

Supporting Information

Open-shell spherical aromaticity: The $2N^2+2N+1$ (with $S = N + 1/2$) rule

Jordi Poater^a and Miquel Solà^{*a}

5

- Complete reference 16:** M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision A.02 ed., Gaussian, Inc., Pittsburgh, PA, 2009.

Table S1. Optimized Cartesian xyz coordinates (in Å) of all analyzed species.

20 C₅H₅⁻

C	0.00000000	0.00000000	1.20277388
C	0.00000000	1.14446647	0.37190541
H	0.00000000	2.18149170	0.70944130
C	0.00000000	0.70709342	-0.97327141
25 H	0.00000000	1.34714608	-1.85631668
C	0.00000000	-1.14446647	0.37190541
H	0.00000000	-2.18149170	0.70944130
C	0.00000000	-0.70709342	-0.97327141
H	0.00000000	-1.34714608	-1.85631668
30 H	0.00000000	0.00000000	2.29349958

C₅H₅⁺

C	0.00000000	0.00000000	1.21314727
C	0.00000000	1.15391432	0.37501229
35 H	0.00000000	2.18463951	0.71034373
C	0.00000000	0.71309739	-0.98158434
H	0.00000000	1.34961720	-1.85889739
C	0.00000000	-1.15391432	0.37501229
H	0.00000000	-2.18463951	0.71034373
40 C	0.00000000	-0.71309739	-0.98158434
H	0.00000000	-1.34961720	-1.85889739
H	0.00000000	0.00000000	2.29708817

C₆H₆

45 C	0.00000000	1.39648969	0.00000000
C	1.20939554	0.69824485	0.00000000
C	1.20939554	-0.69824485	0.00000000
C	0.00000000	-1.39648969	0.00000000

C	-1.20939554	-0.69824485	0.00000000
C	-1.20939554	0.69824485	0.00000000
H	0.00000000	2.48319063	0.00000000
H	2.15050617	1.24159531	0.00000000
5 H	2.15050617	-1.24159531	0.00000000
H	0.00000000	-2.48319063	0.00000000
H	-2.15050617	-1.24159531	0.00000000
H	-2.15050617	1.24159531	0.00000000

10 C₆H₆²⁺

C	0.00000000	1.43306823	0.00000000
C	1.24107349	0.71653411	0.00000000
C	1.24107349	-0.71653411	0.00000000
C	0.00000000	-1.43306823	0.00000000
15 C	-1.24107349	-0.71653411	0.00000000
C	-1.24107349	0.71653411	0.00000000
H	0.00000000	2.52383484	0.00000000
H	2.18570509	1.26191742	0.00000000
H	2.18570509	-1.26191742	0.00000000
20 H	0.00000000	-2.52383484	0.00000000
H	-2.18570509	-1.26191742	0.00000000
H	-2.18570509	1.26191742	0.00000000

C₂₀

25 C	1.18387443	-0.41547354	1.57401052
C	0.72176653	0.95383007	1.54558476
C	0.00000005	-1.31154237	1.63001890
C	-1.18387443	-0.41547356	1.57401063
C	-0.72176653	0.95383010	1.54558484
30 C	0.00000003	-2.04826449	0.43980973
C	-1.18218980	-1.59224434	-0.33473738
C	-1.95572583	-0.65399826	0.40353065
C	1.18218984	-1.59224429	-0.33473740
C	0.72176659	-0.95383007	-1.54558479
35 C	-0.72176655	-0.95383010	-1.54558486
C	1.95572569	-0.65399820	0.40353059
C	1.95572573	0.65399822	-0.40353059
C	1.18387448	0.41547353	-1.57401055
C	1.18218978	1.59224427	0.33473741
40 C	0.00000003	2.04826446	-0.43980970
C	0.00000005	1.31154236	-1.63001892
C	-1.18387443	0.41547356	-1.57401063
C	-1.95572585	0.65399830	-0.40353061
C	-1.18218979	1.59224435	0.33473742

45

C₂₀²⁺

C	1.17103792	-0.38049328	1.61179542
C	0.72374124	0.99614435	1.61179542
C	0.00000000	-1.23130214	1.61179542

	C	-1.17103792	-0.38049328	1.61179542
	C	-0.72374124	0.99614435	1.61179542
	C	0.00000000	-1.99228870	0.38049328
	C	-1.17103792	-1.61179542	-0.38049328
5	C	-1.89477916	-0.61565107	0.38049328
	C	1.17103792	-1.61179542	-0.38049328
	C	0.72374124	-0.99614435	-1.61179542
	C	-0.72374124	-0.99614435	-1.61179542
	C	1.89477916	-0.61565107	0.38049328
10	C	1.89477916	0.61565107	-0.38049328
	C	1.17103792	0.38049328	-1.61179542
	C	1.17103792	1.61179542	0.38049328
	C	0.00000000	1.99228870	-0.38049328
	C	0.00000000	1.23130214	-1.61179542
15	C	-1.17103792	0.38049328	-1.61179542
	C	-1.89477916	0.61565107	-0.38049328
	C	-1.17103792	1.61179542	0.38049328

C_{20}^{7+}

20	C	1.20848444	-0.39266040	1.66333613
	C	0.74688446	1.02799827	1.66333613
	C	0.00000000	-1.27067573	1.66333613
	C	-1.20848444	-0.39266040	1.66333613
	C	-0.74688446	1.02799827	1.66333613
25	C	0.00000000	-2.05599653	0.39266040
	C	-1.20848444	-1.66333613	-0.39266040
	C	-1.95536890	-0.63533787	0.39266040
	C	1.20848444	-1.66333613	-0.39266040
	C	0.74688446	-1.02799827	-1.66333613
30	C	-0.74688446	-1.02799827	-1.66333613
	C	1.95536890	-0.63533787	0.39266040
	C	1.95536890	0.63533787	-0.39266040
	C	1.20848444	0.39266040	-1.66333613
	C	1.20848444	1.66333613	0.39266040
35	C	0.00000000	2.05599653	-0.39266040
	C	0.00000000	1.27067573	-1.66333613
	C	-1.20848444	0.39266040	-1.66333613
	C	-1.95536890	0.63533787	-0.39266040
	C	-1.20848444	1.66333613	0.39266040

40

C_{20}^{5-}

	C	1.22036910	-0.39652196	1.67969397
	C	0.75422958	1.03810796	1.67969397
	C	0.00000000	-1.28317201	1.67969397
45	C	-1.22036910	-0.39652196	1.67969397
	C	-0.75422958	1.03810796	1.67969397
	C	0.00000000	-2.07621593	0.39652196
	C	-1.22036910	-1.67969397	-0.39652196
	C	-1.97459869	-0.64158601	0.39652196

C	1.22036910	-1.67969397	-0.39652196
C	0.75422958	-1.03810796	-1.67969397
C	-0.75422958	-1.03810796	-1.67969397
C	1.97459869	-0.64158601	0.39652196
5 C	1.97459869	0.64158601	-0.39652196
C	1.22036910	0.39652196	-1.67969397
C	1.22036910	1.67969397	0.39652196
C	0.00000000	2.07621593	-0.39652196
C	0.00000000	1.28317201	-1.67969397
10 C	-1.22036910	0.39652196	-1.67969397
C	-1.97459869	0.64158601	-0.39652196
C	-1.22036910	1.67969397	0.39652196

C₆₀

15 C	0.72671577	-1.00023846	3.32766488
C	-0.72671577	-1.00023846	3.32766488
C	-1.42445978	-1.96060069	2.59401341
C	-0.69774401	-2.96083915	1.82989923
C	0.69774401	-2.96083915	1.82989923
20 C	1.42445978	-1.96060069	2.59401341
C	1.17585083	0.38205709	3.32766488
C	0.00000000	1.23636273	3.32766488
C	-1.17585083	0.38205709	3.32766488
C	-2.30482435	0.74888283	2.59401341
25 C	-2.60031061	-1.57854360	1.82989923
C	-1.42445978	-3.19696342	0.59353650
C	-0.72671577	-3.42367419	-0.59353650
C	0.72671577	-3.42367419	-0.59353650
C	1.42445978	-3.19696342	0.59353650
30 C	2.60031061	-2.34265778	0.59353650
C	2.60031061	-1.57854360	1.82989923
C	3.03154012	-0.25135563	1.82989923
C	2.30482435	0.74888283	2.59401341
C	0.00000000	2.42343573	2.59401341
35 C	1.17585083	2.80549282	1.82989923
C	2.30482435	1.98524555	1.82989923
C	3.03154012	1.74912128	0.59353650
C	3.48067517	0.36682573	0.59353650
C	3.48067517	-0.36682573	-0.59353650
40 C	3.03154012	-1.74912128	-0.59353650
C	2.30482435	-1.98524555	-1.82989923
C	1.17585083	-2.80549282	-1.82989923
C	-2.60031061	-2.34265778	0.59353650
C	-1.17585083	-0.38205709	-3.32766488
45 C	-2.30482435	-0.74888283	-2.59401341
C	-3.03154012	0.25135563	-1.82989923
C	-2.60031061	1.57854360	-1.82989923
C	-1.42445978	1.96060069	-2.59401341
C	0.72671577	1.00023846	-3.32766488

C	1.17585083	-0.38205709	-3.32766488
C	0.00000000	-1.23636273	-3.32766488
C	0.00000000	-2.42343573	-2.59401341
C	-1.17585083	-2.80549282	-1.82989923
5 C	-2.30482435	-1.98524555	-1.82989923
C	-3.48067517	-0.36682573	-0.59353650
C	-3.48067517	0.36682573	0.59353650
C	-3.03154012	1.74912128	0.59353650
C	-2.60031061	2.34265778	-0.59353650
10 C	-1.42445978	3.19696342	-0.59353650
C	-0.69774401	2.96083915	-1.82989923
C	0.69774401	2.96083915	-1.82989923
C	1.42445978	1.96060069	-2.59401341
C	2.30482435	-0.74888283	-2.59401341
15 C	3.03154012	0.25135563	-1.82989923
C	2.60031061	1.57854360	-1.82989923
C	2.60031061	2.34265778	-0.59353650
C	1.42445978	3.19696342	-0.59353650
C	0.72671577	3.42367419	0.59353650
20 C	-0.72671577	3.42367419	0.59353650
C	-1.17585083	2.80549282	1.82989923
C	-2.30482435	1.98524555	1.82989923
C	-3.03154012	-1.74912128	-0.59353650
C	-3.03154012	-0.25135563	1.82989923
25 C	-0.72671577	1.00023846	-3.32766488

C_{60}^{1-}			
C	0.71979493	-0.99071273	3.34879325
C	-0.71979493	-0.99071273	3.34879325
30 C	-1.43866272	-1.98014936	2.59293092
C	-0.71886779	-2.97086209	1.83609374
C	0.71886779	-2.97086209	1.83609374
C	1.43866272	-1.98014936	2.59293092
C	1.16465266	0.37841859	3.34879325
35 C	0.00000000	1.22458828	3.34879325
C	-1.16465266	0.37841859	3.34879325
C	-2.32780518	0.75634975	2.59293092
C	-2.60331539	-1.60173077	1.83609374
C	-1.43866272	-3.20473764	0.61150547
40 C	-0.71979493	-3.43831194	-0.61150547
C	0.71979493	-3.43831194	-0.61150547
C	1.43866272	-3.20473764	0.61150547
C	2.60331539	-2.35856795	0.61150547
C	2.60331539	-1.60173077	1.83609374
45 C	3.04760011	-0.23436298	1.83609374
C	2.32780518	0.75634975	2.59293092
C	0.00000000	2.44759921	2.59293092
C	1.16465266	2.82601780	1.83609374
C	2.32780518	1.98093803	1.83609374

C	3.04760011	1.74706248	0.61150547
C	3.49245784	0.37793116	0.61150547
C	3.49245784	-0.37793116	-0.61150547
C	3.04760011	-1.74706248	-0.61150547
5 C	2.32780518	-1.98093803	-1.83609374
C	1.16465266	-2.82601780	-1.83609374
C	-2.60331539	-2.35856795	0.61150547
C	-1.16465266	-0.37841859	-3.34879325
C	-2.32780518	-0.75634975	-2.59293092
10 C	-3.04760011	0.23436298	-1.83609374
C	-2.60331539	1.60173077	-1.83609374
C	-1.43866272	1.98014936	-2.59293092
C	0.71979493	0.99071273	-3.34879325
C	1.16465266	-0.37841859	-3.34879325
15 C	0.00000000	-1.22458828	-3.34879325
C	0.00000000	-2.44759921	-2.59293092
C	-1.16465266	-2.82601780	-1.83609374
C	-2.32780518	-1.98093803	-1.83609374
C	-3.49245784	-0.37793116	-0.61150547
20 C	-3.49245784	0.37793116	0.61150547
C	-3.04760011	1.74706248	0.61150547
C	-2.60331539	2.35856795	-0.61150547
C	-1.43866272	3.20473764	-0.61150547
C	-0.71886779	2.97086209	-1.83609374
25 C	0.71886779	2.97086209	-1.83609374
C	1.43866272	1.98014936	-2.59293092
C	2.32780518	-0.75634975	-2.59293092
C	3.04760011	0.23436298	-1.83609374
C	2.60331539	1.60173077	-1.83609374
30 C	2.60331539	2.35856795	-0.61150547
C	1.43866272	3.20473764	-0.61150547
C	0.71979493	3.43831194	0.61150547
C	-0.71979493	3.43831194	0.61150547
C	-1.16465266	2.82601780	1.83609374
35 C	-2.32780518	1.98093803	1.83609374
C	-3.04760011	-1.74706248	-0.61150547
C	-3.04760011	-0.23436298	1.83609374
C	-0.71979493	0.99071273	-3.34879325
40 C ₆₀ ¹⁹⁺			
C	0.76172002	-1.04841767	3.53338742
C	-0.76172002	-1.04841767	3.53338742
C	-1.51696014	-2.08791652	2.73928096
C	-0.75524012	-3.13633419	1.93836113
45 C	0.75524012	-3.13633419	1.93836113
C	1.51696014	-2.08791652	2.73928096
C	1.23248889	0.40045992	3.53338742
C	0.00000000	1.29591551	3.53338742
C	-1.23248889	0.40045992	3.53338742

C	-2.45449308	0.79751315	2.73928096
C	-2.74944904	-1.68745660	1.93836113
C	-1.51696014	-3.38383203	0.64244562
C	-0.76172002	-3.62922442	-0.64244562
5 C	0.76172002	-3.62922442	-0.64244562
C	1.51696014	-3.38383203	0.64244562
C	2.74944904	-2.48837643	0.64244562
C	2.74944904	-1.68745660	1.93836113
C	3.21621310	-0.25090453	1.93836113
10 C	2.45449308	0.79751315	2.73928096
C	0.00000000	2.58080674	2.73928096
C	1.23248889	2.98126666	1.93836113
C	2.45449308	2.09342865	1.93836113
C	3.21621310	1.84593081	0.64244562
15 C	3.68698196	0.39705323	0.64244562
C	3.68698196	-0.39705323	-0.64244562
C	3.21621310	-1.84593081	-0.64244562
C	2.45449308	-2.09342865	-1.93836113
C	1.23248889	-2.98126666	-1.93836113
20 C	-2.74944904	-2.48837643	0.64244562
C	-1.23248889	-0.40045992	-3.53338742
C	-2.45449308	-0.79751315	-2.73928096
C	-3.21621310	0.25090453	-1.93836113
C	-2.74944904	1.68745660	-1.93836113
25 C	-1.51696014	2.08791652	-2.73928096
C	0.76172002	1.04841767	-3.53338742
C	1.23248889	-0.40045992	-3.53338742
C	0.00000000	-1.29591551	-3.53338742
C	0.00000000	-2.58080674	-2.73928096
30 C	-1.23248889	-2.98126666	-1.93836113
C	-2.45449308	-2.09342865	-1.93836113
C	-3.68698196	-0.39705323	-0.64244562
C	-3.68698196	0.39705323	0.64244562
C	-3.21621310	1.84593081	0.64244562
35 C	-2.74944904	2.48837643	-0.64244562
C	-1.51696014	3.38383203	-0.64244562
C	-0.75524012	3.13633419	-1.93836113
C	0.75524012	3.13633419	-1.93836113
C	1.51696014	2.08791652	-2.73928096
40 C	2.45449308	-0.79751315	-2.73928096
C	3.21621310	0.25090453	-1.93836113
C	2.74944904	1.68745660	-1.93836113
C	2.74944904	2.48837643	-0.64244562
C	1.51696014	3.38383203	-0.64244562
45 C	0.76172002	3.62922442	0.64244562
C	-0.76172002	3.62922442	0.64244562
C	-1.23248889	2.98126666	1.93836113
C	-2.45449308	2.09342865	1.93836113
C	-3.21621310	-1.84593081	-0.64244562

C	-3.21621310	-0.25090453	1.93836113
C	-0.76172002	1.04841767	-3.53338742
C_{60}^{10+}			
5 C	0.73015276	-1.00496905	3.37059545
C	-0.73015276	-1.00496905	3.37059545
C	-1.44549266	-1.98954995	2.61844257
C	-0.71533990	-2.99451901	1.85071453
C	0.71533990	-2.99451901	1.85071453
10 C	1.44549266	-1.98954995	2.61844257
C	1.18141198	0.38386402	3.37059545
C	0.00000000	1.24221007	3.37059545
C	-1.18141198	0.38386402	3.37059545
C	-2.33885624	0.75994046	2.61844257
15 C	-2.62690463	-1.60568594	1.85071453
C	-1.44549266	-3.23176002	0.60850446
C	-0.73015276	-3.46418804	-0.60850446
C	0.73015276	-3.46418804	-0.60850446
C	1.44549266	-3.23176002	0.60850446
20 C	2.62690463	-2.37341398	0.60850446
C	2.62690463	-1.60568594	1.85071453
C	3.06900900	-0.24502859	1.85071453
C	2.33885624	0.75994046	2.61844257
C	0.00000000	2.45921899	2.61844257
25 C	1.18141198	2.84308301	1.85071453
C	2.33885624	2.00215052	1.85071453
C	3.06900900	1.76490952	0.60850446
C	3.52026822	0.37607644	0.60850446
C	3.52026822	-0.37607644	-0.60850446
30 C	3.06900900	-1.76490952	-0.60850446
C	2.33885624	-2.00215052	-1.85071453
C	1.18141198	-2.84308301	-1.85071453
C	-2.62690463	-2.37341398	0.60850446
C	-1.18141198	-0.38386402	-3.37059545
35 C	-2.33885624	-0.75994046	-2.61844257
C	-3.06900900	0.24502859	-1.85071453
C	-2.62690463	1.60568594	-1.85071453
C	-1.44549266	1.98954995	-2.61844257
C	0.73015276	1.00496905	-3.37059545
40 C	1.18141198	-0.38386402	-3.37059545
C	0.00000000	-1.24221007	-3.37059545
C	0.00000000	-2.45921899	-2.61844257
C	-1.18141198	-2.84308301	-1.85071453
C	-2.33885624	-2.00215052	-1.85071453
45 C	-3.52026822	-0.37607644	-0.60850446
C	-3.52026822	0.37607644	0.60850446
C	-3.06900900	1.76490952	0.60850446
C	-2.62690463	2.37341398	-0.60850446
C	-1.44549266	3.23176002	-0.60850446

C	-0.71533990	2.99451901	-1.85071453
C	0.71533990	2.99451901	-1.85071453
C	1.44549266	1.98954995	-2.61844257
C	2.33885624	-0.75994046	-2.61844257
5 C	3.06900900	0.24502859	-1.85071453
C	2.62690463	1.60568594	-1.85071453
C	2.62690463	2.37341398	-0.60850446
C	1.44549266	3.23176002	-0.60850446
C	0.73015276	3.46418804	0.60850446
10 C	-0.73015276	3.46418804	0.60850446
C	-1.18141198	2.84308301	1.85071453
C	-2.33885624	2.00215052	1.85071453
C	-3.06900900	-1.76490952	-0.60850446
C	-3.06900900	-0.24502859	1.85071453
15 C	-0.73015276	1.00496905	-3.37059545

C ₈₀			
C	0.00000000	4.08920371	0.24137285
C	0.81329148	3.73282579	1.36681726
20 C	0.15871204	3.23094604	2.53286993
C	-2.63362828	-3.12747447	0.24140738
C	0.48519873	3.90665844	-1.11675910
C	1.95946024	2.57354518	-2.53284962
C	1.78194729	3.37860695	-1.36677769
25 C	2.63362828	3.12747447	-0.24140738
C	2.76963218	2.32000372	1.94398240
C	2.07642124	1.73950174	3.07293017
C	0.78770513	2.24581944	3.37990865
C	2.34894714	0.38203862	3.37990932
30 C	3.62586482	1.53313480	1.11675910
C	4.02528648	-0.71705177	0.24140738
C	3.81693310	0.14609185	1.36677769
C	3.20848563	-0.41016975	2.53284962
C	2.87743737	1.47802436	-2.53286993
35 C	3.63936770	1.16208181	-1.36681726
C	3.54135430	2.04460185	-0.24137285
C	3.93118404	-0.20735291	-1.11669019
C	-3.39399825	1.23856997	1.94398240
C	-2.54466331	0.92848267	3.07293017
40 C	-0.24327978	1.38565283	3.89594417
C	-1.50532872	1.84322858	3.37990932
C	-3.14066610	2.37352365	1.11675910
C	-1.39165820	3.84452623	0.24140738
C	-2.03498580	3.23251510	1.36677769
45 C	-1.24902539	2.98371494	2.53284962
C	-2.71872533	1.75292168	-2.53286993
C	-2.82607622	2.57074398	-1.36681726
C	-3.54135430	2.04460185	-0.24137285
C	-1.78601913	3.50818170	-1.11669019

C	0.24327978	-1.38565283	-3.89594417
C	2.54466331	-0.92848267	-3.07293017
C	1.50532872	-1.84322858	-3.37990932
C	3.39399825	-1.23856997	-1.94398240
5 C	-0.78770513	-2.24581944	-3.37990865
C	-2.76963218	-2.32000372	-1.94398240
C	-2.07642124	-1.73950174	-3.07293017
C	-2.34894714	-0.38203862	-3.37990932
C	0.00000000	-4.08920371	-0.24137285
10 C	-0.81329148	-3.73282579	-1.36681726
C	-0.15871204	-3.23094604	-2.53286993
C	-2.14516491	-3.30082879	-1.11669019
C	3.14066610	-2.37352365	-1.11675910
C	2.03498580	-3.23251510	-1.36677769
15 C	1.24902539	-2.98371494	-2.53284962
C	1.39165820	-3.84452623	-0.24140738
C	3.54135430	-2.04460185	0.24137285
C	2.71872533	-1.75292168	2.53286993
C	2.82607622	-2.57074398	1.36681726
20 C	1.78601913	-3.50818170	1.11669019
C	-3.62586482	-1.53313480	-1.11675910
C	-3.81693310	-0.14609185	-1.36677769
C	-3.20848563	0.41016975	-2.53284962
C	-4.02528648	0.71705177	-0.24140738
25 C	-1.55108412	1.80508238	-3.37990865
C	-0.46824207	2.66798441	-3.07293017
C	-0.62436607	3.55857369	-1.94398240
C	0.84361841	2.22526721	-3.37990932
C	-1.32165044	0.48213995	-3.89594417
30 C	2.33878926	0.44073706	-3.37990865
C	0.00000000	0.00000000	-4.13276964
C	1.07837066	0.90351288	-3.89594417
C	-3.54135430	-2.04460185	0.24137285
C	-2.87743737	-1.47802436	2.53286993
35 C	-3.63936770	-1.16208181	1.36681726
C	-3.93118404	0.20735291	1.11669019
C	-0.48519873	-3.90665844	1.11675910
C	-1.95946024	-2.57354518	2.53284962
C	-1.78194729	-3.37860695	1.36677769
40 C	2.14516491	3.30082879	1.11669019
C	1.55108412	-1.80508238	3.37990865
C	-0.84361841	-2.22526721	3.37990932
C	0.46824207	-2.66798441	3.07293017
C	0.62436607	-3.55857369	1.94398240
45 C	1.32165044	-0.48213995	3.89594417
C	-2.33878926	-0.44073706	3.37990865
C	0.00000000	0.00000000	4.13276964
C	-1.07837066	-0.90351288	3.89594417

C_{80}^{8+}			
C	2.39133356	-2.06174903	2.64900946
C	2.37072217	-0.77029432	3.26301913
C	3.14649516	0.26239940	2.64900946
5 C	0.00000000	1.22963925	-3.93376711
C	1.22187714	-2.91140885	2.64900946
C	-1.22187714	-2.91140885	2.64900946
C	0.00000000	-2.49272480	3.26301913
C	0.00000000	-1.22963925	3.93376711
10 C	0.72276382	0.99479905	3.93376711
C	1.46518687	2.01665673	3.26301913
C	2.69980256	1.63717788	2.64900946
C	0.72276382	3.07358061	2.64900946
C	-0.72276382	0.99479905	3.93376711
15 C	-2.69980256	1.63717788	2.64900946
C	-1.46518687	2.01665673	3.26301913
C	-0.72276382	3.07358061	2.64900946
C	-2.39133356	-2.06174903	2.64900946
C	-2.37072217	-0.77029432	3.26301913
20 C	-1.16945642	-0.37997943	3.93376711
C	-3.14649516	0.26239940	2.64900946
C	3.86925898	-0.02755920	-1.41937020
C	3.83590904	1.24636240	-0.77029432
C	3.14649516	2.25199750	1.41937020
25 C	3.86925898	1.25719845	0.65941135
C	3.86925898	-1.25719845	-0.65941135
C	3.11409738	-2.29658923	1.41937020
C	3.83590904	-1.24636240	0.77029432
C	3.86925898	0.02755920	1.41937020
30 C	1.16945642	-3.68840023	-1.41937020
C	2.37072217	-3.26301913	-0.77029432
C	3.14649516	-2.25199750	-1.41937020
C	2.39133356	-3.29138828	0.65941135
C	-3.14649516	-2.25199750	-1.41937020
35 C	-3.83590904	-1.24636240	0.77029432
C	-3.86925898	-1.25719845	-0.65941135
C	-3.86925898	0.02755920	1.41937020
C	-2.69980256	-1.63717788	-2.64900946
C	-0.72276382	-0.99479905	-3.93376711
40 C	-1.46518687	-2.01665673	-3.26301913
C	-0.72276382	-3.07358061	-2.64900946
C	-2.39133356	2.06174903	-2.64900946
C	-2.37072217	0.77029432	-3.26301913
C	-3.14649516	-0.26239940	-2.64900946
45 C	-1.16945642	0.37997943	-3.93376711
C	-3.86925898	1.25719845	0.65941135
C	-3.83590904	1.24636240	-0.77029432
C	-3.86925898	-0.02755920	-1.41937020
C	-3.11409738	2.29658923	-1.41937020

C	-3.14649516	2.25199750	1.41937020
C	-1.16945642	3.68840023	1.41937020
C	-2.37072217	3.26301913	0.77029432
C	-2.39133356	3.29138828	-0.65941135
5 C	0.72276382	-0.99479905	-3.93376711
C	1.46518687	-2.01665673	-3.26301913
C	0.72276382	-3.07358061	-2.64900946
C	2.69980256	-1.63717788	-2.64900946
C	0.00000000	-4.06837966	-0.65941135
10 C	0.00000000	-4.03331345	0.77029432
C	1.22187714	-3.67136771	1.41937020
C	-1.22187714	-3.67136771	1.41937020
C	-1.16945642	-3.68840023	-1.41937020
C	-3.11409738	-2.29658923	1.41937020
15 C	-2.37072217	-3.26301913	-0.77029432
C	-2.39133356	-3.29138828	0.65941135
C	1.16945642	0.37997943	-3.93376711
C	2.39133356	2.06174903	-2.64900946
C	2.37072217	0.77029432	-3.26301913
20 C	3.14649516	-0.26239940	-2.64900946
C	-1.22187714	2.91140885	-2.64900946
C	1.22187714	2.91140885	-2.64900946
C	0.00000000	2.49272480	-3.26301913
C	1.16945642	-0.37997943	3.93376711
25 C	0.00000000	4.06837966	0.65941135
C	1.22187714	3.67136771	-1.41937020
C	0.00000000	4.03331345	-0.77029432
C	-1.22187714	3.67136771	-1.41937020
C	1.16945642	3.68840023	1.41937020
30 C	3.11409738	2.29658923	-1.41937020
C	2.37072217	3.26301913	0.77029432
C	2.39133356	3.29138828	-0.65941135

C_{80}^{5-}			
35 C	0.00000000	-2.50203608	3.27520775
C	-1.22754796	-2.92197688	2.65744991
C	-2.39963197	-2.07040800	2.65744991
C	-2.37957772	-0.77317167	3.27520775
C	-1.17208401	-0.38083318	3.94817022
40 C	0.00000000	-1.23240206	3.94817022
C	1.17208401	-0.38083318	3.94817022
C	2.37957772	-0.77317167	3.27520775
C	2.39963197	-2.07040800	2.65744991
C	1.22754796	-2.92197688	2.65744991
45 C	1.22754796	-3.68364325	1.42504785
C	0.00000000	-4.04837942	0.77317167
C	-1.22754796	-3.68364325	1.42504785
C	-2.39963197	-3.30281006	0.66338148
C	-3.12401973	-2.30577585	1.42504785

C	-3.85023763	-1.25101804	0.77317167
C	-3.88268609	0.02915912	1.42504785
C	-3.15829834	0.26452697	2.65744991
C	-2.71060208	1.64239437	2.65744991
5 C	-1.47065991	2.02418971	3.27520775
C	-0.72438776	0.99703421	3.94817022
C	0.72438776	0.99703421	3.94817022
C	1.47065991	2.02418971	3.27520775
C	2.71060208	1.64239437	2.65744991
10 C	3.15829834	0.26452697	2.65744991
C	3.88268609	0.02915912	1.42504785
C	3.85023763	-1.25101804	0.77317167
C	3.12401973	-2.30577585	1.42504785
C	2.39963197	-3.30281006	0.66338148
15 C	2.37957772	-3.27520775	-0.77317167
C	1.17208401	-3.70166457	-1.42504785
C	0.00000000	-4.08249776	-0.66338148
C	-1.17208401	-3.70166457	-1.42504785
C	-2.37957772	-3.27520775	-0.77317167
20 C	-3.15829834	-2.25859540	-1.42504785
C	-3.88268609	-1.26156119	-0.66338148
C	-3.88268609	-0.02915912	-1.42504785
C	-3.85023763	1.25101804	-0.77317167
C	-3.88268609	1.26156119	0.66338148
25 C	-3.15829834	2.25859540	1.42504785
C	-2.37957772	3.27520775	0.77317167
C	-1.17208401	3.70166457	1.42504785
C	-0.72438776	3.08546354	2.65744991
C	0.72438776	3.08546354	2.65744991
30 C	1.17208401	3.70166457	1.42504785
C	2.37957772	3.27520775	0.77317167
C	3.15829834	2.25859540	1.42504785
C	3.88268609	1.26156119	0.66338148
C	3.85023763	1.25101804	-0.77317167
35 C	3.88268609	-0.02915912	-1.42504785
C	3.88268609	-1.26156119	-0.66338148
C	3.15829834	-2.25859540	-1.42504785
C	2.71060208	-1.64239437	-2.65744991
C	1.47065991	-2.02418971	-3.27520775
40 C	0.72438776	-3.08546354	-2.65744991
C	-0.72438776	-3.08546354	-2.65744991
C	-1.47065991	-2.02418971	-3.27520775
C	-2.71060208	-1.64239437	-2.65744991
C	-3.15829834	-0.26452697	-2.65744991
45 C	-2.37957772	0.77317167	-3.27520775
C	-2.39963197	2.07040800	-2.65744991
C	-3.12401973	2.30577585	-1.42504785
C	-2.39963197	3.30281006	-0.66338148
C	-1.22754796	3.68364325	-1.42504785

	C	0.00000000	4.04837942	-0.77317167
	C	0.00000000	4.08249776	0.66338148
	C	3.15829834	-0.26452697	-2.65744991
	C	2.37957772	0.77317167	-3.27520775
5	C	1.17208401	0.38083318	-3.94817022
	C	0.72438776	-0.99703421	-3.94817022
	C	-0.72438776	-0.99703421	-3.94817022
	C	-1.17208401	0.38083318	-3.94817022
	C	0.00000000	1.23240206	-3.94817022
10	C	0.00000000	2.50203608	-3.27520775
	C	-1.22754796	2.92197688	-2.65744991
	C	1.22754796	2.92197688	-2.65744991
	C	1.22754796	3.68364325	-1.42504785
	C	2.39963197	3.30281006	-0.66338148
15	C	3.12401973	2.30577585	-1.42504785
	C	2.39963197	2.07040800	-2.65744991

Ge₁₂⁻²

	Ge	0.00000040	-0.00000029	2.55392129
20	Ge	2.17249247	-0.70589228	1.14214912
	Ge	1.34268055	1.84802983	1.14214912
	Ge	-1.34266970	1.84803713	1.14214912
	Ge	-2.17249551	-0.70588046	1.14214912
	Ge	-0.00000582	-2.28429565	1.14214912
25	Ge	0.00000040	-0.00000029	-2.55391842
	Ge	0.00000661	2.28429508	-1.14214624
	Ge	2.17249630	0.70587989	-1.14214624
	Ge	1.34267050	-1.84803771	-1.14214624
	Ge	-1.34267975	-1.84803040	-1.14214624
30	Ge	-2.17249167	0.70589170	-1.14214624