866361
H	2.502823	-4.836012	-5.381205
H	3.052590	-4.447173	-2.994712
H	2.363885	-0.218806	-3.541789
C	-1.449428	-2.158464	-5.279401
C	-2.741013	-2.179953	-5.813069
C	-3.821946	-2.488414	-4.980044
C	-3.607079	-2.790640	-3.639350
C	-2.305664	-2.789215	-3.084209
C	-1.228581	-2.452857	-3.936332
H	-0.596640	-1.898166	-5.906392
H	-2.906736	-1.951427	-6.866361

H	-4.836012	-2.502823	-5.381205
H	-4.447173	-3.052590	-2.994712
H	-0.218806	-2.363885	-3.541789
C	-1.449428	2.158464	5.279401
C	-2.741013	2.179953	5.813069
C	-3.821946	2.488414	4.980044
C	-3.607079	2.790640	3.639350
C	-2.305664	2.789215	3.084209
C	-1.228581	2.452857	3.936332
H	-0.596640	1.898166	5.906392
H	-2.906736	1.951427	6.866361
H	-4.836012	2.502823	5.381205
H	-4.447173	3.052590	2.994712
H	-0.218806	2.363885	3.541789
C	2.488414	3.821946	4.980044
C	2.179953	2.741013	5.813069
C	2.158464	1.449428	5.279401
C	2.452857	1.228581	3.936332
C	2.789215	2.305664	3.084209
C	2.790640	3.607079	3.639350
H	2.502823	4.836012	5.381205
H	1.951427	2.906736	6.866361
H	1.898166	0.596640	5.906392
H	2.363885	0.218806	3.541789

H	3.052590	4.447173	2.994712
C	3.821946	-2.488414	4.980044
C	2.741013	-2.179953	5.813069
C	1.449428	-2.158464	5.279401
C	1.228581	-2.452857	3.936332
C	2.305664	-2.789215	3.084209
C	3.607079	-2.790640	3.639350
H	4.836012	-2.502823	5.381205
H	2.906736	-1.951427	6.866361
H	0.596640	-1.898166	5.906392
H	0.218806	-2.363885	3.541789
H	4.447173	-3.052590	2.994712
C	-2.488414	-3.821946	4.980044
C	-2.179953	-2.741013	5.813069
C	-2.158464	-1.449428	5.279401
C	-2.452857	-1.228581	3.936332
C	-2.789215	-2.305664	3.084209
C	-2.790640	-3.607079	3.639350
H	-2.502823	-4.836012	5.381205
H	-1.951427	-2.906736	6.866361
H	-1.898166	-0.596640	5.906392
H	-2.363885	-0.218806	3.541789
H	-3.052590	-4.447173	2.994712

Table S 107. Coordinates of the calculated structure of 13_5 (n=5) (TPSS-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	1.223862	5.303935	3.704670
C	0.866476	5.252575	5.048223
C	1.033481	4.070467	5.772320
C	1.551430	2.940623	5.137545
C	1.912533	2.988431	3.793435
C	1.758555	4.175887	3.052530
C	2.073056	4.262833	1.626660
C	3.191869	3.610030	0.920522
C	3.049585	3.836836	-0.486232
C	1.820408	4.608619	-0.659637
C	1.236137	4.798461	0.659637
C	4.057567	2.621751	1.405671
C	4.591421	1.714680	0.486232
C	4.419684	1.920087	-0.920522
C	3.747291	3.048810	-1.405671
C	4.694804	0.654305	-1.626660

C	4.945595	-0.307169	-0.659637
C	4.945595	0.307169	0.659637
C	4.694804	-0.654305	1.626660
C	4.419684	-1.920087	0.920522
C	4.591421	-1.714680	-0.486232
C	4.057567	-2.621751	-1.405671
C	3.191869	-3.610030	-0.920522
C	3.049585	-3.836836	0.486232
C	3.747291	-3.048810	1.405671
C	2.073056	-4.262833	-1.626660
C	1.236137	-4.798461	-0.659637
C	1.820408	-4.608619	0.659637
C	-0.211930	-4.896566	-0.486232
C	-0.460354	-4.796709	0.920522
C	0.828493	-4.667216	1.626660
C	-1.741614	-4.506019	1.405671
C	-2.706674	-4.085975	0.486232

C	-2.447001	-4.151209	-0.920522
C	-1.239577	-4.669141	-1.405671
C	-3.413586	-3.288881	-1.626660
C	-4.181620	-2.658442	-0.659637
C	-3.820520	-3.155453	0.659637
C	-4.722401	-1.311564	-0.486232
C	-4.704199	-1.044442	0.920522
C	-4.182767	-2.230193	1.626660
C	-4.823667	0.263937	1.405671
C	-4.722401	1.311564	0.486232
C	-4.704199	1.044442	-0.920522
C	-4.823667	-0.263937	-1.405671
C	-4.182767	2.230193	-1.626660
C	-3.820520	3.155453	-0.659637
C	-4.181620	2.658442	0.659637
C	-3.413586	3.288881	1.626660
C	-2.447001	4.151209	0.920522
C	-2.706674	4.085975	-0.486232
C	-1.239577	4.669141	1.405671
C	-0.211930	4.896566	0.486232
C	-0.460354	4.796709	-0.920522
C	-1.741614	4.506019	-1.405671
C	0.828493	4.667216	-1.626660
C	4.514928	-0.382066	3.052530
C	5.422536	0.475044	3.704670
C	5.263252	0.799067	5.048223
C	4.190607	0.274944	5.772320
C	3.276117	-0.566796	5.137545
C	3.433172	-0.895451	3.793435
C	1.758555	-4.175887	-3.052530
C	1.223862	-5.303935	-3.704670
C	0.866476	-5.252575	-5.048223
C	1.033481	-4.070467	-5.772320
C	1.551430	-2.940623	-5.137545
C	1.912533	-2.988431	-3.793435
C	1.031824	-4.412016	3.052530
C	0.209284	-3.541850	3.793435
C	0.473321	-3.290921	5.137545
C	1.556457	-3.900542	5.772320
C	2.386392	-4.758725	5.048223
C	2.127450	-5.010342	3.704670
C	-3.428081	-2.962906	-3.052530
C	-2.251161	-2.742403	-3.793435
C	-2.317280	-2.384200	-5.137545

C	-3.551881	-2.240742	-5.772320
C	-4.727740	-2.447203	-5.048223
C	-4.666148	-2.802968	-3.704670
C	-3.877226	-2.344711	3.052530
C	-3.303828	-1.293532	3.793435
C	-2.983588	-1.467106	5.137545
C	-3.228664	-2.685612	5.772320
C	-3.788380	-3.740121	5.048223
C	-4.107700	-3.571606	3.704670
C	-3.877226	2.344711	-3.052530
C	-3.303828	1.293532	-3.793435
C	-2.983588	1.467106	-5.137545
C	-3.228664	2.685612	-5.772320
C	-3.788380	3.740121	-5.048223
C	-4.107700	3.571606	-3.704670
C	-3.428081	2.962906	3.052530
C	-4.666148	2.802968	3.704670
C	-4.727740	2.447203	5.048223
C	-3.551881	2.240742	5.772320
C	-2.317280	2.384200	5.137545
C	-2.251161	2.742403	3.793435
C	4.514928	0.382066	-3.052530
C	3.433172	0.895451	-3.793435
C	3.276117	0.566796	-5.137545
C	4.190607	-0.274944	-5.772320
C	5.263252	-0.799067	-5.048223
C	5.422536	-0.475044	-3.704670
C	1.031824	4.412016	-3.052530
C	2.127450	5.010342	-3.704670
C	2.386392	4.758725	-5.048223
C	1.556457	3.900542	-5.772320
C	0.473321	3.290921	-5.137545
C	0.209284	3.541850	-3.793435
H	-4.805118	0.466134	2.470116
H	-4.805118	-0.466134	-2.470116
H	-1.928183	-4.425896	2.470116
H	-1.041544	-4.713982	-2.470116
H	3.613436	-3.201488	2.470116
H	4.161409	-2.447268	-2.470116
H	-1.041544	4.713982	2.470116
H	-1.928183	4.425896	-2.470116
H	4.161409	2.447268	2.470116
H	3.613436	3.201488	-2.470116
H	-3.979107	4.693635	-5.532336

H	-2.981474	2.815553	-6.822179
H	-2.536886	0.643030	-5.685449
H	-3.070059	0.352434	-3.308625
H	-4.553417	4.385312	-3.139691
H	-0.172383	2.611429	-5.685449
H	1.756424	3.705604	-6.822179
H	3.234300	5.234769	-5.532336
H	2.763596	5.685693	-3.139691
H	-0.613516	3.028708	-3.308625
H	5.978015	-1.458369	-5.532336
H	4.067004	-0.525364	-6.822179
H	2.430347	0.970922	-5.685449
H	2.690886	1.519410	-3.308625
H	6.261413	-0.871360	-3.139691
H	1.674421	-2.011366	-5.685449
H	0.757123	-4.030297	-6.822179
H	0.460316	-6.136091	-5.532336
H	1.106170	-6.224223	-3.139691
H	2.276575	-2.089661	-3.308625
H	-5.693524	-2.333943	-5.532336
H	-3.599077	-1.965497	-6.822179
H	-1.395498	-2.214015	-5.685449
H	-1.283886	-2.810892	-3.308625
H	-5.577763	-2.975421	-3.139691
H	2.430347	-0.970922	5.685449
H	4.067004	0.525364	6.822179
H	5.978015	1.458369	5.532336
H	6.261413	0.871360	3.139691
H	2.690886	-1.519410	3.308625
H	3.234300	-5.234769	5.532336
H	1.756424	-3.705604	6.822179
H	-0.172383	-2.611429	5.685449
H	-0.613516	-3.028708	3.308625
H	2.763596	-5.685693	3.139691
H	-3.979107	-4.693635	5.532336
H	-2.981474	-2.815553	6.822179
H	-2.536886	-0.643030	5.685449
H	-3.070059	-0.352434	3.308625
H	-4.553417	-4.385312	3.139691
H	-1.395498	2.214015	5.685449
H	-3.599077	1.965497	6.822179
H	-5.693524	2.333943	5.532336
H	-5.577763	2.975421	3.139691
H	-1.283886	2.810892	3.308625
H	0.460316	6.136091	5.532336
H	0.757123	4.030297	6.822179
H	1.674421	2.011366	5.685449
H	2.276575	2.089661	3.308625
H	1.106170	6.224223	3.139691

Table S 108. Coordinates of the calculated structure of the triplet of 13_5 (n=5) (TPSS-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	1.2257582	5.3100761	3.7036598
C	0.8667659	5.2717668	5.0470673
C	1.0365005	4.0980386	5.7844046
C	1.5600691	2.963756	5.1623366
C	1.9218343	2.9983919	3.817927
C	1.7651155	4.1771359	3.0633331
C	2.0777612	4.2486297	1.6364811
C	3.1765474	3.5957727	0.9334322
C	3.0298914	3.8231335	-0.4895921
C	1.814769	4.5912615	-0.6606581
C	1.2304968	4.7811031	0.6606581
C	4.045205	2.6078729	1.4115681
C	4.572304	1.7001847	0.4895921
C	4.4013901	1.9099212	-0.9334322
C	3.7302716	3.0413415	-1.4115681
C	4.6827505	0.6631695	-1.6364811
C	4.9273437	-0.3071701	-0.6606581
C	4.9273437	0.3071701	0.6606581
C	4.6827505	-0.6631695	1.6364811
C	4.4013901	-1.9099212	0.9334322
C	4.572304	-1.7001847	-0.4895921
C	4.045205	-2.6078729	-1.4115681
C	3.1765474	-3.5957727	-0.9334322
C	3.0298914	-3.8231335	0.4895921
C	3.7302716	-3.0413415	1.4115681
C	2.0777612	-4.2486297	-1.6364811
C	1.2304968	-4.7811031	-0.6606581
C	1.814769	-4.5912615	0.6606581
C	-0.2040521	-4.8739055	-0.4895921
C	-0.4563387	-4.7761689	0.9334322
C	0.8163378	-4.658491	1.6364811

C	-1.7397704	-4.4875254	1.4115681
C	-2.6997281	-4.0630112	0.4895921
C	-2.4381759	-4.132231	-0.9334322
C	-1.2301974	-4.6530956	-1.4115681
C	-3.3986235	-3.2889671	-1.6364811
C	-4.1668548	-2.6477141	-0.6606581
C	-3.8057547	-3.1447258	0.6606581
C	-4.6984151	-1.3120545	-0.4895921
C	-4.683423	-1.0419135	0.9334322
C	-4.178226	-2.2159363	1.6364811
C	-4.8055088	0.2678983	1.4115681
C	-4.6984151	1.3120545	0.4895921
C	-4.683423	1.0419135	-0.9334322
C	-4.8055088	-0.2678983	-1.4115681
C	-4.178226	2.2159363	-1.6364811
C	-3.8057547	3.1447258	-0.6606581
C	-4.1668548	2.6477141	0.6606581
C	-3.3986235	3.2889671	1.6364811
C	-2.4381759	4.132231	0.9334322
C	-2.6997281	4.0630112	-0.4895921
C	-1.2301974	4.6530956	1.4115681
C	-0.2040521	4.8739055	0.4895921
C	-0.4563387	4.7761689	-0.9334322
C	-1.7397704	4.4875254	-1.4115681
C	0.8163378	4.658491	-1.6364811
C	4.518143	-0.3879186	3.0633331
C	5.4289626	0.4751384	3.7036598
C	5.2815935	0.8047222	5.0470673
C	4.2177626	0.2805931	5.7844046
C	3.3007873	-0.5678629	5.1623366
C	3.4455196	-0.901219	3.817927
C	1.7651155	-4.1771359	-3.0633331
C	1.2257582	-5.3100761	-3.7036598
C	0.8667659	-5.2717668	-5.0470673
C	1.0365005	-4.0980386	-5.7844046
C	1.5600691	-2.963756	-5.1623366
C	1.9218343	-2.9983919	-3.817927
C	1.0272505	-4.4168828	3.0633331
C	0.2076139	-3.5553759	3.817927
C	0.4799296	-3.3147146	5.1623366
C	1.5702202	-3.9246226	5.7844046
C	2.3974384	-4.7744211	5.0470673
C	2.1295252	-5.0164244	3.7036598
C	-3.4272417	-2.9695306	-3.0633331

C	-2.2577607	-2.7543271	-3.817927
C	-2.3366116	-2.3995649	-5.1623366
C	-3.5771701	-2.2521341	-5.7844046
C	-4.7459028	-2.4534088	-5.0470673
C	-4.6714024	-2.8066691	-3.7036598
C	-3.8832673	-2.3418651	3.0633331
C	-3.3172072	-1.2961241	3.817927
C	-3.0041745	-1.4807433	5.1623366
C	-3.2473132	-2.7061432	5.7844046
C	-3.7998951	-3.7554767	5.0470673
C	-4.1128437	-3.5754592	3.7036598
C	-3.8832673	2.3418651	-3.0633331
C	-3.3172072	1.2961241	-3.817927
C	-3.0041745	1.4807433	-5.1623366
C	-3.2473132	2.7061432	-5.7844046
C	-3.7998951	3.7554767	-5.0470673
C	-4.1128437	3.5754592	-3.7036598
C	-3.4272417	2.9695306	3.0633331
C	-4.6714024	2.8066691	3.7036598
C	-4.7459028	2.4534088	5.0470673
C	-3.5771701	2.2521341	5.7844046
C	-2.3366116	2.3995649	5.1623366
C	-2.2577607	2.7543271	3.817927
C	4.518143	0.3879186	-3.0633331
C	3.4455196	0.901219	-3.817927
C	3.3007873	0.5678629	-5.1623366
C	4.2177626	-0.2805931	-5.7844046
C	5.2815935	-0.8047222	-5.0470673
C	5.4289626	-0.4751384	-3.7036598
C	1.0272505	4.4168828	-3.0633331
C	2.1295252	5.0164244	-3.7036598
C	2.3974384	4.7744211	-5.0470673
C	1.5702202	3.9246226	-5.7844046
C	0.4799296	3.3147146	-5.1623366
C	0.2076139	3.5553759	-3.817927
H	-4.7919129	0.4750594	2.4750622
H	-4.7919129	-0.4750594	-2.4750622
H	-1.9325909	-4.4105785	2.4750622
H	-1.0289742	-4.7041814	-2.4750622
H	3.597506	-3.2009469	2.4750622
H	4.1559719	-2.4322846	-2.4750622
H	-1.0289742	4.7041814	2.4750622
H	-1.9325909	4.4105785	-2.4750622
H	4.1559719	2.4322846	2.4750622

H	3.597506	3.2009469	-2.4750622
H	-3.9894455	4.714392	-5.5209477
H	-3.003745	2.8456756	-6.8338516
H	-2.5626604	0.6602884	-5.7198983
H	-3.0817281	0.3502078	-3.3433452
H	-4.5516171	4.3864529	-3.1292547
H	-0.1639341	2.6412752	-5.7198983
H	1.7781901	3.7360934	-6.8338516
H	3.2508468	5.2510154	-5.5209477
H	2.7652376	5.6843336	-3.1292547
H	-0.6192389	3.0391177	-3.3433452
H	5.9985793	-1.469086	-5.5209477
H	4.1027269	-0.5366429	-6.8338516
H	2.4613435	0.9721095	-5.7198983
H	2.6990174	1.5280702	-3.3433452
H	6.2606279	-0.8733415	-3.1292547
H	1.685128	-2.0404785	-5.7198983
H	0.7574346	-4.067757	-6.8338516
H	0.4564791	-6.1589605	-5.5209477
H	1.1040433	-6.2240884	-3.1292547
H	2.2873234	-2.0947184	-3.3433452
H	-5.7164597	-2.3373609	-5.5209477
H	-3.6346066	-1.9773692	-6.8338516
H	-1.4198771	-2.2331945	-5.7198983
H	-1.2853738	-2.8226774	-3.3433452
H	-5.5782917	-2.9733566	-3.1292547

H	2.4613435	-0.9721095	5.7198983
H	4.1027269	0.5366429	6.8338516
H	5.9985793	1.469086	5.5209477
H	6.2606279	0.8733415	3.1292547
H	2.6990174	-1.5280702	3.3433452
H	3.2508468	-5.2510154	5.5209477
H	1.7781901	-3.7360934	6.8338516
H	-0.1639341	-2.6412752	5.7198983
H	-0.6192389	-3.0391177	3.3433452
H	2.7652376	-5.6843336	3.1292547
H	-3.9894455	-4.714392	5.5209477
H	-3.003745	-2.8456756	6.8338516
H	-2.5626604	-0.6602884	5.7198983
H	-3.0817281	-0.3502078	3.3433452
H	-4.5516171	-4.3864529	3.1292547
H	-1.4198771	2.2331945	5.7198983
H	-3.6346066	1.9773692	6.8338516
H	-5.7164597	2.3373609	5.5209477
H	-5.5782917	2.9733566	3.1292547
H	-1.2853738	2.8226774	3.3433452
H	0.4564791	6.1589605	5.5209477
H	0.7574346	4.067757	6.8338516
H	1.685128	2.0404785	5.7198983
H	2.2873234	2.0947184	3.3433452
H	1.1040433	6.2240884	3.1292547

Table S 109. Coordinates of the calculated structure of the open-shell singlet of 13_5 (n=5) (TDDFT, BP86-D3/def2-TZVP) in D_5 geometry.

	x	y	z
C	1.183540	5.237070	3.723044
C	0.787664	5.150437	5.055238
C	0.932096	3.947524	5.752711
C	1.467517	2.833368	5.101719
C	1.865686	2.915454	3.768455
C	1.733996	4.124324	3.053844
C	2.072404	4.239188	1.637238
C	3.175450	3.593307	0.935458
C	3.030949	3.826807	-0.489970
C	1.819598	4.600879	-0.661486
C	1.232243	4.791722	0.661486
C	4.045470	2.605600	1.413522
C	4.576125	1.700056	0.489970
C	4.398706	1.909640	-0.935458

C	3.728192	3.042296	-1.413522
C	4.672116	0.660993	-1.637238
C	4.937983	-0.308791	-0.661486
C	4.937983	0.308791	0.661486
C	4.672116	-0.660993	1.637238
C	4.398706	-1.909640	0.935458
C	4.576125	-1.700056	-0.489970
C	4.045470	-2.605600	-1.413522
C	3.175450	-3.593307	-0.935458
C	3.030949	-3.826807	0.489970
C	3.728192	-3.042296	1.413522
C	2.072404	-4.239188	-1.637238
C	1.232243	-4.791722	-0.661486
C	1.819598	-4.600879	0.661486
C	-0.202749	-4.877499	-0.489970

C	-0.456901	-4.773529	0.935458
C	0.815122	-4.647704	1.637238
C	-1.741321	-4.485843	1.413522
C	-2.702895	-4.065153	0.489970
C	-2.436170	-4.130426	-0.935458
C	-1.227954	-4.652646	-1.413522
C	-3.391300	-3.280955	-1.637238
C	-4.176415	-2.652657	-0.661486
C	-3.813409	-3.152290	0.661486
C	-4.701430	-1.314405	-0.489970
C	-4.681086	-1.040563	0.935458
C	-4.168343	-2.211447	1.637238
C	-4.804388	0.269893	1.413522
C	-4.701430	1.314405	0.489970
C	-4.681086	1.040563	-0.935458
C	-4.804388	-0.269893	-1.413522
C	-4.168343	2.211447	-1.637238
C	-3.813409	3.152290	-0.661486
C	-4.176415	2.652657	0.661486
C	-3.391300	3.280955	1.637238
C	-2.436170	4.130426	0.935458
C	-2.702895	4.065153	-0.489970
C	-1.227954	4.652646	1.413522
C	-0.202749	4.877499	0.489970
C	-0.456901	4.773529	-0.935458
C	-1.741321	4.485843	-1.413522
C	0.815122	4.647704	-1.637238
C	4.458300	-0.374642	3.053844
C	5.346484	0.492730	3.723044
C	5.141759	0.842460	5.055238
C	4.042352	0.333376	5.752711
C	3.148181	-0.520133	5.101719
C	3.349290	-0.873448	3.768455
C	1.733996	-4.124324	-3.053844
C	1.183540	-5.237070	-3.723044
C	0.787664	-5.150437	-5.055238
C	0.932096	-3.947524	-5.752711
C	1.467517	-2.833368	-5.101719
C	1.865686	-2.915454	-3.768455
C	1.021385	-4.355865	3.053844
C	0.204289	-3.455275	3.768455
C	0.478165	-3.154828	5.101719
C	1.566215	-3.741486	5.752711
C	2.390118	-4.629769	5.055238

C	2.120769	-4.932546	3.723044
C	-3.386631	-2.923614	-3.053844
C	-2.196233	-2.675298	-3.768455
C	-2.241205	-2.271251	-5.101719
C	-3.466285	-2.106328	-5.752711
C	-4.654955	-2.340686	-5.055238
C	-4.615016	-2.743957	-3.723044
C	-3.827049	-2.317431	3.053844
C	-3.223033	-1.262029	3.768455
C	-2.852659	-1.429658	5.101719
C	-3.074378	-2.645741	5.752711
C	-3.664585	-3.703814	5.055238
C	-4.035777	-3.541211	3.723044
C	-3.827049	2.317431	-3.053844
C	-3.223033	1.262029	-3.768455
C	-2.852659	1.429658	-5.101719
C	-3.074378	2.645741	-5.752711
C	-3.664585	3.703814	-5.055238
C	-4.035777	3.541211	-3.723044
C	-3.386631	2.923614	3.053844
C	-4.615016	2.743957	3.723044
C	-4.654955	2.340686	5.055238
C	-3.466285	2.106328	5.752711
C	-2.241205	2.271251	5.101719
C	-2.196233	2.675298	3.768455
C	4.458300	0.374642	-3.053844
C	3.349290	0.873448	-3.768455
C	3.148181	0.520133	-5.101719
C	4.042352	-0.333376	-5.752711
C	5.141759	-0.842460	-5.055238
C	5.346484	-0.492730	-3.723044
C	1.021385	4.355865	-3.053844
C	2.120769	4.932546	-3.723044
C	2.390118	4.629769	-5.055238
C	1.566215	3.741486	-5.752711
C	0.478165	3.154828	-5.101719
C	0.204289	3.455275	-3.768455
H	-4.786974	0.477565	2.481706
H	-4.786974	-0.477565	-2.481706
H	-1.933448	-4.405107	2.481706
H	-1.025065	-4.700258	-2.481706
H	3.592037	-3.200071	2.481706
H	4.153449	-2.427354	-2.481706
H	-1.025065	4.700258	2.481706

H	-1.933448	4.405107	-2.481706
H	4.153449	2.427354	2.481706
H	3.592037	3.200071	-2.481706
H	-3.838384	4.658431	-5.552989
H	-2.784492	2.772219	-6.796399
H	-2.382551	0.598902	-5.627714
H	-3.002271	0.319923	-3.268836
H	-4.505271	4.360893	-3.177670
H	-0.166659	2.451012	-5.627714
H	1.776082	3.504872	-6.796399
H	3.244305	5.090055	-5.552989
H	2.755250	5.632357	-3.177670
H	-0.623488	2.954191	-3.268836
H	5.843475	-1.512604	-5.552989
H	3.882171	-0.606089	-6.796399
H	2.279550	0.915906	-5.627714
H	2.616934	1.505867	-3.268836
H	6.208109	-0.879905	-3.177670
H	1.575499	-1.884950	-5.627714
H	0.623232	-3.879456	-6.796399
H	0.367161	-6.024895	-5.552989
H	1.081572	-6.176168	-3.177670
H	2.240842	-2.023514	-3.268836
H	-5.616557	-2.210986	-5.552989
H	-3.496993	-1.791546	-6.796399
H	-1.305839	-2.080870	-5.627714
H	-1.232018	-2.756467	-3.268836
H	-5.539661	-2.937177	-3.177670
H	2.279550	-0.915906	5.627714
H	3.882171	0.606089	6.796399
H	5.843475	1.512604	5.552989
H	6.208109	0.879905	3.177670
H	2.616934	-1.505867	3.268836
H	3.244305	-5.090055	5.552989
H	1.776082	-3.504872	6.796399
H	-0.166659	-2.451012	5.627714
H	-0.623488	-2.954191	3.268836
H	2.755250	-5.632357	3.177670
H	-3.838384	-4.658431	5.552989
H	-2.784492	-2.772219	6.796399
H	-2.382551	-0.598902	5.627714
H	-3.002271	-0.319923	3.268836
H	-4.505271	-4.360893	3.177670
H	-1.305839	2.080870	5.627714
H	-3.496993	1.791546	6.796399
H	-5.616557	2.210986	5.552989
H	-5.539661	2.937177	3.177670
H	-1.232018	2.756467	3.268836
H	0.367161	6.024895	5.552989
H	0.623232	3.879456	6.796399
H	1.575499	1.884950	5.627714
H	2.240842	2.023514	3.268836
H	1.081572	6.176168	3.177670

Table S 110. Coordinates of the calculated structure of 13_6 (n=6) (TPSS-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-6.333831	-0.465887	3.733880
C	-6.146207	-0.783692	5.075351
C	-5.079944	-0.227708	5.785671
C	-4.203725	0.646226	5.140288
C	-4.389692	0.967589	3.797979
C	-5.461149	0.416724	3.068972
C	-5.645252	0.677962	1.641227
C	-5.864072	-0.306293	0.662735
C	-5.864072	0.306293	-0.662735
C	-5.561162	1.696563	-0.497137
C	-5.411974	1.920357	0.940166
C	-5.645252	-0.677962	-1.641227
C	-5.411974	-1.920357	-0.940166
C	-5.561162	-1.696563	0.497137
C	-4.848527	-3.106032	-1.418350
C	-4.249847	-3.967826	-0.497137
C	-4.369065	-3.726728	0.940166
C	-5.114166	-2.645932	1.418350
C	-3.197293	-4.925289	-0.662735
C	-2.666779	-5.231581	0.662735
C	-3.409759	-4.549951	1.641227
C	-1.311314	-5.664389	0.497137
C	-1.042909	-5.647085	-0.940166
C	-2.235494	-5.227913	-1.641227
C	-4.848527	3.106032	1.418350
C	-4.249847	3.967826	0.497137
C	-4.369065	3.726728	-0.940166

C	-5.114166	2.645932	-1.418350
C	-3.409759	4.549951	-1.641227
C	-2.666779	5.231581	-0.662735
C	-3.197293	4.925289	0.662735
C	-1.311314	5.664389	-0.497137
C	-1.042909	5.647085	0.940166
C	-2.235494	5.227913	1.641227
C	0.265639	5.751964	1.418350
C	1.311314	5.664389	0.497137
C	1.042909	5.647085	-0.940166
C	-0.265639	5.751964	-1.418350
C	2.235494	5.227913	-1.641227
C	3.197293	4.925289	-0.662735
C	2.666779	5.231581	0.662735
C	3.409759	4.549951	1.641227
C	4.369065	3.726728	0.940166
C	4.249847	3.967826	-0.497137
C	5.114166	2.645932	1.418350
C	5.561162	1.696563	0.497137
C	5.411974	1.920357	-0.940166
C	4.848527	3.106032	-1.418350
C	5.864072	0.306293	0.662735
C	5.864072	-0.306293	-0.662735
C	5.645252	0.677962	-1.641227
C	0.265639	-5.751964	-1.418350
C	1.311314	-5.664389	-0.497137
C	1.042909	-5.647085	0.940166
C	-0.265639	-5.751964	1.418350
C	2.235494	-5.227913	1.641227
C	3.197293	-4.925289	0.662735
C	2.666779	-5.231581	-0.662735
C	4.249847	-3.967826	0.497137
C	4.369065	-3.726728	-0.940166
C	3.409759	-4.549951	-1.641227
C	5.114166	-2.645932	-1.418350
C	5.561162	-1.696563	-0.497137
C	5.411974	-1.920357	0.940166
C	4.848527	-3.106032	1.418350
C	5.645252	-0.677962	1.641227
C	-3.091468	-4.521132	3.068972
C	-3.032803	-3.317791	3.797979
C	-2.661511	-3.317420	5.140288
C	-2.342771	-4.513215	5.785671
C	-2.394407	-5.714617	5.075351

C	-2.763445	-5.718203	3.733880
C	-5.461149	-0.416724	-3.068972
C	-4.389692	-0.967589	-3.797979
C	-4.203725	-0.646226	-5.140288
C	-5.079944	0.227708	-5.785671
C	-6.146207	0.783692	-5.075351
C	-6.333831	0.465887	-3.733880
C	-3.091468	4.521132	-3.068972
C	-3.032803	3.317791	-3.797979
C	-2.661511	3.317420	-5.140288
C	-2.342771	4.513215	-5.785671
C	-2.394407	5.714617	-5.075351
C	-2.763445	5.718203	-3.733880
C	-2.369681	4.937856	3.068972
C	-1.356890	4.285380	3.797979
C	-1.542215	3.963646	5.140288
C	-2.737173	4.285507	5.785671
C	-3.751800	4.930926	5.075351
C	-3.570386	5.252315	3.733880
C	2.369681	4.937856	-3.068972
C	1.356890	4.285380	-3.797979
C	1.542215	3.963646	-5.140288
C	2.737173	4.285507	-5.785671
C	3.751800	4.930926	-5.075351
C	3.570386	5.252315	-3.733880
C	3.091468	4.521132	3.068972
C	3.032803	3.317791	3.797979
C	2.661511	3.317420	5.140288
C	2.342771	4.513215	5.785671
C	2.394407	5.714617	5.075351
C	2.763445	5.718203	3.733880
C	-2.369681	-4.937856	-3.068972
C	-1.356890	-4.285380	-3.797979
C	-1.542215	-3.963646	-5.140288
C	-2.737173	-4.285507	-5.785671
C	-3.751800	-4.930926	-5.075351
C	-3.570386	-5.252315	-3.733880
C	2.369681	-4.937856	3.068972
C	1.356890	-4.285380	3.797979
C	1.542215	-3.963646	5.140288
C	2.737173	-4.285507	5.785671
C	3.751800	-4.930926	5.075351
C	3.570386	-5.252315	3.733880
C	5.461149	0.416724	-3.068972

C	4.389692	0.967589	-3.797979
C	4.203725	0.646226	-5.140288
C	5.079944	-0.227708	-5.785671
C	6.146207	-0.783692	-5.075351
C	6.333831	-0.465887	-3.733880
C	3.091468	-4.521132	-3.068972
C	3.032803	-3.317791	-3.797979
C	2.661511	-3.317420	-5.140288
C	2.342771	-4.513215	-5.785671
C	2.394407	-5.714617	-5.075351
C	2.763445	-5.718203	-3.733880
C	5.461149	-0.416724	3.068972
C	4.389692	-0.967589	3.797979
C	4.203725	-0.646226	5.140288
C	5.079944	0.227708	5.785671
C	6.146207	0.783692	5.075351
C	6.333831	0.465887	3.733880
H	0.471391	5.740884	2.482385
H	-0.471391	5.740884	-2.482385
H	-4.736056	3.278678	2.482385
H	-5.207447	2.462205	-2.482385
H	-5.207447	-2.462205	2.482385
H	-4.736056	-3.278678	-2.482385
H	5.207447	2.462205	2.482385
H	4.736056	3.278678	-2.482385
H	-0.471391	-5.740884	2.482385
H	0.471391	-5.740884	-2.482385
H	4.736056	-3.278678	2.482385
H	5.207447	-2.462205	-2.482385
H	-2.146515	6.650216	-5.568577
H	-2.052624	4.510408	-6.832554
H	-2.616455	2.374900	-5.678266
H	-3.237447	2.375674	-3.301405
H	-2.811277	6.652686	-3.181745
H	4.685999	5.184044	-5.568577
H	2.879816	4.032828	-6.832554
H	0.748497	3.453366	-5.678266
H	0.438671	3.991548	-3.301405
H	4.355757	5.760980	-3.181745
H	6.832513	-1.466172	-5.568577
H	4.932440	-0.477580	-6.832554
H	3.364951	1.078466	-5.678266
H	3.676117	1.615874	-3.301405
H	7.167033	-0.891706	-3.181745

H	2.146515	-6.650216	-5.568577
H	2.052624	-4.510408	-6.832554
H	2.616455	-2.374900	-5.678266
H	3.237447	-2.375674	-3.301405
H	2.811277	-6.652686	-3.181745
H	-4.685999	-5.184044	-5.568577
H	-2.879816	-4.032828	-6.832554
H	-0.748497	-3.453366	-5.678266
H	-0.438671	-3.991548	-3.301405
H	-4.355757	-5.760980	-3.181745
H	-6.832513	1.466172	-5.568577
H	-4.932440	0.477580	-6.832554
H	-3.364951	-1.078466	-5.678266
H	-3.676117	-1.615874	-3.301405
H	-7.167033	0.891706	-3.181745
H	-4.685999	5.184044	5.568577
H	-2.879816	4.032828	6.832554
H	-0.748497	3.453366	5.678266
H	-0.438671	3.991548	3.301405
H	-4.355757	5.760980	3.181745
H	2.146515	6.650216	5.568577
H	2.052624	4.510408	6.832554
H	2.616455	2.374900	5.678266
H	3.237447	2.375674	3.301405
H	2.811277	6.652686	3.181745
H	6.832513	1.466172	5.568577
H	4.932440	0.477580	6.832554
H	3.364951	-1.078466	5.678266
H	3.676117	-1.615874	3.301405
H	7.167033	0.891706	3.181745
H	4.685999	-5.184044	5.568577
H	2.879816	-4.032828	6.832554
H	0.748497	-3.453366	5.678266
H	0.438671	-3.991548	3.301405
H	4.355757	-5.760980	3.181745
H	-2.146515	-6.650216	5.568577
H	-2.052624	-4.510408	6.832554
H	-2.616455	-2.374900	5.678266
H	-3.237447	-2.375674	3.301405
H	-2.811277	-6.652686	3.181745
H	-6.832513	-1.466172	5.568577
H	-4.932440	-0.477580	6.832554
H	-3.364951	1.078466	5.678266
H	-3.676117	1.615874	3.301405

H	-7.167033	-0.891706	3.181745

Table S 111. Coordinates of the calculated structure of the triplet of 13_6 (n=6) (TPSS-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-6.320281	-0.468910	3.735441
C	-6.116346	-0.782701	5.075520
C	-5.041347	-0.224652	5.770773
C	-4.172291	0.646681	5.112201
C	-4.375013	0.964904	3.771664
C	-5.455370	0.411590	3.057872
C	-5.657359	0.670165	1.632281
C	-5.887317	-0.305553	0.661560
C	-5.887317	0.305553	-0.661560
C	-5.581497	1.709002	-0.493744
C	-5.429568	1.928316	0.928159
C	-5.657359	-0.670165	-1.632281
C	-5.429568	-1.928316	-0.928159
C	-5.581497	-1.709002	0.493744
C	-4.866576	-3.113071	-1.412704
C	-4.270788	-3.979217	-0.493744
C	-4.384755	-3.737986	0.928159
C	-5.129286	-2.658043	1.412704
C	-3.208275	-4.945789	-0.661560
C	-2.679042	-5.251343	0.661560
C	-3.409059	-4.564335	1.632281
C	-1.310709	-5.688220	0.493744
C	-1.044813	-5.666302	-0.928159
C	-2.248300	-5.234499	-1.632281
C	-4.866576	3.113071	1.412704
C	-4.270788	3.979217	0.493744
C	-4.384755	3.737986	-0.928159
C	-5.129286	2.658043	-1.412704
C	-3.409059	4.564335	-1.632281
C	-2.679042	5.251343	-0.661560
C	-3.208275	4.945789	0.661560
C	-1.310709	5.688220	-0.493744
C	-1.044813	5.666302	0.928159
C	-2.248300	5.234499	1.632281
C	0.262711	5.771114	1.412704
C	1.310709	5.688220	0.493744
C	1.044813	5.666302	-0.928159
C	-0.262711	5.771114	-1.412704
C	2.248300	5.234499	-1.632281
C	3.208275	4.945789	-0.661560
C	2.679042	5.251343	0.661560
C	3.409059	4.564335	1.632281
C	4.384755	3.737986	0.928159
C	4.270788	3.979217	-0.493744
C	5.129286	2.658043	1.412704
C	5.581497	1.709002	0.493744
C	5.429568	1.928316	-0.928159
C	4.866576	3.113071	-1.412704
C	5.887317	0.305553	0.661560
C	5.887317	-0.305553	-0.661560
C	5.657359	0.670165	-1.632281
C	0.262711	-5.771114	-1.412704
C	1.310709	-5.688220	-0.493744
C	1.044813	-5.666302	0.928159
C	-0.262711	-5.771114	1.412704
C	2.248300	-5.234499	1.632281
C	3.208275	-4.945789	0.661560
C	2.679042	-5.251343	-0.661560
C	4.270788	-3.979217	0.493744
C	4.384755	-3.737986	-0.928159
C	3.409059	-4.564335	-1.632281
C	5.129286	-2.658043	-1.412704
C	5.581497	-1.709002	-0.493744
C	5.429568	-1.928316	0.928159
C	4.866576	-3.113071	1.412704
C	5.657359	-0.670165	1.632281
C	-3.084133	-4.518694	3.057872
C	-3.023138	-3.306420	3.771664
C	-2.646188	-3.289970	5.112201
C	-2.326119	-4.478261	5.770773
C	-2.380334	-5.688261	5.075520
C	-2.754052	-5.707978	3.735441
C	-5.455370	-0.411590	-3.057872
C	-4.375013	-0.964904	-3.771664
C	-4.172291	-0.646681	-5.112201
C	-5.041347	0.224652	-5.770773
C	-6.116346	0.782701	-5.075520
C	-6.320281	0.468910	-3.735441
C	-3.084133	4.518694	-3.057872

C	-3.023138	3.306420	-3.771664
C	-2.646188	3.289970	-5.112201
C	-2.326119	4.478261	-5.770773
C	-2.380334	5.688261	-5.075520
C	-2.754052	5.707978	-3.735441
C	-2.371238	4.930284	3.057872
C	-1.351875	4.271324	3.771664
C	-1.526104	3.936651	5.112201
C	-2.715228	4.253609	5.770773
C	-3.736012	4.905560	5.075520
C	-3.566228	5.239069	3.735441
C	2.371238	4.930284	-3.057872
C	1.351875	4.271324	-3.771664
C	1.526104	3.936651	-5.112201
C	2.715228	4.253609	-5.770773
C	3.736012	4.905560	-5.075520
C	3.566228	5.239069	-3.735441
C	3.084133	4.518694	3.057872
C	3.023138	3.306420	3.771664
C	2.646188	3.289970	5.112201
C	2.326119	4.478261	5.770773
C	2.380334	5.688261	5.075520
C	2.754052	5.707978	3.735441
C	-2.371238	-4.930284	-3.057872
C	-1.351875	-4.271324	-3.771664
C	-1.526104	-3.936651	-5.112201
C	-2.715228	-4.253609	-5.770773
C	-3.736012	-4.905560	-5.075520
C	-3.566228	-5.239069	-3.735441
C	2.371238	-4.930284	3.057872
C	1.351875	-4.271324	3.771664
C	1.526104	-3.936651	5.112201
C	2.715228	-4.253609	5.770773
C	3.736012	-4.905560	5.075520
C	3.566228	-5.239069	3.735441
C	5.455370	0.411590	-3.057872
C	4.375013	0.964904	-3.771664
C	4.172291	0.646681	-5.112201
C	5.041347	-0.224652	-5.770773
C	6.116346	-0.782701	-5.075520
C	6.320281	-0.468910	-3.735441
C	3.084133	-4.518694	-3.057872
C	3.023138	-3.306420	-3.771664
C	2.646188	-3.289970	-5.112201

C	2.326119	-4.478261	-5.770773
C	2.380334	-5.688261	-5.075520
C	2.754052	-5.707978	-3.735441
C	5.455370	-0.411590	3.057872
C	4.375013	-0.964904	3.771664
C	4.172291	-0.646681	5.112201
C	5.041347	0.224652	5.770773
C	6.116346	0.782701	5.075520
C	6.320281	0.468910	3.735441
H	0.463924	5.758400	2.477618
H	-0.463924	5.758400	-2.477618
H	-4.754959	3.280970	2.477618
H	-5.218883	2.477431	-2.477618
H	-5.218883	-2.477431	2.477618
H	-4.754959	-3.280970	-2.477618
H	5.218883	2.477431	2.477618
H	4.754959	3.280970	-2.477618
H	-0.463924	-5.758400	2.477618
H	0.463924	-5.758400	-2.477618
H	4.754959	-3.280970	2.477618
H	5.218883	-2.477431	-2.477618
H	-2.131515	6.617853	-5.579458
H	-2.033525	4.463033	-6.816887
H	-2.599499	2.341200	-5.638830
H	-3.231231	2.370762	-3.264487
H	-2.805731	6.648686	-3.194453
H	4.665472	5.154872	-5.579458
H	2.848337	3.992601	-6.816887
H	0.727789	3.421832	-5.638830
H	0.437525	3.983709	-3.264487
H	4.355065	5.754177	-3.194453
H	6.796986	-1.462981	-5.579458
H	4.881862	-0.470432	-6.816887
H	3.327288	1.080633	-5.638830
H	3.668756	1.612947	-3.264487
H	7.160796	-0.894509	-3.194453
H	2.131515	-6.617853	-5.579458
H	2.033525	-4.463033	-6.816887
H	2.599499	-2.341200	-5.638830
H	3.231231	-2.370762	-3.264487
H	2.805731	-6.648686	-3.194453
H	-4.665472	-5.154872	-5.579458
H	-2.848337	-3.992601	-6.816887
H	-0.727789	-3.421832	-5.638830

H	-0.437525	-3.983709	-3.264487
H	-4.355065	-5.754177	-3.194453
H	-6.796986	1.462981	-5.579458
H	-4.881862	0.470432	-6.816887
H	-3.327288	-1.080633	-5.638830
H	-3.668756	-1.612947	-3.264487
H	-7.160796	0.894509	-3.194453
H	-4.665472	5.154872	5.579458
H	-2.848337	3.992601	6.816887
H	-0.727789	3.421832	5.638830
H	-0.437525	3.983709	3.264487
H	-4.355065	5.754177	3.194453
H	2.131515	6.617853	5.579458
H	2.033525	4.463033	6.816887
H	2.599499	2.341200	5.638830
H	3.231231	2.370762	3.264487
H	2.805731	6.648686	3.194453
H	6.796986	1.462981	5.579458
H	4.881862	0.470432	6.816887
H	3.327288	-1.080633	5.638830
H	3.668756	-1.612947	3.264487
H	7.160796	0.894509	3.194453
H	4.665472	-5.154872	5.579458
H	2.848337	-3.992601	6.816887
H	0.727789	-3.421832	5.638830
H	0.437525	-3.983709	3.264487
H	4.355065	-5.754177	3.194453
H	-2.131515	-6.617853	5.579458
H	-2.033525	-4.463033	6.816887
H	-2.599499	-2.341200	5.638830
H	-3.231231	-2.370762	3.264487
H	-2.805731	-6.648686	3.194453
H	-6.796986	-1.462981	5.579458
H	-4.881862	-0.470432	6.816887
H	-3.327288	1.080633	5.638830
H	-3.668756	1.612947	3.264487
H	-7.160796	-0.894509	3.194453

Table S 112. Coordinates of the calculated structure of the open-shell singlet of 13_6 (n=6) (TDDFT, BP86-D3/def2-TZVP) in D_6 geometry.

	x	y	z
C	-6.231336	-0.498325	3.755022
C	-5.981659	-0.839954	5.081794
C	-4.891150	-0.283561	5.757719
C	-4.054219	0.615936	5.091894
C	-4.300371	0.958943	3.763416
C	-5.395792	0.405866	3.067293
C	-5.628131	0.678019	1.650721
C	-5.860778	-0.308206	0.665889
C	-5.860778	0.308206	-0.665889
C	-5.554258	1.690838	-0.498777
C	-5.399506	1.915701	0.950628
C	-5.628131	-0.678019	-1.650721
C	-5.399506	-1.915701	-0.950628
C	-5.554258	-1.690838	0.498777
C	-4.839196	-3.103713	-1.424103
C	-4.241437	-3.964710	-0.498777
C	-4.358798	-3.718259	0.950628
C	-5.107492	-2.639011	1.424103
C	-3.197303	-4.921480	-0.665889
C	-2.663475	-5.229685	0.665889
C	-3.401247	-4.535095	1.650721
C	-1.312821	-5.655547	0.498777
C	-1.040707	-5.633959	-0.950628
C	-2.226884	-5.213113	-1.650721
C	-4.839196	3.103713	1.424103
C	-4.241437	3.964710	0.498777
C	-4.358798	3.718259	-0.950628
C	-5.107492	2.639011	-1.424103
C	-3.401247	4.535095	-1.650721
C	-2.663475	5.229685	-0.665889
C	-3.197303	4.921480	0.665889
C	-1.312821	5.655547	-0.498777
C	-1.040707	5.633959	0.950628
C	-2.226884	5.213113	1.650721
C	0.268296	5.742723	1.424103
C	1.312821	5.655547	0.498777
C	1.040707	5.633959	-0.950628
C	-0.268296	5.742723	-1.424103
C	2.226884	5.213113	-1.650721
C	3.197303	4.921480	-0.665889
C	2.663475	5.229685	0.665889
C	3.401247	4.535095	1.650721
C	4.358798	3.718259	0.950628

C	4.241437	3.964710	-0.498777
C	5.107492	2.639011	1.424103
C	5.554258	1.690838	0.498777
C	5.399506	1.915701	-0.950628
C	4.839196	3.103713	-1.424103
C	5.860778	0.308206	0.665889
C	5.860778	-0.308206	-0.665889
C	5.628131	0.678019	-1.650721
C	0.268296	-5.742723	-1.424103
C	1.312821	-5.655547	-0.498777
C	1.040707	-5.633959	0.950628
C	-0.268296	-5.742723	1.424103
C	2.226884	-5.213113	1.650721
C	3.197303	-4.921480	0.665889
C	2.663475	-5.229685	-0.665889
C	4.241437	-3.964710	0.498777
C	4.358798	-3.718259	-0.950628
C	3.401247	-4.535095	-1.650721
C	5.107492	-2.639011	-1.424103
C	5.554258	-1.690838	-0.498777
C	5.399506	-1.915701	0.950628
C	4.839196	-3.103713	1.424103
C	5.628131	-0.678019	1.650721
C	-3.049386	-4.469960	3.067293
C	-2.980654	-3.244759	3.763416
C	-2.560525	-3.203088	5.091894
C	-2.200004	-4.377641	5.757719
C	-2.263408	-5.600246	5.081794
C	-2.684106	-5.645658	3.755022
C	-5.395792	-0.405866	-3.067293
C	-4.300371	-0.958943	-3.763416
C	-4.054219	-0.615936	-5.091894
C	-4.891150	0.283561	-5.757719
C	-5.981659	0.839954	-5.081794
C	-6.231336	0.498325	-3.755022
C	-3.049386	4.469960	-3.067293
C	-2.980654	3.244759	-3.763416
C	-2.560525	3.203088	-5.091894
C	-2.200004	4.377641	-5.757719
C	-2.263408	5.600246	-5.081794
C	-2.684106	5.645658	-3.755022
C	-2.346406	4.875826	3.067293
C	-1.319717	4.203702	3.763416
C	-1.493693	3.819024	5.091894

C	-2.691146	4.094080	5.757719
C	-3.718251	4.760292	5.081794
C	-3.547230	5.147333	3.755022
C	2.346406	4.875826	-3.067293
C	1.319717	4.203702	-3.763416
C	1.493693	3.819024	-5.091894
C	2.691146	4.094080	-5.757719
C	3.718251	4.760292	-5.081794
C	3.547230	5.147333	-3.755022
C	3.049386	4.469960	3.067293
C	2.980654	3.244759	3.763416
C	2.560525	3.203088	5.091894
C	2.200004	4.377641	5.757719
C	2.263408	5.600246	5.081794
C	2.684106	5.645658	3.755022
C	-2.346406	-4.875826	-3.067293
C	-1.319717	-4.203702	-3.763416
C	-1.493693	-3.819024	-5.091894
C	-2.691146	-4.094080	-5.757719
C	-3.718251	-4.760292	-5.081794
C	-3.547230	-5.147333	-3.755022
C	2.346406	-4.875826	3.067293
C	1.319717	-4.203702	3.763416
C	1.493693	-3.819024	5.091894
C	2.691146	-4.094080	5.757719
C	3.718251	-4.760292	5.081794
C	3.547230	-5.147333	3.755022
C	5.395792	0.405866	-3.067293
C	4.300371	0.958943	-3.763416
C	4.054219	0.615936	-5.091894
C	4.891150	-0.283561	-5.757719
C	5.981659	-0.839954	-5.081794
C	6.231336	-0.498325	-3.755022
C	3.049386	-4.469960	-3.067293
C	2.980654	-3.244759	-3.763416
C	2.560525	-3.203088	-5.091894
C	2.200004	-4.377641	-5.757719
C	2.263408	-5.600246	-5.081794
C	2.684106	-5.645658	-3.755022
C	5.395792	-0.405866	3.067293
C	4.300371	-0.958943	3.763416
C	4.054219	-0.615936	5.091894
C	4.891150	0.283561	5.757719
C	5.981659	0.839954	5.081794

C	6.231336	0.498325	3.755022
H	0.478660	5.734219	2.491811
H	-0.478660	5.734219	-2.491811
H	-4.726650	3.281641	2.491811
H	-5.205310	2.452578	-2.491811
H	-5.205310	-2.452578	2.491811
H	-4.726650	-3.281641	-2.491811
H	5.205310	2.452578	2.491811
H	4.726650	3.281641	-2.491811
H	-0.478660	-5.734219	2.491811
H	0.478660	-5.734219	-2.491811
H	4.726650	-3.281641	2.491811
H	5.205310	-2.452578	-2.491811
H	-1.984039	6.522438	-5.592553
H	-1.868814	4.342763	-6.796164
H	-2.510201	2.240858	-5.602383
H	-3.214426	2.313765	-3.248756
H	-2.743102	6.600017	-3.229817
H	4.656577	4.979447	-5.592553
H	2.826536	3.789822	-6.796164
H	0.685540	3.294327	-5.602383
H	0.396566	3.940657	-3.248756
H	4.344231	5.675604	-3.229817
H	6.640616	-1.542991	-5.592553
H	4.695350	-0.552941	-6.796164
H	3.195740	1.053469	-5.602383
H	3.610992	1.626892	-3.248756
H	7.087333	-0.924412	-3.229817
H	1.984039	-6.522438	-5.592553
H	1.868814	-4.342763	-6.796164
H	2.510201	-2.240858	-5.602383
H	3.214426	-2.313765	-3.248756
H	2.743102	-6.600017	-3.229817
H	-4.656577	-4.979447	-5.592553
H	-2.826536	-3.789822	-6.796164
H	-0.685540	-3.294327	-5.602383
H	-0.396566	-3.940657	-3.248756
H	-4.344231	-5.675604	-3.229817
H	-6.640616	1.542991	-5.592553
H	-4.695350	0.552941	-6.796164
H	-3.195740	-1.053469	-5.602383
H	-3.610992	-1.626892	-3.248756
H	-7.087333	0.924412	-3.229817
H	-4.656577	4.979447	5.592553
H	-2.826536	3.789822	6.796164
H	-0.685540	3.294327	5.602383
H	-0.396566	3.940657	3.248756
H	-4.344231	5.675604	3.229817
H	1.984039	6.522438	5.592553
H	1.868814	4.342763	6.796164
H	2.510201	2.240858	5.602383
H	3.214426	2.313765	3.248756
H	2.743102	6.600017	3.229817
H	6.640616	1.542991	5.592553
H	4.695350	0.552941	6.796164
H	3.195740	-1.053469	5.602383
H	3.610992	-1.626892	3.248756
H	7.087333	0.924412	3.229817
H	4.656577	-4.979447	5.592553
H	2.826536	-3.789822	6.796164
H	0.685540	-3.294327	5.602383
H	0.396566	-3.940657	3.248756
H	4.344231	-5.675604	3.229817
H	-1.984039	-6.522438	5.592553
H	-1.868814	-4.342763	6.796164
H	-2.510201	-2.240858	5.602383
H	-3.214426	-2.313765	3.248756
H	-2.743102	-6.600017	3.229817
H	-6.640616	-1.542991	5.592553
H	-4.695350	-0.552941	6.796164
H	-3.195740	1.053469	5.602383
H	-3.610992	1.626892	3.248756
H	-7.087333	-0.924412	3.229817

Table S 113. Coordinates of the calculated structure of 13_7 (n=7) (TPSS-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.872744	-0.303611	-0.661643
C	6.600893	-1.726282	-0.493303
C	6.463004	-1.948000	0.914699
C	6.652540	-0.669203	1.623210
C	6.872744	0.303611	0.661643
C	6.202917	-2.702536	-1.408300
C	5.552625	-3.838422	-0.914699

C	5.465251	-4.084467	0.493303
C	5.980383	-3.164632	1.408300
C	4.670995	-4.783924	-1.623210
C	4.047713	-5.562626	-0.661643
C	4.522458	-5.184029	0.661643
C	2.765928	-6.237105	-0.493303
C	2.506610	-6.267538	0.914699
C	3.624587	-5.618406	1.623210
C	1.254499	-6.648768	1.408300
C	0.214163	-6.819529	0.493303
C	0.461006	-6.734434	-0.914699
C	1.754528	-6.534639	-1.408300
C	-0.827905	-6.634658	-1.623210
C	-1.825328	-6.632870	-0.661643
C	-1.233331	-6.767989	0.661643
C	-2.132754	-6.336835	1.623210
C	-3.337313	-5.867492	0.914699
C	-3.151837	-6.051261	-0.493303
C	-4.416049	-5.126246	1.408300
C	-5.198194	-4.419346	0.493303
C	-4.977760	-4.559279	-0.914699
C	-4.015057	-5.446026	-1.408300
C	-5.703375	-3.489360	-1.623210
C	-6.323860	-2.708428	-0.661643
C	-6.060396	-3.255516	0.661643
C	-6.284087	-2.283498	1.623210
C	-6.668171	-1.049105	0.914699
C	-6.696205	-1.308694	-0.493303
C	-6.761222	0.256444	1.408300
C	-6.696205	1.308694	0.493303
C	-6.668171	1.049105	-0.914699
C	-6.761222	-0.256444	-1.408300
C	-6.323860	2.708428	0.661643
C	-6.060396	3.255516	-0.661643
C	-6.284087	2.283498	-1.623210
C	-5.198194	4.419346	-0.493303
C	-4.977760	4.559279	0.914699
C	-5.703375	3.489360	1.623210
C	-4.015057	5.446026	1.408300
C	-3.151837	6.051261	0.493303
C	-3.337313	5.867492	-0.914699
C	-4.416049	5.126246	-1.408300
C	-2.132754	6.336835	-1.623210
C	-1.233331	6.767989	-0.661643

C	-1.825328	6.632870	0.661643
C	0.214163	6.819529	-0.493303
C	0.461006	6.734434	0.914699
C	-0.827905	6.634658	1.623210
C	1.754528	6.534639	1.408300
C	2.765928	6.237105	0.493303
C	2.506610	6.267538	-0.914699
C	1.254499	6.648768	-1.408300
C	6.652540	0.669203	-1.623210
H	1.942099	-6.482586	-2.474660
H	1.062918	-6.683254	2.474660
H	-3.857411	-5.560221	-2.474660
H	-4.562459	-4.997963	2.474660
H	-6.752212	-0.450895	-2.474660
H	-6.752212	0.450895	2.474660
H	6.279169	-2.523432	-2.474660
H	5.887897	-3.335918	2.474660
H	-4.562459	4.997963	-2.474660
H	-3.857411	5.560221	2.474660
H	1.062918	6.683254	-2.474660
H	1.942099	6.482586	2.474660
C	3.624587	5.618406	-1.623210
C	4.047713	5.562626	0.661643
C	4.522458	5.184029	-0.661643
C	5.465251	4.084467	-0.493303
C	4.670995	4.783924	1.623210
C	5.552625	3.838422	0.914699
C	5.980383	3.164632	-1.408300
C	6.202917	2.702536	1.408300
C	6.463004	1.948000	-0.914699
C	6.600893	1.726282	0.493303
H	5.887897	3.335918	-2.474660
H	6.279169	2.523432	2.474660
C	4.982020	5.028912	-5.087102
C	3.848503	4.576588	-5.766085
C	2.630372	4.484413	-5.090558
C	2.541139	4.843192	-3.748060
C	3.675656	5.299214	-3.049759
C	4.896531	5.386198	-3.745000
H	5.933631	5.104512	-5.605454
H	3.915543	4.298491	-6.814147
H	1.743011	4.128576	-5.606360
H	1.597067	4.731864	-3.226050
H	5.773345	5.751009	-3.217519

C	7.038000	-0.759625	-5.087102
C	5.977623	-0.155425	-5.766085
C	5.146066	0.739478	-5.090558
C	5.370934	1.032938	-3.748060
C	6.434827	0.430262	-3.049759
C	7.264036	-0.470023	-3.745000
H	7.690427	-1.456488	-5.605454
H	5.801996	-0.381229	-6.814147
H	4.314600	1.211384	-5.606360
H	4.695275	1.701632	-3.226050
H	8.095942	-0.928087	-3.217519
C	3.786667	-3.562299	-5.090558
C	3.605471	-4.770400	-5.766085
C	3.794223	-5.976148	-5.087102
C	4.161574	-5.972307	-3.745000
C	4.348441	-4.762686	-3.049759
C	4.156306	-3.555139	-3.748060
H	3.637207	-2.618004	-5.606360
H	3.319429	-4.773876	-6.814147
H	3.656175	-6.920724	-5.605454
H	4.322129	-6.908316	-3.217519
H	4.257845	-2.609964	-3.226050
C	-2.306682	-6.692510	-5.087102
C	-1.481675	-5.793166	-5.766085
C	-0.424169	-5.181593	-5.090558
C	-0.188105	-5.466124	-3.748060
C	-1.012409	-6.369234	-3.049759
C	-2.074639	-6.977322	-3.745000
H	-3.131252	-7.173513	-5.605454
H	-1.662737	-5.571697	-6.814147
H	0.220924	-4.475982	-5.606360
H	0.614171	-4.956203	-3.226050
H	-2.706335	-7.686441	-3.217519
C	-4.315597	-2.899041	-5.090558
C	-5.453089	-2.453560	-5.766085
C	-6.670608	-2.369276	-5.087102
C	-6.748606	-2.728271	-3.745000
C	-5.610895	-3.179620	-3.049759
C	-4.390869	-3.261006	-3.748060
H	-3.361720	-2.963454	-5.606360
H	-5.392827	-2.173916	-6.814147
H	-7.560782	-2.024501	-5.605454
H	-7.696874	-2.676520	-3.217519
H	-3.491986	-3.570321	-3.226050

C	-4.957293	1.566547	-5.090558
C	-5.318216	2.733627	-5.766085
C	-6.011430	3.738072	-5.087102
C	-6.340735	3.575223	-3.745000
C	-5.984262	2.404314	-3.049759
C	-5.287219	1.399716	-3.748060
H	-4.412920	0.780615	-5.606360
H	-5.062009	2.860868	-6.814147
H	-6.296889	4.649002	-5.605454
H	-6.891510	4.348876	-3.217519
H	-4.968607	0.504086	-3.226050
C	-0.825523	7.030575	-5.087102
C	-1.178618	5.862337	-5.766085
C	-1.866045	4.852494	-5.090558
C	-2.202185	5.006423	-3.748060
C	-1.851358	6.177750	-3.049759
C	-1.158162	7.186502	-3.745000
H	-0.291310	7.821711	-5.605454
H	-0.919395	5.741360	-6.814147
H	-2.141101	3.936865	-5.606360
H	-2.703765	4.198906	-3.226050
H	-0.896698	8.099479	-3.217519
C	3.794223	5.976148	5.087102
C	3.605471	4.770400	5.766085
C	3.786667	3.562299	5.090558
C	4.156306	3.555139	3.748060
C	4.348441	4.762686	3.049759
C	4.161574	5.972307	3.745000
H	3.656175	6.920724	5.605454
H	3.319429	4.773876	6.814147
H	3.637207	2.618004	5.606360
H	4.257845	2.609964	3.226050
H	4.322129	6.908316	3.217519
C	7.038000	0.759625	5.087102
C	5.977623	0.155425	5.766085
C	5.146066	-0.739478	5.090558
C	5.370934	-1.032938	3.748060
C	6.434827	-0.430262	3.049759
C	7.264036	0.470023	3.745000
H	7.690427	1.456488	5.605454
H	5.801996	0.381229	6.814147
H	4.314600	-1.211384	5.606360
H	4.695275	-1.701632	3.226050
H	8.095942	0.928087	3.217519

C	4.982020	-5.028912	5.087102
C	3.848503	-4.576588	5.766085
C	2.630372	-4.484413	5.090558
C	2.541139	-4.843192	3.748060
C	3.675656	-5.299214	3.049759
C	4.896531	-5.386198	3.745000
H	5.933631	-5.104512	5.605454
H	3.915543	-4.298491	6.814147
H	1.743011	-4.128576	5.606360
H	1.597067	-4.731864	3.226050
H	5.773345	-5.751009	3.217519
C	-0.825523	-7.030575	5.087102
C	-1.178618	-5.862337	5.766085
C	-1.866045	-4.852494	5.090558
C	-2.202185	-5.006423	3.748060
C	-1.851358	-6.177750	3.049759
C	-1.158162	-7.186502	3.745000
H	-0.291310	-7.821711	5.605454
H	-0.919395	-5.741360	6.814147
H	-2.141101	-3.936865	5.606360
H	-2.703765	-4.198906	3.226050
H	-0.896698	-8.099479	3.217519
C	-6.011430	-3.738072	5.087102
C	-5.318216	-2.733627	5.766085
C	-4.957293	-1.566547	5.090558
C	-5.287219	-1.399716	3.748060
C	-5.984262	-2.404314	3.049759
C	-6.340735	-3.575223	3.745000
H	-6.296889	-4.649002	5.605454
H	-5.062009	-2.860868	6.814147
H	-4.412920	-0.780615	5.606360
H	-4.968607	-0.504086	3.226050
H	-6.891510	-4.348876	3.217519
C	-6.670608	2.369276	5.087102
C	-5.453089	2.453560	5.766085
C	-4.315597	2.899041	5.090558
C	-4.390869	3.261006	3.748060
C	-5.610895	3.179620	3.049759
C	-6.748606	2.728271	3.745000
H	-7.560782	2.024501	5.605454
H	-5.392827	2.173916	6.814147
H	-3.361720	2.963454	5.606360
H	-3.491986	3.570321	3.226050
H	-7.696874	2.676520	3.217519
C	-2.306682	6.692510	5.087102
C	-1.481675	5.793166	5.766085
C	-0.424169	5.181593	5.090558
C	-0.188105	5.466124	3.748060
C	-1.012409	6.369234	3.049759
C	-2.074639	6.977322	3.745000
H	-3.131252	7.173513	5.605454
H	-1.662737	5.571697	6.814147
H	0.220924	4.475982	5.606360
H	0.614171	4.956203	3.226050
H	-2.706335	7.686441	3.217519

Table S 114. Coordinates of the calculated structure of the triplet of 13_7 (n=7) (TPSS-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.851686	-0.303665	-0.662090
C	6.581810	-1.716056	-0.495780
C	6.445535	-1.941407	0.924369
C	6.640297	-0.676286	1.630368
C	6.851686	0.303665	0.662090
C	6.187685	-2.691868	-1.412500
C	5.536578	-3.828874	-0.924369
C	5.445358	-4.075922	0.495780
C	5.962546	-3.159375	1.412500
C	4.668899	-4.769936	-1.630368
C	4.034542	-5.546195	-0.662090
C	4.509371	-5.167532	0.662090
C	2.762024	-6.215810	-0.495780
C	2.500872	-6.249769	0.924369
C	3.611416	-5.613251	1.630368
C	1.247488	-6.631544	1.412500
C	0.208441	-6.798648	0.495780
C	0.458466	-6.715935	-0.924369
C	1.753371	-6.516080	-1.412500
C	-0.818275	-6.624299	-1.630368
C	-1.820695	-6.612328	-0.662090
C	-1.228592	-6.747471	0.662090
C	-2.136936	-6.323323	1.630368
C	-3.326998	-5.851928	0.924369
C	-3.137622	-6.034931	-0.495780

C	-4.406954	-5.110026	1.412500
C	-5.185437	-4.401854	0.495780
C	-4.964881	-4.545760	-0.924369
C	-4.001267	-5.433550	-1.412500
C	-5.689271	-3.490430	-1.630368
C	-6.304911	-2.699243	-0.662090
C	-6.041400	-3.246427	0.662090
C	-6.276131	-2.271804	1.630368
C	-6.649571	-1.047465	0.924369
C	-6.674575	-1.309627	-0.495780
C	-6.742870	0.259447	1.412500
C	-6.674575	1.309627	0.495780
C	-6.649571	1.047465	-0.924369
C	-6.742870	-0.259447	-1.412500
C	-6.304911	2.699243	0.662090
C	-6.041400	3.246427	-0.662090
C	-6.276131	2.271804	-1.630368
C	-5.185437	4.401854	-0.495780
C	-4.964881	4.545760	0.924369
C	-5.689271	3.490430	1.630368
C	-4.001267	5.433550	1.412500
C	-3.137622	6.034931	0.495780
C	-3.326998	5.851928	-0.924369
C	-4.406954	5.110026	-1.412500
C	-2.136936	6.323323	-1.630368
C	-1.228592	6.747471	-0.662090
C	-1.820695	6.612328	0.662090
C	0.208441	6.798648	-0.495780
C	0.458466	6.715935	0.924369
C	-0.818275	6.624299	1.630368
C	1.753371	6.516080	1.412500
C	2.762024	6.215810	0.495780
C	2.500872	6.249769	-0.924369
C	1.247488	6.631544	-1.412500
C	6.640297	0.676286	-1.630368
H	1.945222	-6.465543	-2.478117
H	1.052710	-6.669253	2.478117
H	-3.842139	-5.552036	-2.478117
H	-4.557878	-4.981253	2.478117
H	-6.736291	-0.457732	-2.478117
H	-6.736291	0.457732	2.478117
H	6.267791	-2.510365	-2.478117
H	5.870586	-3.335170	2.478117
H	-4.557878	4.981253	-2.478117

H	-3.842139	5.552036	2.478117
H	1.052710	6.669253	-2.478117
H	1.945222	6.465543	2.478117
C	3.611416	5.613251	-1.630368
C	4.034542	5.546195	0.662090
C	4.509371	5.167532	-0.662090
C	5.445358	4.075922	-0.495780
C	4.668899	4.769936	1.630368
C	5.536578	3.828874	0.924369
C	5.962546	3.159375	-1.412500
C	6.187685	2.691868	1.412500
C	6.445535	1.941407	-0.924369
C	6.581810	1.716056	0.495780
H	5.870586	3.335170	-2.478117
H	6.267791	2.510365	2.478117
C	5.005209	5.057598	-5.085278
C	3.878460	4.615854	-5.782410
C	2.652650	4.519580	-5.121540
C	2.549387	4.862531	-3.775888
C	3.676538	5.308821	-3.059364
C	4.905320	5.400180	-3.740448
H	5.962998	5.136247	-5.591714
H	3.956846	4.348491	-6.832453
H	1.770373	4.171113	-5.650990
H	1.599590	4.745077	-3.265723
H	5.777550	5.756291	-3.199482
C	7.074886	-0.759869	-5.085278
C	6.027000	-0.154365	-5.782410
C	5.187450	0.743987	-5.121540
C	5.391197	1.038547	-3.775888
C	6.442887	0.435563	-3.059364
C	7.280448	-0.468176	-3.740448
H	7.733548	-1.459662	-5.591714
H	5.866840	-0.382347	-6.832453
H	4.364917	1.216513	-5.650990
H	4.707179	1.707897	-3.265723
H	8.102693	-0.928082	-3.199482
C	3.815995	-3.591844	-5.121540
C	3.637086	-4.808343	-5.782410
C	3.817030	-6.005139	-5.085278
C	4.173250	-5.983987	-3.740448
C	4.357611	-4.765683	-3.059364
C	4.173325	-3.567484	-3.775888
H	3.672590	-2.654146	-5.650990

H	3.358984	-4.825269	-6.832453
H	3.680579	-6.956416	-5.591714
H	4.326343	-6.913590	-3.199482
H	4.270165	-2.615364	-3.265723
C	-2.315128	-6.728417	-5.085278
C	-1.491628	-5.841541	-5.782410
C	-0.428983	-5.222943	-5.121540
C	-0.187146	-5.487127	-3.775888
C	-1.009035	-6.378273	-3.059364
C	-2.076490	-6.993733	-3.740448
H	-3.143941	-7.214847	-5.591714
H	-1.678255	-5.634666	-6.832453
H	0.214727	-4.526179	-5.650990
H	0.617631	-4.969203	-3.265723
H	-2.707832	-7.693024	-3.199482
C	-4.350928	-2.921059	-5.121540
C	-5.497116	-2.475940	-5.782410
C	-6.703947	-2.385060	-5.085278
C	-6.762591	-2.737056	-3.740448
C	-5.615857	-3.187893	-3.059364
C	-4.406692	-3.274851	-3.775888
H	-3.404829	-2.989907	-5.650990
H	-5.451734	-2.201044	-6.832453
H	-7.601010	-2.040351	-5.591714
H	-7.702954	-2.679454	-3.199482
H	-3.499993	-3.581130	-3.265723
C	-4.996535	1.580442	-5.121540
C	-5.363163	2.754095	-5.782410
C	-6.044557	3.754297	-5.085278
C	-6.356323	3.580680	-3.740448
C	-5.993825	2.403036	-3.059364
C	-5.307909	1.403454	-3.775888
H	-4.460480	0.797826	-5.650990
H	-5.119946	2.890009	-6.832453
H	-6.334363	4.670571	-5.591714
H	-6.897595	4.351800	-3.199482
H	-4.982050	0.503606	-3.265723
C	-0.833493	7.066591	-5.085278
C	-1.190639	5.910240	-5.782410
C	-1.879650	4.891838	-5.121540
C	-2.212163	5.024930	-3.775888
C	-1.858320	6.184429	-3.059364
C	-1.163614	7.202091	-3.740448
H	-0.297811	7.864457	-5.591714

H	-0.932734	5.804826	-6.832453
H	-2.157298	3.984780	-5.650990
H	-2.712522	4.209117	-3.265723
H	-0.898206	8.106059	-3.199482
C	3.817030	6.005139	5.085278
C	3.637086	4.808343	5.782410
C	3.815995	3.591844	5.121540
C	4.173325	3.567484	3.775888
C	4.357611	4.765683	3.059364
C	4.173250	5.983987	3.740448
H	3.680579	6.956416	5.591714
H	3.358984	4.825269	6.832453
H	3.672590	2.654146	5.650990
H	4.270165	2.615364	3.265723
H	4.326343	6.913590	3.199482
C	7.074886	0.759869	5.085278
C	6.027000	0.154365	5.782410
C	5.187450	-0.743987	5.121540
C	5.391197	-1.038547	3.775888
C	6.442887	-0.435563	3.059364
C	7.280448	0.468176	3.740448
H	7.733548	1.459662	5.591714
H	5.866840	0.382347	6.832453
H	4.364917	-1.216513	5.650990
H	4.707179	-1.707897	3.265723
H	8.102693	0.928082	3.199482
C	5.005209	-5.057598	5.085278
C	3.878460	-4.615854	5.782410
C	2.652650	-4.519580	5.121540
C	2.549387	-4.862531	3.775888
C	3.676538	-5.308821	3.059364
C	4.905320	-5.400180	3.740448
H	5.962998	-5.136247	5.591714
H	3.956846	-4.348491	6.832453
H	1.770373	-4.171113	5.650990
H	1.599590	-4.745077	3.265723
H	5.777550	-5.756291	3.199482
C	-0.833493	-7.066591	5.085278
C	-1.190639	-5.910240	5.782410
C	-1.879650	-4.891838	5.121540
C	-2.212163	-5.024930	3.775888
C	-1.858320	-6.184429	3.059364
C	-1.163614	-7.202091	3.740448
H	-0.297811	-7.864457	5.591714

H	-0.932734	-5.804826	6.832453
H	-2.157298	-3.984780	5.650990
H	-2.712522	-4.209117	3.265723
H	-0.898206	-8.106059	3.199482
C	-6.044557	-3.754297	5.085278
C	-5.363163	-2.754095	5.782410
C	-4.996535	-1.580442	5.121540
C	-5.307909	-1.403454	3.775888
C	-5.993825	-2.403036	3.059364
C	-6.356323	-3.580680	3.740448
H	-6.334363	-4.670571	5.591714
H	-5.119946	-2.890009	6.832453
H	-4.460480	-0.797826	5.650990
H	-4.982050	-0.503606	3.265723
H	-6.897595	-4.351800	3.199482
C	-6.703947	2.385060	5.085278
C	-5.497116	2.475940	5.782410
C	-4.350928	2.921059	5.121540
C	-4.406692	3.274851	3.775888
C	-5.615857	3.187893	3.059364
C	-6.762591	2.737056	3.740448
H	-7.601010	2.040351	5.591714
H	-5.451734	2.201044	6.832453
H	-3.404829	2.989907	5.650990
H	-3.499993	3.581130	3.265723
H	-7.702954	2.679454	3.199482
C	-2.315128	6.728417	5.085278
C	-1.491628	5.841541	5.782410
C	-0.428983	5.222943	5.121540
C	-0.187146	5.487127	3.775888
C	-1.009035	6.378273	3.059364
C	-2.076490	6.993733	3.740448
H	-3.143941	7.214847	5.591714
H	-1.678255	5.634666	6.832453
H	0.214727	4.526179	5.650990
H	0.617631	4.969203	3.265723
H	-2.707832	7.693024	3.199482

Table S 115. Coordinates of the calculated structure of the open-shell singlet of 13_7 (n=7) (TDDFT, BP86-D3/def2-TZVP) in D_7 geometry.

	x	y	z
C	6.862579	-0.305082	-0.663311
C	6.586805	-1.716268	-0.496270
C	6.443998	-1.941762	0.925994
C	6.628397	-0.674810	1.631095
C	6.862579	0.305082	0.663311
C	6.188846	-2.690798	-1.414043
C	5.535898	-3.827452	-0.925994
C	5.448638	-4.079696	0.496270
C	5.962433	-3.160950	1.414043
C	4.660326	-4.761552	-1.631095
C	4.040225	-5.555596	-0.663311
C	4.517271	-5.175165	0.663311
C	2.764973	-6.219847	-0.496270
C	2.499637	-6.248790	0.925994
C	3.605150	-5.603026	1.631095
C	1.246187	-6.632438	1.414043
C	0.207536	-6.803565	0.496270
C	0.459154	-6.714516	-0.925994
C	1.754932	-6.516320	-1.414043
C	-0.817066	-6.612369	-1.631095
C	-1.824501	-6.622633	-0.663311
C	-1.229634	-6.758407	0.663311
C	-2.132848	-6.312050	1.631095
C	-3.327003	-5.850351	0.925994
C	-3.138940	-6.039754	-0.496270
C	-4.408464	-5.109565	1.414043
C	-5.189845	-4.404212	0.496270
C	-4.963343	-4.545413	-0.925994
C	-4.000482	-5.434920	-1.414043
C	-5.679190	-3.483936	-1.631095
C	-6.315340	-2.702692	-0.663311
C	-6.050600	-3.252431	0.663311
C	-6.264768	-2.267971	1.631095
C	-6.648341	-1.046479	0.925994
C	-6.679167	-1.311603	-0.496270
C	-6.743451	0.260914	1.414043
C	-6.679167	1.311603	0.496270
C	-6.648341	1.046479	-0.925994
C	-6.743451	-0.260914	-1.414043
C	-6.315340	2.702692	0.663311
C	-6.050600	3.252431	-0.663311
C	-6.264768	2.267971	-1.631095
C	-5.189845	4.404212	-0.496270

C	-4.963343	4.545413	0.925994
C	-5.679190	3.483936	1.631095
C	-4.000482	5.434920	1.414043
C	-3.138940	6.039754	0.496270
C	-3.327003	5.850351	-0.925994
C	-4.408464	5.109565	-1.414043
C	-2.132848	6.312050	-1.631095
C	-1.229634	6.758407	-0.663311
C	-1.824501	6.622633	0.663311
C	0.207536	6.803565	-0.496270
C	0.459154	6.714516	0.925994
C	-0.817066	6.612369	1.631095
C	1.754932	6.516320	1.414043
C	2.764973	6.219847	0.496270
C	2.499637	6.248790	-0.925994
C	1.246187	6.632438	-1.414043
C	6.628397	0.674810	-1.631095
H	1.946541	-6.462649	-2.484186
H	1.050265	-6.667218	2.484186
H	-3.839054	-5.551263	-2.484186
H	-4.557812	-4.978073	2.484186
H	-6.733763	-0.459663	-2.484186
H	-6.733763	0.459663	2.484186
H	6.266351	-2.507529	-2.484186
H	5.867471	-3.335812	2.484186
H	-4.557812	4.978073	-2.484186
H	-3.839054	5.551263	2.484186
H	1.050265	6.667218	-2.484186
H	1.946541	6.462649	2.484186
C	3.605150	5.603026	-1.631095
C	4.040225	5.555596	0.663311
C	4.517271	5.175165	-0.663311
C	5.448638	4.079696	-0.496270
C	4.660326	4.761552	1.631095
C	5.535898	3.827452	0.925994
C	5.962433	3.160950	-1.414043
C	6.188846	2.690798	1.414043
C	6.443998	1.941762	-0.925994
C	6.586805	1.716268	0.496270
H	5.867471	3.335812	-2.484186
H	6.266351	2.507529	2.484186
C	4.926042	4.879333	-5.086793
C	3.780746	4.410521	-5.737986
C	2.566083	4.361125	-5.048419

C	2.493047	4.773701	-3.719089
C	3.640013	5.245574	-3.047432
C	4.855898	5.294009	-3.758924
H	5.877567	4.923128	-5.617728
H	3.836526	4.086594	-6.777872
H	1.665626	3.994126	-5.542246
H	1.548976	4.689633	-3.182858
H	5.744386	5.674207	-3.253239
C	6.886153	-0.809120	-5.086793
C	5.805541	-0.205992	-5.737986
C	5.009591	0.712872	-5.048419
C	5.286620	1.027211	-3.719089
C	6.370666	0.424686	-3.047432
C	7.166626	-0.495733	-3.758924
H	7.513659	-1.525747	-5.617728
H	5.587063	-0.451567	-6.777872
H	4.161234	1.188058	-5.542246
H	4.632273	1.712900	-3.182858
H	8.017840	-0.953331	-3.253239
C	3.680775	-3.472188	-5.048419
C	3.458645	-4.667388	-5.737986
C	3.660850	-5.888290	-5.086793
C	4.080738	-5.912178	-3.758924
C	4.304078	-4.716000	-3.047432
C	4.099260	-3.492790	-3.719089
H	3.523348	-2.512642	-5.542246
H	3.130428	-4.649689	-6.777872
H	3.491813	-6.825703	-5.617728
H	4.253697	-6.862992	-3.253239
H	4.227375	-2.553681	-3.182858
C	-2.321147	-6.533457	-5.086793
C	-1.492681	-5.614146	-5.737986
C	-0.419740	-5.042619	-5.048419
C	-0.174927	-5.382649	-3.719089
C	-1.003569	-6.305441	-3.047432
C	-2.078029	-6.876633	-3.758924
H	-3.159440	-6.985765	-5.617728
H	-1.683484	-5.346501	-6.777872
H	0.232309	-4.321271	-5.542246
H	0.639177	-4.897289	-3.182858
H	-2.713567	-7.604679	-3.253239
C	-4.204182	-2.815856	-5.048419
C	-5.319988	-2.333338	-5.737986
C	-6.555274	-2.258798	-5.086793

C	-6.671997	-2.662842	-3.758924
C	-5.555508	-3.146757	-3.047432
C	-4.317389	-3.219264	-3.719089
H	-3.233663	-2.875895	-5.542246
H	-5.229698	-2.017288	-6.777872
H	-7.431570	-1.885404	-5.617728
H	-7.637459	-2.619888	-3.253239
H	-3.430335	-3.553138	-3.182858
C	-4.822789	1.531305	-5.048419
C	-5.141235	2.704522	-5.737986
C	-5.853145	3.716782	-5.086793
C	-6.241816	3.556123	-3.758924
C	-5.924036	2.381500	-3.047432
C	-5.208770	1.368293	-3.719089
H	-4.264621	0.735088	-5.542246
H	-4.837842	2.830984	-6.777872
H	-6.107576	4.634705	-5.617728
H	-6.810189	4.337732	-3.253239
H	-4.916734	0.466598	-3.182858
C	-0.743479	6.893549	-5.086793
C	-1.091027	5.705821	-5.737986
C	-1.809738	4.725361	-5.048419
C	-2.177841	4.925497	-3.719089
C	-1.831644	6.116439	-3.047432
C	-1.111420	7.097255	-3.758924
H	-0.184453	7.664787	-5.617728
H	-0.802993	5.547467	-6.777872
H	-2.084233	3.792535	-5.542246
H	-2.700732	4.134977	-3.182858
H	-0.854708	8.028952	-3.253239
C	3.660850	5.888290	5.086793
C	3.458645	4.667388	5.737986
C	3.680775	3.472188	5.048419
C	4.099260	3.492790	3.719089
C	4.304078	4.716000	3.047432
C	4.080738	5.912178	3.758924
H	3.491813	6.825703	5.617728
H	3.130428	4.649689	6.777872
H	3.523348	2.512642	5.542246
H	4.227375	2.553681	3.182858
H	4.253697	6.862992	3.253239
C	6.886153	0.809120	5.086793
C	5.805541	0.205992	5.737986
C	5.009591	-0.712872	5.048419

C	5.286620	-1.027211	3.719089
C	6.370666	-0.424686	3.047432
C	7.166626	0.495733	3.758924
H	7.513659	1.525747	5.617728
H	5.587063	0.451567	6.777872
H	4.161234	-1.188058	5.542246
H	4.632273	-1.712900	3.182858
H	8.017840	0.953331	3.253239
C	4.926042	-4.879333	5.086793
C	3.780746	-4.410521	5.737986
C	2.566083	-4.361125	5.048419
C	2.493047	-4.773701	3.719089
C	3.640013	-5.245574	3.047432
C	4.855898	-5.294009	3.758924
H	5.877567	-4.923128	5.617728
H	3.836526	-4.086594	6.777872
H	1.665626	-3.994126	5.542246
H	1.548976	-4.689633	3.182858
H	5.744386	-5.674207	3.253239
C	-0.743479	-6.893549	5.086793
C	-1.091027	-5.705821	5.737986
C	-1.809738	-4.725361	5.048419
C	-2.177841	-4.925497	3.719089
C	-1.831644	-6.116439	3.047432
C	-1.111420	-7.097255	3.758924
H	-0.184453	-7.664787	5.617728
H	-0.802993	-5.547467	6.777872
H	-2.084233	-3.792535	5.542246
H	-2.700732	-4.134977	3.182858
H	-0.854708	-8.028952	3.253239
C	-5.853145	-3.716782	5.086793
C	-5.141235	-2.704522	5.737986
C	-4.822789	-1.531305	5.048419
C	-5.208770	-1.368293	3.719089
C	-5.924036	-2.381500	3.047432
C	-6.241816	-3.556123	3.758924
H	-6.107576	-4.634705	5.617728
H	-4.837842	-2.830984	6.777872
H	-4.264621	-0.735088	5.542246
H	-4.916734	-0.466598	3.182858
H	-6.810189	-4.337732	3.253239
C	-6.555274	2.258798	5.086793
C	-5.319988	2.333338	5.737986
C	-4.204182	2.815856	5.048419

C	-4.317389	3.219264	3.719089
C	-5.555508	3.146757	3.047432
C	-6.671997	2.662842	3.758924
H	-7.431570	1.885404	5.617728
H	-5.229698	2.017288	6.777872
H	-3.233663	2.875895	5.542246
H	-3.430335	3.553138	3.182858
H	-7.637459	2.619888	3.253239
C	-2.321147	6.533457	5.086793
C	-1.492681	5.614146	5.737986
C	-0.419740	5.042619	5.048419
C	-0.174927	5.382649	3.719089
C	-1.003569	6.305441	3.047432
C	-2.078029	6.876633	3.758924
H	-3.159440	6.985765	5.617728
H	-1.683484	5.346501	6.777872
H	0.232309	4.321271	5.542246
H	0.639177	4.897289	3.182858
H	-2.713567	7.604679	3.253239

Table S 116. Coordinates of the calculated structure of 13_8 (n=8) (TPSS-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.732888	0.254294	1.408737
C	-7.676872	1.307874	0.494930
C	-7.648860	1.050945	-0.913678
C	-7.732888	-0.254294	-1.408737
H	-7.728760	-0.447392	-2.475294
C	-7.676872	-1.307874	-0.494930
C	-7.648860	-1.050945	0.913678
C	-7.314659	-2.299512	1.623541
C	-7.124100	-3.278223	0.661997
C	-7.355554	-2.719446	-0.661997
C	-6.798245	-3.546245	-1.623541
C	-6.353175	-4.503562	0.494930
C	-5.647791	-5.288165	1.408737
H	-5.781412	-5.148705	2.475294
C	-6.151691	-4.665431	-0.913678
C	-4.665431	-6.151691	0.913678
C	-4.503562	-6.353175	-0.494930
C	-5.288165	-5.647791	-1.408737
C	-3.546245	-6.798245	1.623541
C	-2.719446	-7.355554	0.661997
C	-3.278223	-7.124100	-0.661997
C	-2.299512	-7.314659	-1.623541
C	-1.050945	-7.648860	-0.913678
C	-1.307874	-7.676872	0.494930
C	-0.254294	-7.732888	1.408737
C	0.254294	-7.732888	-1.408737
C	1.307874	-7.676872	-0.494930
C	1.050945	-7.648860	0.913678
C	2.299512	-7.314659	1.623541
C	3.278223	-7.124100	0.661997
C	2.719446	-7.355554	-0.661997
C	3.546245	-6.798245	-1.623541
C	4.665431	-6.151691	-0.913678
C	4.503562	-6.353175	0.494930
C	5.288165	-5.647791	1.408737
C	5.647791	-5.288165	-1.408737
C	6.353175	-4.503562	-0.494930
C	6.151691	-4.665431	0.913678
C	6.798245	-3.546245	1.623541
C	7.124100	-3.278223	-0.661997
C	7.355554	-2.719446	0.661997
C	7.314659	-2.299512	-1.623541
C	7.648860	-1.050945	-0.913678
C	7.676872	-1.307874	0.494930
C	7.732888	-0.254294	1.408737
C	7.732888	0.254294	-1.408737
C	7.676872	1.307874	-0.494930
C	7.648860	1.050945	0.913678
C	7.355554	2.719446	-0.661997
C	7.314659	2.299512	1.623541
C	6.798245	3.546245	-1.623541
C	7.124100	3.278223	0.661997
C	6.151691	4.665431	-0.913678
C	6.353175	4.503562	0.494930
C	5.288165	5.647791	-1.408737
C	5.647791	5.288165	1.408737
C	4.665431	6.151691	0.913678
C	4.503562	6.353175	-0.494930
C	3.278223	7.124100	-0.661997
C	3.546245	6.798245	1.623541
C	2.719446	7.355554	0.661997

C	2.299512	7.314659	-1.623541
C	1.050945	7.648860	-0.913678
C	1.307874	7.676872	0.494930
C	0.254294	7.732888	1.408737
C	-0.254294	7.732888	-1.408737
C	-1.307874	7.676872	-0.494930
C	-1.050945	7.648860	0.913678
C	-2.299512	7.314659	1.623541
C	-7.355554	2.719446	0.661997
C	-7.314659	2.299512	-1.623541
C	-7.124100	3.278223	-0.661997
H	-7.728760	0.447392	2.475294
H	-5.148705	-5.781412	-2.475294
H	-0.447392	-7.728760	2.475294
H	0.447392	-7.728760	-2.475294
H	5.781412	-5.148705	-2.475294
H	5.148705	-5.781412	2.475294
H	7.728760	0.447392	-2.475294
H	7.728760	-0.447392	2.475294
H	5.148705	5.781412	-2.475294
H	5.781412	5.148705	2.475294
H	-0.447392	7.728760	-2.475294
H	0.447392	7.728760	2.475294
C	-2.719446	7.355554	-0.661997
C	-3.278223	7.124100	0.661997
C	-3.546245	6.798245	-1.623541
C	-4.503562	6.353175	0.494930
C	-4.665431	6.151691	-0.913678
C	-5.288165	5.647791	1.408737
C	-5.647791	5.288165	-1.408737
C	-6.151691	4.665431	0.913678
C	-6.353175	4.503562	-0.494930
H	-5.148705	5.781412	2.475294
H	-5.781412	5.148705	-2.475294
C	-6.798245	3.546245	1.623541
C	7.731731	2.398033	-5.087620
C	6.538357	2.594837	-5.786023
C	5.430371	3.125754	-5.123113
C	5.510920	3.458934	-3.773517
C	6.706063	3.262983	-3.055287
C	7.814840	2.729081	-3.738705
H	8.599422	1.987650	-5.596304
H	6.474017	2.337113	-6.839423
H	4.495359	3.278402	-5.654851

H	4.632100	3.835340	-3.261346
H	8.746465	2.592373	-3.197085
C	6.050094	-1.629610	-5.123113
C	6.458143	-2.788490	-5.786023
C	7.162825	-3.771494	-5.087620
C	7.455678	-3.596174	-3.738705
C	7.049180	-2.434625	-3.055287
C	6.342644	-1.450974	-3.773517
H	5.496879	-0.860519	-5.654851
H	6.230410	-2.925233	-6.839423
H	7.486191	-4.675229	-5.596304
H	8.017769	-4.351600	-3.197085
H	5.987384	-0.563395	-3.261346
C	3.125754	-5.430371	-5.123113
C	2.594837	-6.538357	-5.786023
C	2.398033	-7.731731	-5.087620
C	2.729081	-7.814840	-3.738705
C	3.262983	-6.706063	-3.055287
C	3.458934	-5.510920	-3.773517
H	3.278402	-4.495359	-5.654851
H	2.337113	-6.474017	-6.839423
H	1.987650	-8.599422	-5.596304
H	2.592373	-8.746465	-3.197085
H	3.835340	-4.632100	-3.261346
C	-3.771494	-7.162825	-5.087620
C	-2.788490	-6.458143	-5.786023
C	-1.629610	-6.050094	-5.123113
C	-1.450974	-6.342644	-3.773517
C	-2.434625	-7.049180	-3.055287
C	-3.596174	-7.455678	-3.738705
H	-4.675229	-7.486191	-5.596304
H	-2.925233	-6.230410	-6.839423
H	-0.860519	-5.496879	-5.654851
H	-0.563395	-5.987384	-3.261346
H	-4.351600	-8.017769	-3.197085
C	-5.430371	-3.125754	-5.123113
C	-6.538357	-2.594837	-5.786023
C	-7.731731	-2.398033	-5.087620
C	-7.814840	-2.729081	-3.738705
C	-6.706063	-3.262983	-3.055287
C	-5.510920	-3.458934	-3.773517
H	-4.495359	-3.278402	-5.654851
H	-6.474017	-2.337113	-6.839423
H	-8.599422	-1.987650	-5.596304

H	-8.746465	-2.592373	-3.197085
H	-4.632100	-3.835340	-3.261346
C	-6.050094	1.629610	-5.123113
C	-6.458143	2.788490	-5.786023
C	-7.162825	3.771494	-5.087620
C	-7.455678	3.596174	-3.738705
C	-7.049180	2.434625	-3.055287
C	-6.342644	1.450974	-3.773517
H	-5.496879	0.860519	-5.654851
H	-6.230410	2.925233	-6.839423
H	-7.486191	4.675229	-5.596304
H	-8.017769	4.351600	-3.197085
H	-5.987384	0.563395	-3.261346
C	-2.398033	7.731731	-5.087620
C	-2.594837	6.538357	-5.786023
C	-3.125754	5.430371	-5.123113
C	-3.458934	5.510920	-3.773517
C	-3.262983	6.706063	-3.055287
C	-2.729081	7.814840	-3.738705
H	-1.987650	8.599422	-5.596304
H	-2.337113	6.474017	-6.839423
H	-3.278402	4.495359	-5.654851
H	-3.835340	4.632100	-3.261346
H	-2.592373	8.746465	-3.197085
C	1.629610	6.050094	-5.123113
C	2.788490	6.458143	-5.786023
C	3.771494	7.162825	-5.087620
C	3.596174	7.455678	-3.738705
C	2.434625	7.049180	-3.055287
C	1.450974	6.342644	-3.773517
H	0.860519	5.496879	-5.654851
H	2.925233	6.230410	-6.839423
H	4.675229	7.486191	-5.596304
H	4.351600	8.017769	-3.197085
H	0.563395	5.987384	-3.261346
C	7.162825	3.771494	5.087620
C	6.458143	2.788490	5.786023
C	6.050094	1.629610	5.123113
C	6.342644	1.450974	3.773517
C	7.049180	2.434625	3.055287
C	7.455678	3.596174	3.738705
H	7.486191	4.675229	5.596304
H	6.230410	2.925233	6.839423
H	5.496879	0.860519	5.654851

H	5.987384	0.563395	3.261346
H	8.017769	4.351600	3.197085
C	7.731731	-2.398033	5.087620
C	6.538357	-2.594837	5.786023
C	5.430371	-3.125754	5.123113
C	5.510920	-3.458934	3.773517
C	6.706063	-3.262983	3.055287
C	7.814840	-2.729081	3.738705
H	8.599422	-1.987650	5.596304
H	6.474017	-2.337113	6.839423
H	4.495359	-3.278402	5.654851
H	4.632100	-3.835340	3.261346
H	8.746465	-2.592373	3.197085
C	3.771494	-7.162825	5.087620
C	2.788490	-6.458143	5.786023
C	1.629610	-6.050094	5.123113
C	1.450974	-6.342644	3.773517
C	2.434625	-7.049180	3.055287
C	3.596174	-7.455678	3.738705
H	4.675229	-7.486191	5.596304
H	2.925233	-6.230410	6.839423
H	0.860519	-5.496879	5.654851
H	0.563395	-5.987384	3.261346
H	4.351600	-8.017769	3.197085
C	-2.398033	-7.731731	5.087620
C	-2.594837	-6.538357	5.786023
C	-3.125754	-5.430371	5.123113
C	-3.458934	-5.510920	3.773517
C	-3.262983	-6.706063	3.055287
C	-2.729081	-7.814840	3.738705
H	-1.987650	-8.599422	5.596304
H	-2.337113	-6.474017	6.839423
H	-3.278402	-4.495359	5.654851
H	-3.835340	-4.632100	3.261346
H	-2.592373	-8.746465	3.197085
C	-7.162825	-3.771494	5.087620
C	-6.458143	-2.788490	5.786023
C	-6.050094	-1.629610	5.123113
C	-6.342644	-1.450974	3.773517
C	-7.049180	-2.434625	3.055287
C	-7.455678	-3.596174	3.738705
H	-7.486191	-4.675229	5.596304
H	-6.230410	-2.925233	6.839423
H	-5.496879	-0.860519	5.654851

H	-5.987384	-0.563395	3.261346
H	-8.017769	-4.351600	3.197085
C	-5.430371	3.125754	5.123113
C	-6.538357	2.594837	5.786023
C	-7.731731	2.398033	5.087620
C	-7.814840	2.729081	3.738705
C	-6.706063	3.262983	3.055287
C	-5.510920	3.458934	3.773517
H	-4.495359	3.278402	5.654851
H	-6.474017	2.337113	6.839423
H	-8.599422	1.987650	5.596304
H	-8.746465	2.592373	3.197085
H	-4.632100	3.835340	3.261346
C	-3.771494	7.162825	5.087620
C	-2.788490	6.458143	5.786023
C	-1.629610	6.050094	5.123113
C	-1.450974	6.342644	3.773517
C	-2.434625	7.049180	3.055287
C	-3.596174	7.455678	3.738705
H	-4.675229	7.486191	5.596304
H	-2.925233	6.230410	6.839423
H	-0.860519	5.496879	5.654851
H	-0.563395	5.987384	3.261346
H	-4.351600	8.017769	3.197085
C	2.398033	7.731731	5.087620
C	2.594837	6.538357	5.786023
C	3.125754	5.430371	5.123113
C	3.458934	5.510920	3.773517
C	3.262983	6.706063	3.055287
C	2.729081	7.814840	3.738705
H	1.987650	8.599422	5.596304
H	2.337113	6.474017	6.839423
H	3.278402	4.495359	5.654851
H	3.835340	4.632100	3.261346
H	2.592373	8.746465	3.197085

Table S 117. Coordinates of the calculated structure of the triplet of 13_8 (n=8) (TPSS-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.713276	0.256901	1.412626
C	-7.654508	1.308930	0.497315
C	-7.629333	1.049368	-0.922376
C	-7.713276	-0.256901	-1.412626
H	-7.710396	-0.453298	-2.478523
C	-7.654508	-1.308930	-0.497315
C	-7.629333	-1.049368	0.922376
C	-7.303808	-2.288221	1.629678
C	-7.103308	-3.269945	0.662330
C	-7.334998	-2.710597	-0.662330
C	-6.782589	-3.546555	-1.629678
C	-6.338107	-4.487001	0.497315
C	-5.635767	-5.272454	1.412626
H	-5.772603	-5.131544	2.478523
C	-6.136768	-4.652738	-0.922376
C	-4.652738	-6.136768	0.922376
C	-4.487001	-6.338107	-0.497315
C	-5.272454	-5.635767	-1.412626
C	-3.546555	-6.782589	1.629678
C	-2.710597	-7.334998	0.662330
C	-3.269945	-7.103308	-0.662330
C	-2.288221	-7.303808	-1.629678
C	-1.049368	-7.629333	-0.922376
C	-1.308930	-7.654508	0.497315
C	-0.256901	-7.713276	1.412626
C	0.256901	-7.713276	-1.412626
C	1.308930	-7.654508	-0.497315
C	1.049368	-7.629333	0.922376
C	2.288221	-7.303808	1.629678
C	3.269945	-7.103308	0.662330
C	2.710597	-7.334998	-0.662330
C	3.546555	-6.782589	-1.629678
C	4.652738	-6.136768	-0.922376
C	4.487001	-6.338107	0.497315
C	5.272454	-5.635767	1.412626
C	5.635767	-5.272454	-1.412626
C	6.338107	-4.487001	-0.497315
C	6.136768	-4.652738	0.922376
C	6.782589	-3.546555	1.629678
C	7.103308	-3.269945	-0.662330
C	7.334998	-2.710597	0.662330
C	7.303808	-2.288221	-1.629678
C	7.629333	-1.049368	-0.922376
C	7.654508	-1.308930	0.497315
C	7.713276	-0.256901	1.412626

C	7.713276	0.256901	-1.412626
C	7.654508	1.308930	-0.497315
C	7.629333	1.049368	0.922376
C	7.334998	2.710597	-0.662330
C	7.303808	2.288221	1.629678
C	6.782589	3.546555	-1.629678
C	7.103308	3.269945	0.662330
C	6.136768	4.652738	-0.922376
C	6.338107	4.487001	0.497315
C	5.272454	5.635767	-1.412626
C	5.635767	5.272454	1.412626
C	4.652738	6.136768	0.922376
C	4.487001	6.338107	-0.497315
C	3.269945	7.103308	-0.662330
C	3.546555	6.782589	1.629678
C	2.710597	7.334998	0.662330
C	2.288221	7.303808	-1.629678
C	1.049368	7.629333	-0.922376
C	1.308930	7.654508	0.497315
C	0.256901	7.713276	1.412626
C	-0.256901	7.713276	-1.412626
C	-1.308930	7.654508	-0.497315
C	-1.049368	7.629333	0.922376
C	-2.288221	7.303808	1.629678
C	-7.334998	2.710597	0.662330
C	-7.303808	2.288221	-1.629678
C	-7.103308	3.269945	-0.662330
H	-7.710396	0.453298	2.478523
H	-5.131544	-5.772603	-2.478523
H	-0.453298	-7.710396	2.478523
H	0.453298	-7.710396	-2.478523
H	5.772603	-5.131544	-2.478523
H	5.131544	-5.772603	2.478523
H	7.710396	0.453298	-2.478523
H	7.710396	-0.453298	2.478523
H	5.131544	5.772603	-2.478523
H	5.772603	5.131544	2.478523
H	-0.453298	7.710396	-2.478523
H	0.453298	7.710396	2.478523
C	-2.710597	7.334998	-0.662330
C	-3.269945	7.103308	0.662330
C	-3.546555	6.782589	-1.629678
C	-4.487001	6.338107	0.497315
C	-4.652738	6.136768	-0.922376

C	-5.272454	5.635767	1.412626
C	-5.635767	5.272454	-1.412626
C	-6.136768	4.652738	0.922376
C	-6.338107	4.487001	-0.497315
H	-5.131544	5.772603	2.478523
H	-5.772603	5.131544	-2.478523
C	-6.782589	3.546555	1.629678
C	7.760301	2.411481	-5.085792
C	6.576874	2.612538	-5.799847
C	5.460548	3.141549	-5.149525
C	5.522717	3.467819	-3.797264
C	6.707919	3.268754	-3.063396
C	7.825221	2.736486	-3.734485
H	8.634502	2.002222	-5.584176
H	6.526483	2.358942	-6.854988
H	4.532730	3.296770	-5.693007
H	4.636455	3.840598	-3.295336
H	8.749374	2.595699	-3.181152
C	6.082601	-1.639780	-5.149525
C	6.497896	-2.803209	-5.799847
C	7.192536	-3.782187	-5.085792
C	7.468254	-3.598279	-3.734485
C	7.054573	-2.431857	-3.063396
C	6.357269	-1.453032	-3.797264
H	5.536292	-0.873955	-5.693007
H	6.282944	-2.946897	-6.854988
H	7.521300	-4.689730	-5.584176
H	8.022178	-4.351306	-3.181152
H	5.994182	-0.562756	-3.295336
C	3.141549	-5.460548	-5.149525
C	2.612538	-6.576874	-5.799847
C	2.411481	-7.760301	-5.085792
C	2.736486	-7.825221	-3.734485
C	3.268754	-6.707919	-3.063396
C	3.467819	-5.522717	-3.797264
H	3.296770	-4.532730	-5.693007
H	2.358942	-6.526483	-6.854988
H	2.002222	-8.634502	-5.584176
H	2.595699	-8.749374	-3.181152
H	3.840598	-4.636455	-3.295336
C	-3.782187	-7.192536	-5.085792
C	-2.803209	-6.497896	-5.799847
C	-1.639780	-6.082601	-5.149525
C	-1.453032	-6.357269	-3.797264

C	-2.431857	-7.054573	-3.063396
C	-3.598279	-7.468254	-3.734485
H	-4.689730	-7.521300	-5.584176
H	-2.946897	-6.282944	-6.854988
H	-0.873955	-5.536292	-5.693007
H	-0.562756	-5.994182	-3.295336
H	-4.351306	-8.022178	-3.181152
C	-5.460548	-3.141549	-5.149525
C	-6.576874	-2.612538	-5.799847
C	-7.760301	-2.411481	-5.085792
C	-7.825221	-2.736486	-3.734485
C	-6.707919	-3.268754	-3.063396
C	-5.522717	-3.467819	-3.797264
H	-4.532730	-3.296770	-5.693007
H	-6.526483	-2.358942	-6.854988
H	-8.634502	-2.002222	-5.584176
H	-8.749374	-2.595699	-3.181152
H	-4.636455	-3.840598	-3.295336
C	-6.082601	1.639780	-5.149525
C	-6.497896	2.803209	-5.799847
C	-7.192536	3.782187	-5.085792
C	-7.468254	3.598279	-3.734485
C	-7.054573	2.431857	-3.063396
C	-6.357269	1.453032	-3.797264
H	-5.536292	0.873955	-5.693007
H	-6.282944	2.946897	-6.854988
H	-7.521300	4.689730	-5.584176
H	-8.022178	4.351306	-3.181152
H	-5.994182	0.562756	-3.295336
C	-2.411481	7.760301	-5.085792
C	-2.612538	6.576874	-5.799847
C	-3.141549	5.460548	-5.149525
C	-3.467819	5.522717	-3.797264
C	-3.268754	6.707919	-3.063396
C	-2.736486	7.825221	-3.734485
H	-2.002222	8.634502	-5.584176
H	-2.358942	6.526483	-6.854988
H	-3.296770	4.532730	-5.693007
H	-3.840598	4.636455	-3.295336
H	-2.595699	8.749374	-3.181152
C	1.639780	6.082601	-5.149525
C	2.803209	6.497896	-5.799847
C	3.782187	7.192536	-5.085792
C	3.598279	7.468254	-3.734485

C	2.431857	7.054573	-3.063396
C	1.453032	6.357269	-3.797264
H	0.873955	5.536292	-5.693007
H	2.946897	6.282944	-6.854988
H	4.689730	7.521300	-5.584176
H	4.351306	8.022178	-3.181152
H	0.562756	5.994182	-3.295336
C	7.192536	3.782187	5.085792
C	6.497896	2.803209	5.799847
C	6.082601	1.639780	5.149525
C	6.357269	1.453032	3.797264
C	7.054573	2.431857	3.063396
C	7.468254	3.598279	3.734485
H	7.521300	4.689730	5.584176
H	6.282944	2.946897	6.854988
H	5.536292	0.873955	5.693007
H	5.994182	0.562756	3.295336
H	8.022178	4.351306	3.181152
C	7.760301	-2.411481	5.085792
C	6.576874	-2.612538	5.799847
C	5.460548	-3.141549	5.149525
C	5.522717	-3.467819	3.797264
C	6.707919	-3.268754	3.063396
C	7.825221	-2.736486	3.734485
H	8.634502	-2.002222	5.584176
H	6.526483	-2.358942	6.854988
H	4.532730	-3.296770	5.693007
H	4.636455	-3.840598	3.295336
H	8.749374	-2.595699	3.181152
C	3.782187	-7.192536	5.085792
C	2.803209	-6.497896	5.799847
C	1.639780	-6.082601	5.149525
C	1.453032	-6.357269	3.797264
C	2.431857	-7.054573	3.063396
C	3.598279	-7.468254	3.734485
H	4.689730	-7.521300	5.584176
H	2.946897	-6.282944	6.854988
H	0.873955	-5.536292	5.693007
H	0.562756	-5.994182	3.295336
H	4.351306	-8.022178	3.181152
C	-2.411481	-7.760301	5.085792
C	-2.612538	-6.576874	5.799847
C	-3.141549	-5.460548	5.149525
C	-3.467819	-5.522717	3.797264

C	-3.268754	-6.707919	3.063396
C	-2.736486	-7.825221	3.734485
H	-2.002222	-8.634502	5.584176
H	-2.358942	-6.526483	6.854988
H	-3.296770	-4.532730	5.693007
H	-3.840598	-4.636455	3.295336
H	-2.595699	-8.749374	3.181152
C	-7.192536	-3.782187	5.085792
C	-6.497896	-2.803209	5.799847
C	-6.082601	-1.639780	5.149525
C	-6.357269	-1.453032	3.797264
C	-7.054573	-2.431857	3.063396
C	-7.468254	-3.598279	3.734485
H	-7.521300	-4.689730	5.584176
H	-6.282944	-2.946897	6.854988
H	-5.536292	-0.873955	5.693007
H	-5.994182	-0.562756	3.295336
H	-8.022178	-4.351306	3.181152
C	-5.460548	3.141549	5.149525
C	-6.576874	2.612538	5.799847
C	-7.760301	2.411481	5.085792
C	-7.825221	2.736486	3.734485
C	-6.707919	3.268754	3.063396
C	-5.522717	3.467819	3.797264
H	-4.532730	3.296770	5.693007
H	-6.526483	2.358942	6.854988
H	-8.634502	2.002222	5.584176
H	-8.749374	2.595699	3.181152
H	-4.636455	3.840598	3.295336
C	-3.782187	7.192536	5.085792
C	-2.803209	6.497896	5.799847
C	-1.639780	6.082601	5.149525
C	-1.453032	6.357269	3.797264
C	-2.431857	7.054573	3.063396
C	-3.598279	7.468254	3.734485
H	-4.689730	7.521300	5.584176
H	-2.946897	6.282944	6.854988
H	-0.873955	5.536292	5.693007
H	-0.562756	5.994182	3.295336
H	-4.351306	8.022178	3.181152
C	2.411481	7.760301	5.085792
C	2.612538	6.576874	5.799847
C	3.141549	5.460548	5.149525
C	3.467819	5.522717	3.797264
C	3.268754	6.707919	3.063396
C	2.736486	7.825221	3.734485
H	2.002222	8.634502	5.584176
H	2.358942	6.526483	6.854988
H	3.296770	4.532730	5.693007
H	3.840598	4.636455	3.295336
H	2.595699	8.749374	3.181152

Table S 118. Coordinates of the calculated structure of the open-shell singlet of 13_8 (n=8) (TDDFT, BP86-D3/def2-TZVP) in D_8 geometry.

	x	y	z
C	-7.719418	0.257623	1.413447
C	-7.664494	1.310293	0.496546
C	-7.632913	1.049013	-0.923123
C	-7.719418	-0.257623	-1.413447
H	-7.716332	-0.455074	-2.483728
C	-7.664494	-1.310293	-0.496546
C	-7.632913	-1.049013	0.923123
C	-7.299475	-2.290035	1.631087
C	-7.118960	-3.277550	0.663607
C	-7.351442	-2.716287	-0.663607
C	-6.780808	-3.542209	-1.631087
C	-6.346132	-4.493099	0.496546
C	-5.640620	-5.276286	1.413447
H	-5.778057	-5.134485	2.483728
C	-6.139049	-4.655520	-0.923123
C	-4.655520	-6.139049	0.923123
C	-4.493099	-6.346132	-0.496546
C	-5.276286	-5.640620	-1.413447
C	-3.542209	-6.780808	1.631087
C	-2.716287	-7.351442	0.663607
C	-3.277550	-7.118960	-0.663607
C	-2.290035	-7.299475	-1.631087
C	-1.049013	-7.632913	-0.923123
C	-1.310293	-7.664494	0.496546
C	-0.257623	-7.719418	1.413447
C	0.257623	-7.719418	-1.413447
C	1.310293	-7.664494	-0.496546
C	1.049013	-7.632913	0.923123
C	2.290035	-7.299475	1.631087

C	3.277550	-7.118960	0.663607
C	2.716287	-7.351442	-0.663607
C	3.542209	-6.780808	-1.631087
C	4.655520	-6.139049	-0.923123
C	4.493099	-6.346132	0.496546
C	5.276286	-5.640620	1.413447
C	5.640620	-5.276286	-1.413447
C	6.346132	-4.493099	-0.496546
C	6.139049	-4.655520	0.923123
C	6.780808	-3.542209	1.631087
C	7.118960	-3.277550	-0.663607
C	7.351442	-2.716287	0.663607
C	7.299475	-2.290035	-1.631087
C	7.632913	-1.049013	-0.923123
C	7.664494	-1.310293	0.496546
C	7.719418	-0.257623	1.413447
C	7.719418	0.257623	-1.413447
C	7.664494	1.310293	-0.496546
C	7.632913	1.049013	0.923123
C	7.351442	2.716287	-0.663607
C	7.299475	2.290035	1.631087
C	6.780808	3.542209	-1.631087
C	7.118960	3.277550	0.663607
C	6.139049	4.655520	-0.923123
C	6.346132	4.493099	0.496546
C	5.276286	5.640620	-1.413447
C	5.640620	5.276286	1.413447
C	4.655520	6.139049	0.923123
C	4.493099	6.346132	-0.496546
C	3.277550	7.118960	-0.663607
C	3.542209	6.780808	1.631087
C	2.716287	7.351442	0.663607
C	2.290035	7.299475	-1.631087
C	1.049013	7.632913	-0.923123
C	1.310293	7.664494	0.496546
C	0.257623	7.719418	1.413447
C	-0.257623	7.719418	-1.413447
C	-1.310293	7.664494	-0.496546
C	-1.049013	7.632913	0.923123
C	-2.290035	7.299475	1.631087
C	-7.351442	2.716287	0.663607
C	-7.299475	2.290035	-1.631087
C	-7.118960	3.277550	-0.663607
H	-7.716332	0.455074	2.483728

H	-5.134485	-5.778057	-2.483728
H	-0.455074	-7.716332	2.483728
H	0.455074	-7.716332	-2.483728
H	5.778057	-5.134485	-2.483728
H	5.134485	-5.778057	2.483728
H	7.716332	0.455074	-2.483728
H	7.716332	-0.455074	2.483728
H	5.134485	5.778057	-2.483728
H	5.778057	5.134485	2.483728
H	-0.455074	7.716332	-2.483728
H	0.455074	7.716332	2.483728
C	-2.716287	7.351442	-0.663607
C	-3.277550	7.118960	0.663607
C	-3.542209	6.780808	-1.631087
C	-4.493099	6.346132	0.496546
C	-4.655520	6.139049	-0.923123
C	-5.276286	5.640620	1.413447
C	-5.640620	5.276286	-1.413447
C	-6.139049	4.655520	0.923123
C	-6.346132	4.493099	-0.496546
H	-5.134485	5.778057	2.483728
H	-5.778057	5.134485	-2.483728
C	-6.780808	3.542209	1.631087
C	7.636484	2.299571	-5.084684
C	6.431482	2.496963	-5.766430
C	5.345231	3.067754	-5.097001
C	5.457123	3.435354	-3.757356
C	6.663857	3.237662	-3.054233
C	7.752118	2.668395	-3.746673
H	8.490429	1.858467	-5.599952
H	6.341800	2.208899	-6.814457
H	4.398660	3.223413	-5.615949
H	4.589547	3.838687	-3.237346
H	8.696916	2.533922	-3.218667
C	5.948878	-1.610420	-5.097001
C	6.313364	-2.782125	-5.766430
C	7.025852	-3.773768	-5.084684
C	7.368415	-3.594735	-3.746673
C	7.001431	-2.422686	-3.054233
C	6.287931	-1.429606	-3.757356
H	5.389620	-0.831025	-5.615949
H	6.046258	-2.922402	-6.814457
H	7.317774	-4.689506	-5.599952
H	7.941402	-4.357895	-3.218667

H	5.959661	-0.530938	-3.237346
C	3.067754	-5.345231	-5.097001
C	2.496963	-6.431482	-5.766430
C	2.299571	-7.636484	-5.084684
C	2.668395	-7.752118	-3.746673
C	3.237662	-6.663857	-3.054233
C	3.435354	-5.457123	-3.757356
H	3.223413	-4.398660	-5.615949
H	2.208899	-6.341800	-6.814457
H	1.858467	-8.490429	-5.599952
H	2.533922	-8.696916	-3.218667
H	3.838687	-4.589547	-3.237346
C	-3.773768	-7.025852	-5.084684
C	-2.782125	-6.313364	-5.766430
C	-1.610420	-5.948878	-5.097001
C	-1.429606	-6.287931	-3.757356
C	-2.422686	-7.001431	-3.054233
C	-3.594735	-7.368415	-3.746673
H	-4.689506	-7.317774	-5.599952
H	-2.922402	-6.046258	-6.814457
H	-0.831025	-5.389620	-5.615949
H	-0.530938	-5.959661	-3.237346
H	-4.357895	-7.941402	-3.218667
C	-5.345231	-3.067754	-5.097001
C	-6.431482	-2.496963	-5.766430
C	-7.636484	-2.299571	-5.084684
C	-7.752118	-2.668395	-3.746673
C	-6.663857	-3.237662	-3.054233
C	-5.457123	-3.435354	-3.757356
H	-4.398660	-3.223413	-5.615949
H	-6.341800	-2.208899	-6.814457
H	-8.490429	-1.858467	-5.599952
H	-8.696916	-2.533922	-3.218667
H	-4.589547	-3.838687	-3.237346
C	-5.948878	1.610420	-5.097001
C	-6.313364	2.782125	-5.766430
C	-7.025852	3.773768	-5.084684
C	-7.368415	3.594735	-3.746673
C	-7.001431	2.422686	-3.054233
C	-6.287931	1.429606	-3.757356
H	-5.389620	0.831025	-5.615949
H	-6.046258	2.922402	-6.814457
H	-7.317774	4.689506	-5.599952
H	-7.941402	4.357895	-3.218667

H	-5.959661	0.530938	-3.237346
C	-2.299571	7.636484	-5.084684
C	-2.496963	6.431482	-5.766430
C	-3.067754	5.345231	-5.097001
C	-3.435354	5.457123	-3.757356
C	-3.237662	6.663857	-3.054233
C	-2.668395	7.752118	-3.746673
H	-1.858467	8.490429	-5.599952
H	-2.208899	6.341800	-6.814457
H	-3.223413	4.398660	-5.615949
H	-3.838687	4.589547	-3.237346
H	-2.533922	8.696916	-3.218667
C	1.610420	5.948878	-5.097001
C	2.782125	6.313364	-5.766430
C	3.773768	7.025852	-5.084684
C	3.594735	7.368415	-3.746673
C	2.422686	7.001431	-3.054233
C	1.429606	6.287931	-3.757356
H	0.831025	5.389620	-5.615949
H	2.922402	6.046258	-6.814457
H	4.689506	7.317774	-5.599952
H	4.357895	7.941402	-3.218667
H	0.530938	5.959661	-3.237346
C	7.025852	3.773768	5.084684
C	6.313364	2.782125	5.766430
C	5.948878	1.610420	5.097001
C	6.287931	1.429606	3.757356
C	7.001431	2.422686	3.054233
C	7.368415	3.594735	3.746673
H	7.317774	4.689506	5.599952
H	6.046258	2.922402	6.814457
H	5.389620	0.831025	5.615949
H	5.959661	0.530938	3.237346
H	7.941402	4.357895	3.218667
C	7.636484	-2.299571	5.084684
C	6.431482	-2.496963	5.766430
C	5.345231	-3.067754	5.097001
C	5.457123	-3.435354	3.757356
C	6.663857	-3.237662	3.054233
C	7.752118	-2.668395	3.746673
H	8.490429	-1.858467	5.599952
H	6.341800	-2.208899	6.814457
H	4.398660	-3.223413	5.615949
H	4.589547	-3.838687	3.237346

H	8.696916	-2.533922	3.218667
C	3.773768	-7.025852	5.084684
C	2.782125	-6.313364	5.766430
C	1.610420	-5.948878	5.097001
C	1.429606	-6.287931	3.757356
C	2.422686	-7.001431	3.054233
C	3.594735	-7.368415	3.746673
H	4.689506	-7.317774	5.599952
H	2.922402	-6.046258	6.814457
H	0.831025	-5.389620	5.615949
H	0.530938	-5.959661	3.237346
H	4.357895	-7.941402	3.218667
C	-2.299571	-7.636484	5.084684
C	-2.496963	-6.431482	5.766430
C	-3.067754	-5.345231	5.097001
C	-3.435354	-5.457123	3.757356
C	-3.237662	-6.663857	3.054233
C	-2.668395	-7.752118	3.746673
H	-1.858467	-8.490429	5.599952
H	-2.208899	-6.341800	6.814457
H	-3.223413	-4.398660	5.615949
H	-3.838687	-4.589547	3.237346
H	-2.533922	-8.696916	3.218667
C	-7.025852	-3.773768	5.084684
C	-6.313364	-2.782125	5.766430
C	-5.948878	-1.610420	5.097001
C	-6.287931	-1.429606	3.757356
C	-7.001431	-2.422686	3.054233
C	-7.368415	-3.594735	3.746673
H	-7.317774	-4.689506	5.599952
H	-6.046258	-2.922402	6.814457
H	-5.389620	-0.831025	5.615949
H	-5.959661	-0.530938	3.237346
H	-7.941402	-4.357895	3.218667

C	-5.345231	3.067754	5.097001
C	-6.431482	2.496963	5.766430
C	-7.636484	2.299571	5.084684
C	-7.752118	2.668395	3.746673
C	-6.663857	3.237662	3.054233
C	-5.457123	3.435354	3.757356
H	-4.398660	3.223413	5.615949
H	-6.341800	2.208899	6.814457
H	-8.490429	1.858467	5.599952
H	-8.696916	2.533922	3.218667
H	-4.589547	3.838687	3.237346
C	-3.773768	7.025852	5.084684
C	-2.782125	6.313364	5.766430
C	-1.610420	5.948878	5.097001
C	-1.429606	6.287931	3.757356
C	-2.422686	7.001431	3.054233
C	-3.594735	7.368415	3.746673
H	-4.689506	7.317774	5.599952
H	-2.922402	6.046258	6.814457
H	-0.831025	5.389620	5.615949
H	-0.530938	5.959661	3.237346
H	-4.357895	7.941402	3.218667
C	2.299571	7.636484	5.084684
C	2.496963	6.431482	5.766430
C	3.067754	5.345231	5.097001
C	3.435354	5.457123	3.757356
C	3.237662	6.663857	3.054233
C	2.668395	7.752118	3.746673
H	1.858467	8.490429	5.599952
H	2.208899	6.341800	6.814457
H	3.223413	4.398660	5.615949
H	3.838687	4.589547	3.237346
H	2.533922	8.696916	3.218667