Orbital Contributions to the Magnetic Shielding of Cyclo[2*n*]carbons (*n* = 3 – 12)

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Supplementary Information

Absolute energies and x, y, z coordinates of optimized structures

Cyclo[6]carbon

E = -228.2353012 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.080376	0.000000
2	6	0	1.271856	0.734306	0.000000
3	6	0	0.935633	-0.540188	0.000000
4	6	0	0.000000	-1.468612	0.000000
5	6	0	-0.935633	-0.540188	0.000000
6	6	0	-1.271856	0.734306	0.000000

Cyclo[8]carbon

E = -304.3731121 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.664473	1.715966	0.000000
2	6	0	-0.664473	1.338567	0.000000
3	6	0	-1.715966	0.664473	0.000000
4	6	0	-1.338567	-0.664473	0.000000
5	6	0	-0.664473	-1.715966	0.000000
6	6	0	0.664473	-1.338567	0.000000
7	6	0	1.715966	-0.664473	0.000000
8	6	0	1.338567	0.664473	0.000000

Cyclo[10]carbon

E = -380.6228357 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.923867	0.000000
2	6	0	1.277008	1.757651	0.000000
3	6	0	1.829707	0.594508	0.000000
4	6	0	2.066243	-0.671363	0.000000
5	6	0	1.130821	-1.556441	0.000000
6	6	0	0.000000	-2.172576	0.000000
7	6	0	-1.130821	-1.556441	0.000000
8	6	0	-2.066243	-0.671363	0.000000
9	6	0	-1.829707	0.594508	0.000000
10	6	0	-1.277008	1.757651	0.000000

Cyclo[12]carbon

E = -456.7388599 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.361362	0.000000
2	6	0	-1.227779	2.264466	0.000000
3	6	0	-2.044999	1.180681	0.000000
4	6	0	-2.574974	0.068945	0.000000
5	6	0	-2.044999	-1.180681	0.000000
6	6	0	-1.347195	-2.195521	0.000000
7	6	0	0.000000	-2.361362	0.000000
8	6	0	1.227779	-2.264466	0.000000
9	6	0	2.044999	-1.180681	0.000000
10	6	0	2.574974	-0.068945	0.000000
11	6	0	2.044999	1.180681	0.000000
12	6	0	1.347195	2.195521	0.000000

Cyclo[14]carbon

E = -532.9374548 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.618958	2.711831	0.000000
2	6	0	-1.808584	2.307097	0.000000
3	6	0	-2.506109	1.206878	0.000000
4	6	0	-2.931395	0.024444	0.000000
5	6	0	-2.506109	-1.206878	0.000000
6	6	0	-1.846806	-2.276616	0.000000
7	6	0	-0.618958	-2.711831	0.000000
8	6	0	0.628466	-2.863338	0.000000
9	6	0	1.734281	-2.174720	0.000000
10	6	0	2.630490	-1.293908	0.000000
11	6	0	2.781571	0.000000	0.000000
12	6	0	2.651701	1.249862	0.000000
13	6	0	1.734281	2.174720	0.000000
14	6	0	0.676128	2.852460	0.000000

Cyclo[16]carbon

E = -609.0779286 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.076528	3.300549	0.000000
2	6	0	-1.263117	3.049435	0.000000
3	6	0	-2.387954	2.279727	0.000000
4	6	0	-3.049435	1.263117	0.000000
5	6	0	-3.300549	-0.076528	0.000000
6	6	0	-3.049435	-1.263117	0.000000
7	6	0	-2.279727	-2.387954	0.000000
8	6	0	-1.263117	-3.049435	0.000000
9	6	0	0.076528	-3.300549	0.000000
10	6	0	1.263117	-3.049435	0.000000
11	6	0	2.387954	-2.279727	0.000000
12	6	0	3.049435	-1.263117	0.000000
13	6	0	3.300549	0.076528	0.000000
14	6	0	3.049435	1.263117	0.000000
15	6	0	2.279727	2.387954	0.000000
16	6	0	1.263117	3.049435	0.000000

Cyclo[18]carbon

E = -685.2534457 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.610165	3.642263	0.000000
2	6	0	-0.610165	3.642263	0.000000
3	6	0	-1.873788	3.182342	0.000000
4	6	0	-2.808615	2.397929	0.000000
5	6	0	-3.480975	1.233367	0.000000
6	6	0	-3.692883	0.031578	0.000000
7	6	0	-3.459375	-1.292714	0.000000
8	6	0	-2.849210	-2.349550	0.000000
9	6	0	-1.819095	-3.213919	0.000000
10	6	0	-0.672360	-3.631296	0.000000
11	6	0	0.672360	-3.631296	0.000000
12	6	0	1.819095	-3.213919	0.000000
13	6	0	2.849210	-2.349550	0.000000
14	6	0	3.459375	-1.292714	0.000000
15	6	0	3.692883	0.031578	0.000000
16	6	0	3.480975	1.233367	0.000000
17	6	0	2.808615	2.397929	0.000000
18	6	0	1.873788	3.182342	0.000000

Cyclo[20]carbon

E = -761.4040775 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.606797	4.063428	0.000000
2	6	0	-0.606797	4.063428	0.000000
3	6	0	-1.897514	3.644048	0.000000
4	6	0	-2.879332	2.930716	0.000000
5	6	0	-3.677039	1.832766	0.000000
6	6	0	-4.052060	0.678570	0.000000
7	6	0	-4.052060	-0.678570	0.000000
8	6	0	-3.677039	-1.832766	0.000000
9	6	0	-2.879332	-2.930716	0.000000
10	6	0	-1.897514	-3.644048	0.000000
11	6	0	-0.606797	-4.063428	0.000000
12	6	0	0.606797	-4.063428	0.000000
13	6	0	1.897514	-3.644048	0.000000
14	6	0	2.879332	-2.930716	0.000000
15	6	0	3.677039	-1.832766	0.000000
16	6	0	4.052060	-0.678570	0.000000
17	6	0	4.052060	0.678570	0.000000
18	6	0	3.677039	1.832766	0.000000
19	6	0	2.879332	2.930716	0.000000
20	6	0	1.897514	3.644048	0.000000

Cyclo[22]carbon

E = -837.5675672 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.608247	4.466506	0.000000
2	6	0	0.608247	4.466506	0.000000
3	6	0	1.903085	4.086307	0.000000
4	6	0	2.926466	3.428621	0.000000
5	6	0	3.810202	2.408735	0.000000
6	6	0	4.315552	1.302173	0.000000
7	6	0	4.507606	-0.033594	0.000000
8	6	0	4.334481	-1.237706	0.000000
9	6	0	3.773877	-2.465257	0.000000
10	6	0	2.977243	-3.384622	0.000000
11	6	0	1.841969	-4.114218	0.000000
12	6	0	0.674751	-4.456944	0.000000
13	6	0	-0.674751	-4.456944	0.000000
14	6	0	-1.841969	-4.114218	0.000000
15	6	0	-2.977243	-3.384622	0.000000
16	6	0	-3.773877	-2.465257	0.000000
17	6	0	-4.334481	-1.237706	0.000000
18	6	0	-4.507606	-0.033594	0.000000
19	6	0	-4.315552	1.302173	0.000000

20	6	0	-3.810202	2.408735	0.000000
21	6	0	-2.926466	3.428621	0.000000
22	6	0	-1.903085	4.086307	0.000000

Cyclo[24]carbon

E = -913.7206029 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.606859	4.881282	0.000000
2	6	0	0.606859	4.881282	0.000000
3	6	0	1.915086	4.530743	0.000000
4	6	0	2.966196	3.923885	0.000000
5	6	0	3.923885	2.966196	0.000000
6	6	0	4.530743	1.915086	0.000000
7	6	0	4.881282	0.606859	0.000000
8	6	0	4.881282	-0.606859	0.000000
9	6	0	4.530743	-1.915086	0.000000
10	6	0	3.923885	-2.966196	0.000000
11	6	0	2.966196	-3.923885	0.000000
12	6	0	1.915086	-4.530743	0.000000
13	6	0	0.606859	-4.881282	0.000000
14	6	0	-0.606859	-4.881282	0.000000
15	6	0	-1.915086	-4.530743	0.000000
16	6	0	-2.966196	-3.923885	0.000000
17	6	0	-3.923885	-2.966196	0.000000
18	6	0	-4.530743	-1.915086	0.000000
19	6	0	-4.881282	-0.606859	0.000000
20	6	0	-4.881282	0.606859	0.000000
21	6	0	-4.530743	1.915086	0.000000
22	6	0	-3.923885	2.966196	0.000000
23	6	0	-2.966196	3.923885	0.000000
24	6	0	-1.915086	4.530743	0.000000