

Supporting information for:

Increasing Radical Character of Large [n]cyclacenes Unveiled by Wavefunction Theory

Stefano Battaglia,^{†,‡} Noelia Faginas-Lago,[‡] Dirk Andrae,[¶] Stefano Evangelisti,[†]
and Thierry Leininger^{*,†}

*Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université de Toulouse, CNRS, UPS,
118 Route de Narbonne, 31062 Toulouse Cedex, France, Dipartimento di Chimica, Biologia e
Biotecnologie, Università degli Studi di Perugia, Vie Elce di Sotto 8, 06123 Perugia, Italy, and
Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Freie Universität
Berlin, Takustraße 3, 14195 Berlin, Germany*

E-mail: Thierry.Leininger@irsamc.ups-tlse.fr

^{*}To whom correspondence should be addressed

[†]Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université de Toulouse, CNRS, UPS, 118 Route de Narbonne, 31062 Toulouse Cedex, France

[‡]Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Vie Elce di Sotto 8, 06123 Perugia, Italy

[¶]Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin, Germany

Restricted Hartree-Fock Occupations

The electronic configurations of the two lowest-lying singlet closed-shell electronic states at RHF level of theory are listed in Table S1. The geometries used in the correlated calculations have been relaxed in the electronic configuration $(\pi_+)^2(\pi_-)^0$, even though for $n = 6, 8, 10$ they do not yield the lowest energy. The data in Table S1 show that the degeneracy of HOMO and LUMO seen in the simple Hückel method is an artifact. In a self-consistent field approach, all data (molecular orbitals, orbital energies) adapt to the case under consideration, until self-consistency is achieved.

Table S1: Electron Configurations for Lowest Closed-Shell Singlet States $^1A_{1g}$ (1A_g in D_{2h}) of $[n]$ cyclacenes, with Corresponding Total Energies (in a. u.) at RHF/ANO-DZ Level of Theory (Geometries Relaxed for each Electronic State Considered).

n	Irrep in D_{2h}								E a. u.	HOMO	LUMO
	a_g	b_{3u}	b_{2u}	b_{1g}	b_{1u}	b_{2g}	b_{3g}	a_u			
6	13	10	11	8	11	10	8	7	−915.12287924	$10b_{2g}$	$11b_{3u}$
	13	11	11	8	11	9	8	7	−915.15505998	$11b_{3u}$	$10b_{2g}$
8	16	14	14	12	15	12	12	9	−1220.45159651	$15b_{1u}$	$17a_g$
	17	14	14	12	14	12	12	9	−1220.46805165	$17a_g$	$15b_{1u}$
10	20	17	18	15	17	16	14	13	−1525.72404294	$16b_{2g}$	$18b_{3u}$
	20	18	18	15	17	15	14	13	−1525.72539816	$18b_{3u}$	$16b_{2g}$
12	23	21	21	19	21	18	18	15	−1830.97018339	$21b_{1u}$	$24a_g$
	24	21	21	19	20	18	18	15	−1830.95746391	$24a_g$	$21b_{1u}$
14	27	24	25	22	23	22	20	19	−2136.20207912	$22b_{2g}$	$25b_{3u}$
	27	25	25	22	23	21	20	19	−2136.17657936	$25b_{3u}$	$22b_{2g}$
16	30	28	28	26	27	24	24	21	−2441.42540910	$27b_{1u}$	$31a_g$
	31	28	28	26	26	24	24	21	−2441.38849839	$31a_g$	$27b_{1u}$
18	34	31	32	29	29	28	26	25	−2746.64318030	$28b_{2g}$	$32b_{3u}$
	34	32	32	29	29	27	26	25	−2746.59617206	$32b_{3u}$	$28b_{2g}$
20	37	35	35	33	33	30	30	27	−3051.85712703	$33b_{1u}$	$38a_g$
	38	35	35	33	32	30	30	27	−3051.80121039	$38a_g$	$33b_{1u}$
22	41	38	39	36	35	34	32	31	−3357.06832402	$34b_{2g}$	$39b_{3u}$
	41	39	39	36	35	33	32	31	−3357.00454295	$39b_{3u}$	$34b_{2g}$
24	44	42	42	40	39	36	36	33	−3662.27747887	$39b_{1u}$	$45a_g$
	45	42	42	40	38	36	36	33	−3662.20672622	$45a_g$	$39b_{1u}$
28	51	49	49	47	45	42	42	39	−4272.69142472	$45b_{1u}$	$52a_g$
	52	49	49	47	44	42	42	39	−4272.60892214	$52a_g$	$45b_{1u}$

Geometry Benchmarks

The geometrical parameters are defined as follows: $CC_{\parallel}$ is the C–C bond parallel to the principal axis of the $[n]$ cyclacenes, $CC_{\perp}$ is the C–C bond forming the zigzag edge (note that there is no dimerization), CH is the C–H bond length, R_{C1} is the radius of the internal carbon atoms, R_{C2} is the radius of the external carbon atoms and R_H is the radius of the hydrogen atoms.

Table S2: Geometrical Parameters of $[8]$ cyclacene Optimized with Different Methods and Basis Sets. F-ANO-DZP (F-ANO-TZP) Refers to the Contraction Scheme (3s2p1d/2s1p) ((4s3p2d1f/3s2p1d)). All Values Are Given in Å.

Method/Basis	$CC_{\parallel}$	$CC_{\perp}$	CH	R_{C1}	R_{C2}	R_H
RHF/ANO-DZ	1.454	1.407	1.078	3.157	3.164	3.143
RHF/ANO-TZ	1.454	1.406	1.073	3.158	3.158	3.130
RHF/ANO-DZP	1.454	1.404	1.080	3.148	3.150	3.095
RHF/F-ANO-DZP	1.454	1.404	1.079	3.147	3.150	3.105
RHF/ANO-TZP	1.453	1.401	1.074	3.141	3.145	3.106
RHF/F-ANO-TZP	1.452	1.400	1.072	3.139	3.143	3.103
RMP2/ANO-DZ	1.481	1.438	1.102	3.214	3.226	3.203
RMP2/ANO-TZ	1.471	1.428	1.092	3.201	3.196	3.154
RMP2/ANO-DZP	1.462	1.422	1.099	3.176	3.184	3.130
RMP2/F-ANO-DZP	1.463	1.422	1.097	3.175	3.183	3.130
RMP2/ANO-TZP	1.459	1.415	1.088	3.164	3.167	3.126
RB3LYP/ANO-DZ	1.468	1.420	1.092	3.188	3.192	3.161
RB3LYP/ANO-TZ	1.465	1.416	1.084	3.180	3.182	3.158
RB3LYP/ANO-DZP	1.464	1.416	1.093	3.175	3.179	3.120
RB3LYP/F-ANO-DZP	1.465	1.416	1.092	3.175	3.179	3.129
RB3LYP/ANO-TZP	1.461	1.410	1.084	3.163	3.167	3.127
RB3LYP/F-ANO-TZP	1.460	1.409	1.082	3.160	3.165	3.122
UB3LYP/ANO-DZP	1.458	1.416	1.093	3.176	3.186	3.141

Table S3: Comparison of the Geometrical Parameters of [8]cyclooctene for a Representative Set of Methods/Basis Sets. The Values Represent Differences with Respect to the RHF/ANO-DZ Geometry and Are Given in Å. Numbers in Parenthesis Are Percentages of Absolute Differences.

Method/Basis	CC	CC _⊥	CH	R _{C1}	R _{C2}	R _H
RHF/ANO-DZ	1.454	1.407	1.078	3.157	3.164	3.143
RHF/ANO-DZP	0.000 (0.0 %)	-0.003 (0.2 %)	+0.002 (0.2 %)	-0.009 (0.3 %)	-0.014 (0.4 %)	-0.048 (1.5 %)
RHF/ANO-TZP	-0.001 (0.1 %)	-0.006 (0.4 %)	-0.004 (0.4 %)	-0.016 (0.5 %)	-0.019 (0.6 %)	-0.037 (1.2 %)
RMP2/ANO-DZP	+0.008 (0.6 %)	+0.015 (1.1 %)	+0.021 (1.9 %)	+0.019 (0.6 %)	+0.020 (0.6 %)	-0.013 (0.4 %)
RMP2/ANO-TZP	+0.005 (0.3 %)	+0.008 (0.6 %)	+0.010 (0.9 %)	+0.007 (0.2 %)	+0.003 (0.1 %)	-0.017 (0.5 %)
RB3LYP/ANO-DZP	+0.010 (0.7 %)	+0.008 (0.6 %)	+0.015 (1.4 %)	+0.018 (0.6 %)	+0.015 (0.5 %)	-0.023 (0.7 %)
RB3LYP/ANO-TZP	+0.007 (0.5 %)	+0.003 (0.2 %)	+0.006 (0.6 %)	+0.006 (0.2 %)	+0.003 (0.1 %)	-0.016 (0.5 %)
UB3LYP/ANO-DZP	+0.004 (0.3 %)	+0.009 (0.6 %)	+0.015 (1.4 %)	+0.019 (0.6 %)	+0.022 (0.7 %)	-0.002 (0.1 %)

Table S4: Comparison of the Geometrical Parameters of Three [n]cycloalkenes Optimized at RB3LYP/ANO-DZP Level of Theory. The Values Represent Differences with Respect to the RHF/ANO-DZ Geometries and Are Given in Å. Numbers in Parenthesis Are Percentages of Absolute Differences.

<i>n</i>	CC	CC _⊥	CH	R _{C1}	R _{C2}	R _H
8	+0.010 (0.7 %)	+0.008 (0.6 %)	+0.015 (1.4 %)	+0.018 (0.6 %)	+0.015 (0.5 %)	-0.023 (0.7 %)
16	+0.010 (0.7 %)	+0.009 (0.6 %)	+0.015 (1.4 %)	+0.043 (0.7 %)	+0.041 (0.7 %)	+0.022 (0.4 %)
20	+0.011 (0.8 %)	+0.009 (0.6 %)	+0.015 (1.4 %)	+0.055 (0.7 %)	+0.052 (0.7 %)	+0.037 (0.5 %)

Table S5: Comparison of the ST Energy Gap of [8]cyclacene for a Set of Representative Geometries Optimized at Different Levels of Theory. The Values Represent Differences with Respect to the Gap Calculated on the RHF/ANO-DZ Geometry and Are Given in eV.

Method/Basis	CASSCF(k,k)	NEVPT2
RHF/ANO-DZ	0.72	0.41
RMP2/ANO-DZP	-0.05	-0.03
RMP2/ANO-TZP	-0.03	-0.02
RB3LYP/ANO-DZP	-0.03	-0.03
UB3LYP/ANO-DZP	-0.02	-0.01

Table S6: Comparison of the ST Gap for Three $[n]$ cyclacenes Optimized at RB3LYP/ANO-DZP Level of Theory. The Values Represent Differences with Respect to the Gaps Calculated on RHF/ANO-DZ Geometries and Are Given in eV.

n	CASSCF(k,k)	NEVPT2
8	-0.03	-0.02
16	+0.00	+0.00
20	+0.00	-

[*n*]cyclacenes Geometries

[6]cyclacene

H	2.381154	0.000000	2.480694
H	1.190577	2.062140	2.480694
H	-1.190577	2.062140	2.480694
H	-2.381154	0.000000	2.480694
H	-1.190577	-2.062140	2.480694
H	1.190577	-2.062140	2.480694
C	2.406213	0.000000	1.403424
C	1.203107	2.083842	1.403424
C	-1.203107	2.083842	1.403424
C	-2.406213	0.000000	1.403424
C	-1.203107	-2.083842	1.403424
C	1.203107	-2.083842	1.403424
C	2.074789	1.197880	0.724279
C	0.000000	2.395760	0.724279
C	-2.074789	1.197880	0.724279
C	-2.074789	-1.197880	0.724279
C	0.000000	-2.395760	0.724279
C	2.074789	-1.197880	0.724279
C	2.074789	1.197880	-0.724279
C	0.000000	2.395760	-0.724279
C	-2.074789	1.197880	-0.724279
C	-2.074789	-1.197880	-0.724279
C	0.000000	-2.395760	-0.724279
C	2.074789	-1.197880	-0.724279
C	2.406213	0.000000	-1.403424
C	1.203107	2.083842	-1.403424
C	-1.203107	2.083842	-1.403424
C	-2.406213	0.000000	-1.403424
C	-1.203107	-2.083842	-1.403424
C	1.203107	-2.083842	-1.403424
H	2.381154	0.000000	-2.480694
H	1.190577	2.062140	-2.480694
H	-1.190577	2.062140	-2.480694
H	-2.381154	0.000000	-2.480694
H	-1.190577	-2.062140	-2.480694
H	1.190577	-2.062140	-2.480694

[8]cyclacene

H	3.142960	0.000000	2.483223
H	2.222409	2.222409	2.483223
H	0.000000	3.142960	2.483223
H	-2.222409	2.222409	2.483223
H	-3.142960	0.000000	2.483223
H	-2.222409	-2.222409	2.483223
H	0.000000	-3.142960	2.483223
H	2.222409	-2.222409	2.483223
C	3.163637	0.000000	1.405644
C	2.237029	2.237029	1.405644
C	0.000000	3.163637	1.405644
C	-2.237029	2.237029	1.405644
C	-3.163637	0.000000	1.405644
C	-2.237029	-2.237029	1.405644
C	0.000000	-3.163637	1.405644
C	2.237029	-2.237029	1.405644
C	2.916457	1.208036	0.727181
C	1.208036	2.916457	0.727181
C	-1.208036	2.916457	0.727181
C	-2.916457	1.208036	0.727181
C	-2.916457	-1.208036	0.727181
C	-1.208036	-2.916457	0.727181
C	1.208036	-2.916457	0.727181
C	2.916457	-1.208036	0.727181
C	2.916457	1.208036	-0.727181
C	1.208036	2.916457	-0.727181
C	-1.208036	2.916457	-0.727181
C	-2.916457	1.208036	-0.727181
C	-2.916457	-1.208036	-0.727181
C	-1.208036	-2.916457	-0.727181
C	1.208036	-2.916457	-0.727181
C	2.916457	-1.208036	-0.727181
C	3.163637	0.000000	-1.405644
C	2.237029	2.237029	-1.405644
C	0.000000	3.163637	-1.405644
C	-2.237029	2.237029	-1.405644
C	-3.163637	0.000000	-1.405644
C	-2.237029	-2.237029	-1.405644
C	0.000000	-3.163637	-1.405644
C	2.237029	-2.237029	-1.405644
H	3.142960	0.000000	-2.483223
H	2.222409	2.222409	-2.483223
H	0.000000	3.142960	-2.483223
H	-2.222409	2.222409	-2.483223
H	-3.142960	0.000000	-2.483223

H	-2.222409	-2.222409	-2.483223
H	0.000000	-3.142960	-2.483223
H	2.222409	-2.222409	-2.483223

[10]cyclacene

H	3.913396	0.000000	2.484085
H	3.166004	2.300236	2.484085
H	1.209306	3.721861	2.484085
H	-1.209306	3.721861	2.484085
H	-3.166004	2.300236	2.484085
H	-3.913396	0.000000	2.484085
H	-3.166004	-2.300236	2.484085
H	-1.209306	-3.721861	2.484085
H	1.209306	-3.721861	2.484085
H	3.166004	-2.300236	2.484085
C	3.930815	0.000000	1.406329
C	3.180096	2.310475	1.406329
C	1.214689	3.738427	1.406329
C	-1.214689	3.738427	1.406329
C	-3.180096	2.310475	1.406329
C	-3.930815	0.000000	1.406329
C	-3.180096	-2.310475	1.406329
C	-1.214689	-3.738427	1.406329
C	1.214689	-3.738427	1.406329
C	3.180096	-2.310475	1.406329
C	3.733646	1.213135	0.728440
C	2.307520	3.176029	0.728440
C	0.000000	3.925788	0.728440
C	-2.307520	3.176029	0.728440
C	-3.733646	1.213135	0.728440
C	-3.733646	-1.213135	0.728440
C	-2.307520	-3.176029	0.728440
C	0.000000	-3.925788	0.728440
C	2.307520	-3.176029	0.728440
C	3.733646	-1.213135	0.728440
C	3.733646	1.213135	-0.728440
C	2.307520	3.176029	-0.728440
C	0.000000	3.925788	-0.728440
C	-2.307520	3.176029	-0.728440
C	-3.733646	1.213135	-0.728440
C	-3.733646	-1.213135	-0.728440
C	-2.307520	-3.176029	-0.728440
C	0.000000	-3.925788	-0.728440
C	2.307520	-3.176029	-0.728440

C	3.733646	-1.213135	-0.728440
C	3.930815	0.000000	-1.406329
C	3.180096	2.310475	-1.406329
C	1.214689	3.738427	-1.406329
C	-1.214689	3.738427	-1.406329
C	-3.180096	2.310475	-1.406329
C	-3.930815	0.000000	-1.406329
C	-3.180096	-2.310475	-1.406329
C	-1.214689	-3.738427	-1.406329
C	1.214689	-3.738427	-1.406329
C	3.180096	-2.310475	-1.406329
H	3.913396	0.000000	-2.484085
H	3.166004	2.300236	-2.484085
H	1.209306	3.721861	-2.484085
H	-1.209306	3.721861	-2.484085
H	-3.166004	2.300236	-2.484085
H	-3.913396	0.000000	-2.484085
H	-3.166004	-2.300236	-2.484085
H	-1.209306	-3.721861	-2.484085
H	1.209306	-3.721861	-2.484085
H	3.166004	-2.300236	-2.484085

[12]cyclacene

H	4.687318	0.000000	2.484432
H	4.059336	2.343659	2.484432
H	2.343659	4.059336	2.484432
H	0.000000	4.687318	2.484432
H	-2.343659	4.059336	2.484432
H	-4.059336	2.343659	2.484432
H	-4.687318	0.000000	2.484432
H	-4.059336	-2.343659	2.484432
H	-2.343659	-4.059336	2.484432
H	0.000000	-4.687318	2.484432
H	2.343659	-4.059336	2.484432
H	4.059336	-2.343659	2.484432
C	4.702316	0.000000	1.406566
C	4.072325	2.351158	1.406566
C	2.351158	4.072325	1.406566
C	0.000000	4.702316	1.406566
C	-2.351158	4.072325	1.406566
C	-4.072325	2.351158	1.406566
C	-4.702316	0.000000	1.406566
C	-4.072325	-2.351158	1.406566
C	-2.351158	-4.072325	1.406566

C	0.000000	-4.702316	1.406566
C	2.351158	-4.072325	1.406566
C	4.072325	-2.351158	1.406566
C	4.538288	1.216031	0.729028
C	3.322258	3.322258	0.729028
C	1.216031	4.538288	0.729028
C	-1.216031	4.538288	0.729028
C	-3.322258	3.322258	0.729028
C	-4.538288	1.216031	0.729028
C	-4.538288	-1.216031	0.729028
C	-3.322258	-3.322258	0.729028
C	-1.216031	-4.538288	0.729028
C	1.216031	-4.538288	0.729028
C	3.322258	-3.322258	0.729028
C	4.538288	-1.216031	0.729028
C	4.538288	1.216031	-0.729028
C	3.322258	3.322258	-0.729028
C	1.216031	4.538288	-0.729028
C	-1.216031	4.538288	-0.729028
C	-3.322258	3.322258	-0.729028
C	-4.538288	1.216031	-0.729028
C	-4.538288	-1.216031	-0.729028
C	-3.322258	-3.322258	-0.729028
C	-1.216031	-4.538288	-0.729028
C	1.216031	-4.538288	-0.729028
C	3.322258	-3.322258	-0.729028
C	4.538288	-1.216031	-0.729028
C	4.702316	0.000000	-1.406566
C	4.072325	2.351158	-1.406566
C	2.351158	4.072325	-1.406566
C	0.000000	4.702316	-1.406566
C	-2.351158	4.072325	-1.406566
C	-4.072325	2.351158	-1.406566
C	-4.702316	0.000000	-1.406566
C	-4.072325	-2.351158	-1.406566
C	-2.351158	-4.072325	-1.406566
C	0.000000	-4.702316	-1.406566
C	2.351158	-4.072325	-1.406566
C	4.072325	-2.351158	-1.406566
H	4.687318	0.000000	-2.484432
H	4.059336	2.343659	-2.484432
H	2.343659	4.059336	-2.484432
H	0.000000	4.687318	-2.484432
H	-2.343659	4.059336	-2.484432
H	-4.059336	2.343659	-2.484432

H	-4.687318	0.000000	-2.484432
H	-4.059336	-2.343659	-2.484432
H	-2.343659	-4.059336	-2.484432
H	0.000000	-4.687318	-2.484432
H	2.343659	-4.059336	-2.484432
H	4.059336	-2.343659	-2.484432

[14]cyclacene

H	5.462910	0.000000	2.484581
H	4.921912	2.370268	2.484581
H	3.406069	4.271075	2.484581
H	1.215612	5.325943	2.484581
H	-1.215612	5.325943	2.484581
H	-3.406069	4.271075	2.484581
H	-4.921912	2.370268	2.484581
H	-5.462910	0.000000	2.484581
H	-4.921912	-2.370268	2.484581
H	-3.406069	-4.271075	2.484581
H	-1.215612	-5.325943	2.484581
H	1.215612	-5.325943	2.484581
H	3.406069	-4.271075	2.484581
H	4.921912	-2.370268	2.484581
C	5.476075	0.000000	1.406643
C	4.933773	2.375980	1.406643
C	3.414277	4.281368	1.406643
C	1.218541	5.338778	1.406643
C	-1.218541	5.338778	1.406643
C	-3.414277	4.281368	1.406643
C	-4.933773	2.375980	1.406643
C	-5.476075	0.000000	1.406643
C	-4.933773	-2.375980	1.406643
C	-3.414277	-4.281368	1.406643
C	-1.218541	-5.338778	1.406643
C	1.218541	-5.338778	1.406643
C	3.414277	-4.281368	1.406643
C	4.933773	-2.375980	1.406643
C	5.335627	1.217822	0.729319
C	4.278841	3.412262	0.729319
C	2.374577	4.930861	0.729319
C	0.000000	5.472843	0.729319
C	-2.374577	4.930861	0.729319
C	-4.278841	3.412262	0.729319
C	-5.335627	1.217822	0.729319
C	-5.335627	-1.217822	0.729319

C	-4.278841	-3.412262	0.729319
C	-2.374577	-4.930861	0.729319
C	0.000000	-5.472843	0.729319
C	2.374577	-4.930861	0.729319
C	4.278841	-3.412262	0.729319
C	5.335627	-1.217822	0.729319
C	5.335627	1.217822	-0.729319
C	4.278841	3.412262	-0.729319
C	2.374577	4.930861	-0.729319
C	0.000000	5.472843	-0.729319
C	-2.374577	4.930861	-0.729319
C	-4.278841	3.412262	-0.729319
C	-5.335627	1.217822	-0.729319
C	-5.335627	-1.217822	-0.729319
C	-4.278841	-3.412262	-0.729319
C	-2.374577	-4.930861	-0.729319
C	0.000000	-5.472843	-0.729319
C	2.374577	-4.930861	-0.729319
C	4.278841	-3.412262	-0.729319
C	5.335627	-1.217822	-0.729319
C	5.476075	0.000000	-1.406643
C	4.933773	2.375980	-1.406643
C	3.414277	4.281368	-1.406643
C	1.218541	5.338778	-1.406643
C	-1.218541	5.338778	-1.406643
C	-3.414277	4.281368	-1.406643
C	-4.933773	2.375980	-1.406643
C	-5.476075	0.000000	-1.406643
C	-4.933773	-2.375980	-1.406643
C	-3.414277	-4.281368	-1.406643
C	-1.218541	-5.338778	-1.406643
C	1.218541	-5.338778	-1.406643
C	3.414277	-4.281368	-1.406643
C	4.933773	-2.375980	-1.406643
H	5.462910	0.000000	-2.484581
H	4.921912	2.370268	-2.484581
H	3.406069	4.271075	-2.484581
H	1.215612	5.325943	-2.484581
H	-1.215612	5.325943	-2.484581
H	-3.406069	4.271075	-2.484581
H	-4.921912	2.370268	-2.484581
H	-5.462910	0.000000	-2.484581
H	-4.921912	-2.370268	-2.484581
H	-3.406069	-4.271075	-2.484581
H	-1.215612	-5.325943	-2.484581

H	1.215612	-5.325943	-2.484581
H	3.406069	-4.271075	-2.484581
H	4.921912	-2.370268	-2.484581

[16]cyclacene

H	6.239446	0.000000	2.484654
H	5.764496	2.387733	2.484654
H	4.411955	4.411955	2.484654
H	2.387733	5.764496	2.484654
H	0.000000	6.239446	2.484654
H	-2.387733	5.764496	2.484654
H	-4.411955	4.411955	2.484654
H	-5.764496	2.387733	2.484654
H	-6.239446	0.000000	2.484654
H	-5.764496	-2.387733	2.484654
H	-4.411955	-4.411955	2.484654
H	-2.387733	-5.764496	2.484654
H	0.000000	-6.239446	2.484654
H	2.387733	-5.764496	2.484654
H	4.411955	-4.411955	2.484654
H	5.764496	-2.387733	2.484654
C	6.251161	0.000000	1.406667
C	5.775319	2.392216	1.406667
C	4.420238	4.420238	1.406667
C	2.392216	5.775319	1.406667
C	0.000000	6.251161	1.406667
C	-2.392216	5.775319	1.406667
C	-4.420238	4.420238	1.406667
C	-5.775319	2.392216	1.406667
C	-6.251161	0.000000	1.406667
C	-5.775319	-2.392216	1.406667
C	-4.420238	-4.420238	1.406667
C	-2.392216	-5.775319	1.406667
C	0.000000	-6.251161	1.406667
C	2.392216	-5.775319	1.406667
C	4.420238	-4.420238	1.406667
C	5.775319	-2.392216	1.406667
C	6.128357	1.219006	0.729480
C	5.195370	3.471435	0.729480
C	3.471435	5.195370	0.729480
C	1.219006	6.128357	0.729480
C	-1.219006	6.128357	0.729480
C	-3.471435	5.195370	0.729480
C	-5.195370	3.471435	0.729480

C	-6.128357	1.219006	0.729480
C	-6.128357	-1.219006	0.729480
C	-5.195370	-3.471435	0.729480
C	-3.471435	-5.195370	0.729480
C	-1.219006	-6.128357	0.729480
C	1.219006	-6.128357	0.729480
C	3.471435	-5.195370	0.729480
C	5.195370	-3.471435	0.729480
C	6.128357	-1.219006	0.729480
C	6.128357	1.219006	-0.729480
C	5.195370	3.471435	-0.729480
C	3.471435	5.195370	-0.729480
C	1.219006	6.128357	-0.729480
C	-1.219006	6.128357	-0.729480
C	-3.471435	5.195370	-0.729480
C	-5.195370	3.471435	-0.729480
C	-6.128357	1.219006	-0.729480
C	-6.128357	-1.219006	-0.729480
C	-5.195370	-3.471435	-0.729480
C	-3.471435	-5.195370	-0.729480
C	-1.219006	-6.128357	-0.729480
C	1.219006	-6.128357	-0.729480
C	3.471435	-5.195370	-0.729480
C	5.195370	-3.471435	-0.729480
C	6.128357	-1.219006	-0.729480
C	6.251161	0.000000	-1.406667
C	5.775319	2.392216	-1.406667
C	4.420238	4.420238	-1.406667
C	2.392216	5.775319	-1.406667
C	0.000000	6.251161	-1.406667
C	-2.392216	5.775319	-1.406667
C	-4.420238	4.420238	-1.406667
C	-5.775319	2.392216	-1.406667
C	-6.251161	0.000000	-1.406667
C	-5.775319	-2.392216	-1.406667
C	-4.420238	-4.420238	-1.406667
C	-2.392216	-5.775319	-1.406667
C	0.000000	-6.251161	-1.406667
C	2.392216	-5.775319	-1.406667
C	4.420238	-4.420238	-1.406667
C	5.775319	-2.392216	-1.406667
H	6.239446	0.000000	-2.484654
H	5.764496	2.387733	-2.484654
H	4.411955	4.411955	-2.484654
H	2.387733	5.764496	-2.484654

H	0.000000	6.239446	-2.484654
H	-2.387733	5.764496	-2.484654
H	-4.411955	4.411955	-2.484654
H	-5.764496	2.387733	-2.484654
H	-6.239446	0.000000	-2.484654
H	-5.764496	-2.387733	-2.484654
H	-4.411955	-4.411955	-2.484654
H	-2.387733	-5.764496	-2.484654
H	0.000000	-6.239446	-2.484654
H	2.387733	-5.764496	-2.484654
H	4.411955	-4.411955	-2.484654
H	5.764496	-2.387733	-2.484654

[18]cyclacene

H	7.016528	0.000000	2.484687
H	6.593380	2.399794	2.484687
H	5.374973	4.510138	2.484687
H	3.508264	6.076492	2.484687
H	1.218407	6.909932	2.484687
H	-1.218407	6.909932	2.484687
H	-3.508264	6.076492	2.484687
H	-5.374973	4.510138	2.484687
H	-6.593380	2.399794	2.484687
H	-7.016528	0.000000	2.484687
H	-6.593380	-2.399794	2.484687
H	-5.374973	-4.510138	2.484687
H	-3.508264	-6.076492	2.484687
H	-1.218407	-6.909932	2.484687
H	1.218407	-6.909932	2.484687
H	3.508264	-6.076492	2.484687
H	5.374973	-4.510138	2.484687
H	6.593380	-2.399794	2.484687
C	7.027077	0.000000	1.406665
C	6.603293	2.403402	1.406665
C	5.383054	4.516918	1.406665
C	3.513539	6.085628	1.406665
C	1.220239	6.920320	1.406665
C	-1.220239	6.920320	1.406665
C	-3.513539	6.085628	1.406665
C	-5.383054	4.516918	1.406665
C	-6.603293	2.403402	1.406665
C	-7.027077	0.000000	1.406665
C	-6.603293	-2.403402	1.406665
C	-5.383054	-4.516918	1.406665

C	-3.513539	-6.085628	1.406665
C	-1.220239	-6.920320	1.406665
C	1.220239	-6.920320	1.406665
C	3.513539	-6.085628	1.406665
C	5.383054	-4.516918	1.406665
C	6.603293	-2.403402	1.406665
C	6.917969	1.219825	0.729572
C	6.083560	3.512345	0.729572
C	4.515384	5.381225	0.729572
C	2.402586	6.601049	0.729572
C	0.000000	7.024690	0.729572
C	-2.402586	6.601049	0.729572
C	-4.515384	5.381225	0.729572
C	-6.083560	3.512345	0.729572
C	-6.917969	1.219825	0.729572
C	-6.917969	-1.219825	0.729572
C	-6.083560	-3.512345	0.729572
C	-4.515384	-5.381225	0.729572
C	-2.402586	-6.601049	0.729572
C	0.000000	-7.024690	0.729572
C	2.402586	-6.601049	0.729572
C	4.515384	-5.381225	0.729572
C	6.083560	-3.512345	0.729572
C	6.917969	-1.219825	0.729572
C	6.917969	1.219825	-0.729572
C	6.083560	3.512345	-0.729572
C	4.515384	5.381225	-0.729572
C	2.402586	6.601049	-0.729572
C	0.000000	7.024690	-0.729572
C	-2.402586	6.601049	-0.729572
C	-4.515384	5.381225	-0.729572
C	-6.083560	3.512345	-0.729572
C	-6.917969	1.219825	-0.729572
C	-6.917969	-1.219825	-0.729572
C	-6.083560	-3.512345	-0.729572
C	-4.515384	-5.381225	-0.729572
C	-2.402586	-6.601049	-0.729572
C	0.000000	-7.024690	-0.729572
C	2.402586	-6.601049	-0.729572
C	4.515384	-5.381225	-0.729572
C	6.083560	-3.512345	-0.729572
C	6.917969	-1.219825	-0.729572
C	7.027077	0.000000	-1.406665
C	6.603293	2.403402	-1.406665
C	5.383054	4.516918	-1.406665

C	3.513539	6.085628	-1.406665
C	1.220239	6.920320	-1.406665
C	-1.220239	6.920320	-1.406665
C	-3.513539	6.085628	-1.406665
C	-5.383054	4.516918	-1.406665
C	-6.603293	2.403402	-1.406665
C	-7.027077	0.000000	-1.406665
C	-6.603293	-2.403402	-1.406665
C	-5.383054	-4.516918	-1.406665
C	-3.513539	-6.085628	-1.406665
C	-1.220239	-6.920320	-1.406665
C	1.220239	-6.920320	-1.406665
C	3.513539	-6.085628	-1.406665
C	5.383054	-4.516918	-1.406665
C	6.603293	-2.403402	-1.406665
H	7.016528	0.000000	-2.484687
H	6.593380	2.399794	-2.484687
H	5.374973	4.510138	-2.484687
H	3.508264	6.076492	-2.484687
H	1.218407	6.909932	-2.484687
H	-1.218407	6.909932	-2.484687
H	-3.508264	6.076492	-2.484687
H	-5.374973	4.510138	-2.484687
H	-6.593380	2.399794	-2.484687
H	-7.016528	0.000000	-2.484687
H	-6.593380	-2.399794	-2.484687
H	-5.374973	-4.510138	-2.484687
H	-3.508264	-6.076492	-2.484687
H	-1.218407	-6.909932	-2.484687
H	1.218407	-6.909932	-2.484687
H	3.508264	-6.076492	-2.484687
H	5.374973	-4.510138	-2.484687
H	6.593380	-2.399794	-2.484687

[20]cyclacene

H	7.793977	0.000000	2.484706
H	7.412512	2.408471	2.484706
H	6.305460	4.581185	2.484706
H	4.581185	6.305460	2.484706
H	2.408471	7.412512	2.484706
H	0.000000	7.793977	2.484706
H	-2.408471	7.412512	2.484706
H	-4.581185	6.305460	2.484706
H	-6.305460	4.581185	2.484706

H	-7.412512	2.408471	2.484706
H	-7.793977	0.000000	2.484706
H	-7.412512	-2.408471	2.484706
H	-6.305460	-4.581185	2.484706
H	-4.581185	-6.305460	2.484706
H	-2.408471	-7.412512	2.484706
H	0.000000	-7.793977	2.484706
H	2.408471	-7.412512	2.484706
H	4.581185	-6.305460	2.484706
H	6.305460	-4.581185	2.484706
H	7.412512	-2.408471	2.484706
C	7.803559	0.000000	1.406658
C	7.421626	2.411433	1.406658
C	6.313212	4.586817	1.406658
C	4.586817	6.313212	1.406658
C	2.411433	7.421626	1.406658
C	0.000000	7.803559	1.406658
C	-2.411433	7.421626	1.406658
C	-4.586817	6.313212	1.406658
C	-6.313212	4.586817	1.406658
C	-7.421626	2.411433	1.406658
C	-7.803559	0.000000	1.406658
C	-7.421626	-2.411433	1.406658
C	-6.313212	-4.586817	1.406658
C	-4.586817	-6.313212	1.406658
C	-2.411433	-7.421626	1.406658
C	0.000000	-7.803559	1.406658
C	2.411433	-7.421626	1.406658
C	4.586817	-6.313212	1.406658
C	6.313212	-4.586817	1.406658
C	7.421626	-2.411433	1.406658
C	7.705396	1.220415	0.729632
C	6.951138	3.541782	0.729632
C	5.516455	5.516455	0.729632
C	3.541782	6.951138	0.729632
C	1.220415	7.705396	0.729632
C	-1.220415	7.705396	0.729632
C	-3.541782	6.951138	0.729632
C	-5.516455	5.516455	0.729632
C	-6.951138	3.541782	0.729632
C	-7.705396	1.220415	0.729632
C	-7.705396	-1.220415	0.729632
C	-6.951138	-3.541782	0.729632
C	-5.516455	-5.516455	0.729632
C	-3.541782	-6.951138	0.729632

C	-1.220415	-7.705396	0.729632
C	1.220415	-7.705396	0.729632
C	3.541782	-6.951138	0.729632
C	5.516455	-5.516455	0.729632
C	6.951138	-3.541782	0.729632
C	7.705396	-1.220415	0.729632
C	7.705396	1.220415	-0.729632
C	6.951138	3.541782	-0.729632
C	5.516455	5.516455	-0.729632
C	3.541782	6.951138	-0.729632
C	1.220415	7.705396	-0.729632
C	-1.220415	7.705396	-0.729632
C	-3.541782	6.951138	-0.729632
C	-5.516455	5.516455	-0.729632
C	-6.951138	3.541782	-0.729632
C	-7.705396	1.220415	-0.729632
C	-7.705396	-1.220415	-0.729632
C	-6.951138	-3.541782	-0.729632
C	-5.516455	-5.516455	-0.729632
C	-3.541782	-6.951138	-0.729632
C	-1.220415	-7.705396	-0.729632
C	1.220415	-7.705396	-0.729632
C	3.541782	-6.951138	-0.729632
C	5.516455	-5.516455	-0.729632
C	6.951138	-3.541782	-0.729632
C	7.705396	-1.220415	-0.729632
C	7.803559	0.000000	-1.406658
C	7.421626	2.411433	-1.406658
C	6.313212	4.586817	-1.406658
C	4.586817	6.313212	-1.406658
C	2.411433	7.421626	-1.406658
C	0.000000	7.803559	-1.406658
C	-2.411433	7.421626	-1.406658
C	-4.586817	6.313212	-1.406658
C	-6.313212	4.586817	-1.406658
C	-7.421626	2.411433	-1.406658
C	-7.803559	0.000000	-1.406658
C	-7.421626	-2.411433	-1.406658
C	-6.313212	-4.586817	-1.406658
C	-4.586817	-6.313212	-1.406658
C	-2.411433	-7.421626	-1.406658
C	0.000000	-7.803559	-1.406658
C	2.411433	-7.421626	-1.406658
C	4.586817	-6.313212	-1.406658
C	6.313212	-4.586817	-1.406658

C	7.421626	-2.411433	-1.406658
H	7.793977	0.000000	-2.484706
H	7.412512	2.408471	-2.484706
H	6.305460	4.581185	-2.484706
H	4.581185	6.305460	-2.484706
H	2.408471	7.412512	-2.484706
H	0.000000	7.793977	-2.484706
H	-2.408471	7.412512	-2.484706
H	-4.581185	6.305460	-2.484706
H	-6.305460	4.581185	-2.484706
H	-7.412512	2.408471	-2.484706
H	-7.793977	0.000000	-2.484706
H	-7.412512	-2.408471	-2.484706
H	-6.305460	-4.581185	-2.484706
H	-4.581185	-6.305460	-2.484706
H	-2.408471	-7.412512	-2.484706
H	0.000000	-7.793977	-2.484706
H	2.408471	-7.412512	-2.484706
H	4.581185	-6.305460	-2.484706
H	6.305460	-4.581185	-2.484706
H	7.412512	-2.408471	-2.484706

[22]cyclacene

H	8.571659	0.000000	2.484719
H	8.224447	2.414915	2.484719
H	7.210939	4.634189	2.484719
H	5.613243	6.478028	2.484719
H	3.560796	7.797056	2.484719
H	1.219874	8.484412	2.484719
H	-1.219874	8.484412	2.484719
H	-3.560796	7.797056	2.484719
H	-5.613243	6.478028	2.484719
H	-7.210939	4.634189	2.484719
H	-8.224447	2.414915	2.484719
H	-8.571659	0.000000	2.484719
H	-8.224447	-2.414915	2.484719
H	-7.210939	-4.634189	2.484719
H	-5.613243	-6.478028	2.484719
H	-3.560796	-7.797056	2.484719
H	-1.219874	-8.484412	2.484719
H	1.219874	-8.484412	2.484719
H	3.560796	-7.797056	2.484719
H	5.613243	-6.478028	2.484719
H	7.210939	-4.634189	2.484719

H	8.224447	-2.414915	2.484719
C	8.580433	0.000000	1.406650
C	8.232866	2.417387	1.406650
C	7.218320	4.638933	1.406650
C	5.618989	6.484659	1.406650
C	3.564441	7.805037	1.406650
C	1.221123	8.493097	1.406650
C	-1.221123	8.493097	1.406650
C	-3.564441	7.805037	1.406650
C	-5.618989	6.484659	1.406650
C	-7.218320	4.638933	1.406650
C	-8.232866	2.417387	1.406650
C	-8.580433	0.000000	1.406650
C	-8.232866	-2.417387	1.406650
C	-7.218320	-4.638933	1.406650
C	-5.618989	-6.484659	1.406650
C	-3.564441	-7.805037	1.406650
C	-1.221123	-8.493097	1.406650
C	1.221123	-8.493097	1.406650
C	3.564441	-7.805037	1.406650
C	5.618989	-6.484659	1.406650
C	7.218320	-4.638933	1.406650
C	8.232866	-2.417387	1.406650
C	8.491217	1.220853	0.729675
C	7.803309	3.563652	0.729675
C	6.483223	5.617745	0.729675
C	4.637906	7.216722	0.729675
C	2.416852	8.231043	0.729675
C	0.000000	8.578534	0.729675
C	-2.416852	8.231043	0.729675
C	-4.637906	7.216722	0.729675
C	-6.483223	5.617745	0.729675
C	-7.803309	3.563652	0.729675
C	-8.491217	1.220853	0.729675
C	-8.491217	-1.220853	0.729675
C	-7.803309	-3.563652	0.729675
C	-6.483223	-5.617745	0.729675
C	-4.637906	-7.216722	0.729675
C	-2.416852	-8.231043	0.729675
C	0.000000	-8.578534	0.729675
C	2.416852	-8.231043	0.729675
C	4.637906	-7.216722	0.729675
C	6.483223	-5.617745	0.729675
C	7.803309	-3.563652	0.729675
C	8.491217	-1.220853	0.729675

C	8.491217	1.220853	-0.729675
C	7.803309	3.563652	-0.729675
C	6.483223	5.617745	-0.729675
C	4.637906	7.216722	-0.729675
C	2.416852	8.231043	-0.729675
C	0.000000	8.578534	-0.729675
C	-2.416852	8.231043	-0.729675
C	-4.637906	7.216722	-0.729675
C	-6.483223	5.617745	-0.729675
C	-7.803309	3.563652	-0.729675
C	-8.491217	1.220853	-0.729675
C	-8.491217	-1.220853	-0.729675
C	-7.803309	-3.563652	-0.729675
C	-6.483223	-5.617745	-0.729675
C	-4.637906	-7.216722	-0.729675
C	-2.416852	-8.231043	-0.729675
C	0.000000	-8.578534	-0.729675
C	2.416852	-8.231043	-0.729675
C	4.637906	-7.216722	-0.729675
C	6.483223	-5.617745	-0.729675
C	7.803309	-3.563652	-0.729675
C	8.491217	-1.220853	-0.729675
C	8.580433	0.000000	-1.406650
C	8.232866	2.417387	-1.406650
C	7.218320	4.638933	-1.406650
C	5.618989	6.484659	-1.406650
C	3.564441	7.805037	-1.406650
C	1.221123	8.493097	-1.406650
C	-1.221123	8.493097	-1.406650
C	-3.564441	7.805037	-1.406650
C	-5.618989	6.484659	-1.406650
C	-7.218320	4.638933	-1.406650
C	-8.232866	2.417387	-1.406650
C	-8.580433	0.000000	-1.406650
C	-8.232866	-2.417387	-1.406650
C	-7.218320	-4.638933	-1.406650
C	-5.618989	-6.484659	-1.406650
C	-3.564441	-7.805037	-1.406650
C	-1.221123	-8.493097	-1.406650
C	1.221123	-8.493097	-1.406650
C	3.564441	-7.805037	-1.406650
C	5.618989	-6.484659	-1.406650
C	7.218320	-4.638933	-1.406650
C	8.232866	-2.417387	-1.406650
H	8.571659	0.000000	-2.484719

H	8.224447	2.414915	-2.484719
H	7.210939	4.634189	-2.484719
H	5.613243	6.478028	-2.484719
H	3.560796	7.797056	-2.484719
H	1.219874	8.484412	-2.484719
H	-1.219874	8.484412	-2.484719
H	-3.560796	7.797056	-2.484719
H	-5.613243	6.478028	-2.484719
H	-7.210939	4.634189	-2.484719
H	-8.224447	2.414915	-2.484719
H	-8.571659	0.000000	-2.484719
H	-8.224447	-2.414915	-2.484719
H	-7.210939	-4.634189	-2.484719
H	-5.613243	-6.478028	-2.484719
H	-3.560796	-7.797056	-2.484719
H	-1.219874	-8.484412	-2.484719
H	1.219874	-8.484412	-2.484719
H	3.560796	-7.797056	-2.484719
H	5.613243	-6.478028	-2.484719
H	7.210939	-4.634189	-2.484719
H	8.224447	-2.414915	-2.484719

[24]cyclacene

H	9.349507	0.000000	2.484725
H	9.030931	2.419831	2.484725
H	8.096911	4.674754	2.484725
H	6.611100	6.611100	2.484725
H	4.674754	8.096911	2.484725
H	2.419831	9.030931	2.484725
H	0.000000	9.349507	2.484725
H	-2.419831	9.030931	2.484725
H	-4.674754	8.096911	2.484725
H	-6.611100	6.611100	2.484725
H	-8.096911	4.674754	2.484725
H	-9.030931	2.419831	2.484725
H	-9.349507	0.000000	2.484725
H	-9.030931	-2.419831	2.484725
H	-8.096911	-4.674754	2.484725
H	-6.611100	-6.611100	2.484725
H	-4.674754	-8.096911	2.484725
H	-2.419831	-9.030931	2.484725
H	0.000000	-9.349507	2.484725
H	2.419831	-9.030931	2.484725
H	4.674754	-8.096911	2.484725

H	6.611100	-6.611100	2.484725
H	8.096911	-4.674754	2.484725
H	9.030931	-2.419831	2.484725
C	9.357598	0.000000	1.406641
C	9.038745	2.421925	1.406641
C	8.103917	4.678799	1.406641
C	6.616821	6.616821	1.406641
C	4.678799	8.103917	1.406641
C	2.421925	9.038745	1.406641
C	0.000000	9.357598	1.406641
C	-2.421925	9.038745	1.406641
C	-4.678799	8.103917	1.406641
C	-6.616821	6.616821	1.406641
C	-8.103917	4.678799	1.406641
C	-9.038745	2.421925	1.406641
C	-9.357598	0.000000	1.406641
C	-9.038745	-2.421925	1.406641
C	-8.103917	-4.678799	1.406641
C	-6.616821	-6.616821	1.406641
C	-4.678799	-8.103917	1.406641
C	-2.421925	-9.038745	1.406641
C	0.000000	-9.357598	1.406641
C	2.421925	-9.038745	1.406641
C	4.678799	-8.103917	1.406641
C	6.616821	-6.616821	1.406641
C	8.103917	-4.678799	1.406641
C	9.038745	-2.421925	1.406641
C	9.275831	1.221186	0.729704
C	8.643699	3.580337	0.729704
C	7.422512	5.695494	0.729704
C	5.695494	7.422512	0.729704
C	3.580337	8.643699	0.729704
C	1.221186	9.275831	0.729704
C	-1.221186	9.275831	0.729704
C	-3.580337	8.643699	0.729704
C	-5.695494	7.422512	0.729704
C	-7.422512	5.695494	0.729704
C	-8.643699	3.580337	0.729704
C	-9.275831	1.221186	0.729704
C	-9.275831	-1.221186	0.729704
C	-8.643699	-3.580337	0.729704
C	-7.422512	-5.695494	0.729704
C	-5.695494	-7.422512	0.729704
C	-3.580337	-8.643699	0.729704
C	-1.221186	-9.275831	0.729704

C	1.221186	-9.275831	0.729704
C	3.580337	-8.643699	0.729704
C	5.695494	-7.422512	0.729704
C	7.422512	-5.695494	0.729704
C	8.643699	-3.580337	0.729704
C	9.275831	-1.221186	0.729704
C	9.275831	1.221186	-0.729704
C	8.643699	3.580337	-0.729704
C	7.422512	5.695494	-0.729704
C	5.695494	7.422512	-0.729704
C	3.580337	8.643699	-0.729704
C	1.221186	9.275831	-0.729704
C	-1.221186	9.275831	-0.729704
C	-3.580337	8.643699	-0.729704
C	-5.695494	7.422512	-0.729704
C	-7.422512	5.695494	-0.729704
C	-8.643699	3.580337	-0.729704
C	-9.275831	1.221186	-0.729704
C	-9.275831	-1.221186	-0.729704
C	-8.643699	-3.580337	-0.729704
C	-7.422512	-5.695494	-0.729704
C	-5.695494	-7.422512	-0.729704
C	-3.580337	-8.643699	-0.729704
C	-1.221186	-9.275831	-0.729704
C	1.221186	-9.275831	-0.729704
C	3.580337	-8.643699	-0.729704
C	5.695494	-7.422512	-0.729704
C	7.422512	-5.695494	-0.729704
C	8.643699	-3.580337	-0.729704
C	9.275831	-1.221186	-0.729704
C	9.357598	0.000000	-1.406641
C	9.038745	2.421925	-1.406641
C	8.103917	4.678799	-1.406641
C	6.616821	6.616821	-1.406641
C	4.678799	8.103917	-1.406641
C	2.421925	9.038745	-1.406641
C	0.000000	9.357598	-1.406641
C	-2.421925	9.038745	-1.406641
C	-4.678799	8.103917	-1.406641
C	-6.616821	6.616821	-1.406641
C	-8.103917	4.678799	-1.406641
C	-9.038745	2.421925	-1.406641
C	-9.357598	0.000000	-1.406641
C	-9.038745	-2.421925	-1.406641
C	-8.103917	-4.678799	-1.406641

C	-6.616821	-6.616821	-1.406641
C	-4.678799	-8.103917	-1.406641
C	-2.421925	-9.038745	-1.406641
C	0.000000	-9.357598	-1.406641
C	2.421925	-9.038745	-1.406641
C	4.678799	-8.103917	-1.406641
C	6.616821	-6.616821	-1.406641
C	8.103917	-4.678799	-1.406641
C	9.038745	-2.421925	-1.406641
H	9.349507	0.000000	-2.484725
H	9.030931	2.419831	-2.484725
H	8.096911	4.674754	-2.484725
H	6.611100	6.611100	-2.484725
H	4.674754	8.096911	-2.484725
H	2.419831	9.030931	-2.484725
H	0.000000	9.349507	-2.484725
H	-2.419831	9.030931	-2.484725
H	-4.674754	8.096911	-2.484725
H	-6.611100	6.611100	-2.484725
H	-8.096911	4.674754	-2.484725
H	-9.030931	2.419831	-2.484725
H	-9.349507	0.000000	-2.484725
H	-9.030931	-2.419831	-2.484725
H	-8.096911	-4.674754	-2.484725
H	-6.611100	-6.611100	-2.484725
H	-4.674754	-8.096911	-2.484725
H	-2.419831	-9.030931	-2.484725
H	0.000000	-9.349507	-2.484725
H	2.419831	-9.030931	-2.484725
H	4.674754	-8.096911	-2.484725
H	6.611100	-6.611100	-2.484725
H	8.096911	-4.674754	-2.484725
H	9.030931	-2.419831	-2.484725

[28]cyclacene

H	10.905548	0.000000	2.484732
H	10.632123	2.426713	2.484732
H	9.825560	4.731740	2.484732
H	8.526301	6.799498	2.484732
H	6.799498	8.526301	2.484732
H	4.731740	9.825560	2.484732
H	2.426713	10.632123	2.484732
H	0.000000	10.905548	2.484732
H	-2.426713	10.632123	2.484732

H	-4.731740	9.825560	2.484732
H	-6.799498	8.526301	2.484732
H	-8.526301	6.799498	2.484732
H	-9.825560	4.731740	2.484732
H	-10.632123	2.426713	2.484732
H	-10.905548	0.000000	2.484732
H	-10.632123	-2.426713	2.484732
H	-9.825560	-4.731740	2.484732
H	-8.526301	-6.799498	2.484732
H	-6.799498	-8.526301	2.484732
H	-4.731740	-9.825560	2.484732
H	-2.426713	-10.632123	2.484732
H	0.000000	-10.905548	2.484732
H	2.426713	-10.632123	2.484732
H	4.731740	-9.825560	2.484732
H	6.799498	-8.526301	2.484732
H	8.526301	-6.799498	2.484732
H	9.825560	-4.731740	2.484732
H	10.632123	-2.426713	2.484732
C	10.912537	0.000000	1.406627
C	10.638937	2.428268	1.406627
C	9.831856	4.734772	1.406627
C	8.531765	6.803856	1.406627
C	6.803856	8.531765	1.406627
C	4.734772	9.831856	1.406627
C	2.428268	10.638937	1.406627
C	0.000000	10.912537	1.406627
C	-2.428268	10.638937	1.406627
C	-4.734772	9.831856	1.406627
C	-6.803856	8.531765	1.406627
C	-8.531765	6.803856	1.406627
C	-9.831856	4.734772	1.406627
C	-10.638937	2.428268	1.406627
C	-10.912537	0.000000	1.406627
C	-10.638937	-2.428268	1.406627
C	-9.831856	-4.734772	1.406627
C	-8.531765	-6.803856	1.406627
C	-6.803856	-8.531765	1.406627
C	-4.734772	-9.831856	1.406627
C	-2.428268	-10.638937	1.406627
C	0.000000	-10.912537	1.406627
C	2.428268	-10.638937	1.406627
C	4.734772	-9.831856	1.406627
C	6.803856	-8.531765	1.406627
C	8.531765	-6.803856	1.406627

C	9.831856	-4.734772	1.406627
C	10.638937	-2.428268	1.406627
C	10.842472	1.221653	0.729745
C	10.298785	3.603701	0.729745
C	9.238674	5.805044	0.729745
C	7.715298	7.715298	0.729745
C	5.805044	9.238674	0.729745
C	3.603701	10.298785	0.729745
C	1.221653	10.842472	0.729745
C	-1.221653	10.842472	0.729745
C	-3.603701	10.298785	0.729745
C	-5.805044	9.238674	0.729745
C	-7.715298	7.715298	0.729745
C	-9.238674	5.805044	0.729745
C	-10.298785	3.603701	0.729745
C	-10.842472	1.221653	0.729745
C	-10.842472	-1.221653	0.729745
C	-10.298785	-3.603701	0.729745
C	-9.238674	-5.805044	0.729745
C	-7.715298	-7.715298	0.729745
C	-5.805044	-9.238674	0.729745
C	-3.603701	-10.298785	0.729745
C	-1.221653	-10.842472	0.729745
C	1.221653	-10.842472	0.729745
C	3.603701	-10.298785	0.729745
C	5.805044	-9.238674	0.729745
C	7.715298	-7.715298	0.729745
C	9.238674	-5.805044	0.729745
C	10.298785	-3.603701	0.729745
C	10.842472	-1.221653	0.729745
C	10.842472	1.221653	-0.729745
C	10.298785	3.603701	-0.729745
C	9.238674	5.805044	-0.729745
C	7.715298	7.715298	-0.729745
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C	-1.221653	10.842472	-0.729745
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C	-9.238674	5.805044	-0.729745
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C	-10.842472	1.221653	-0.729745
C	-10.842472	-1.221653	-0.729745

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C	-7.715298	-7.715298	-0.729745
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C	1.221653	-10.842472	-0.729745
C	3.603701	-10.298785	-0.729745
C	5.805044	-9.238674	-0.729745
C	7.715298	-7.715298	-0.729745
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C	10.298785	-3.603701	-0.729745
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C	10.912537	0.000000	-1.406627
C	10.638937	2.428268	-1.406627
C	9.831856	4.734772	-1.406627
C	8.531765	6.803856	-1.406627
C	6.803856	8.531765	-1.406627
C	4.734772	9.831856	-1.406627
C	2.428268	10.638937	-1.406627
C	0.000000	10.912537	-1.406627
C	-2.428268	10.638937	-1.406627
C	-4.734772	9.831856	-1.406627
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C	-8.531765	6.803856	-1.406627
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C	-8.531765	-6.803856	-1.406627
C	-6.803856	-8.531765	-1.406627
C	-4.734772	-9.831856	-1.406627
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C	4.734772	-9.831856	-1.406627
C	6.803856	-8.531765	-1.406627
C	8.531765	-6.803856	-1.406627
C	9.831856	-4.734772	-1.406627
C	10.638937	-2.428268	-1.406627
H	10.905548	0.000000	-2.484732
H	10.632123	2.426713	-2.484732
H	9.825560	4.731740	-2.484732
H	8.526301	6.799498	-2.484732

H	6.799498	8.526301	-2.484732
H	4.731740	9.825560	-2.484732
H	2.426713	10.632123	-2.484732
H	0.000000	10.905548	-2.484732
H	-2.426713	10.632123	-2.484732
H	-4.731740	9.825560	-2.484732
H	-6.799498	8.526301	-2.484732
H	-8.526301	6.799498	-2.484732
H	-9.825560	4.731740	-2.484732
H	-10.632123	2.426713	-2.484732
H	-10.905548	0.000000	-2.484732
H	-10.632123	-2.426713	-2.484732
H	-9.825560	-4.731740	-2.484732
H	-8.526301	-6.799498	-2.484732
H	-6.799498	-8.526301	-2.484732
H	-4.731740	-9.825560	-2.484732
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H	2.426713	-10.632123	-2.484732
H	4.731740	-9.825560	-2.484732
H	6.799498	-8.526301	-2.484732
H	8.526301	-6.799498	-2.484732
H	9.825560	-4.731740	-2.484732
H	10.632123	-2.426713	-2.484732