

Supplementary Information

Bandgaps of Atomically Precise Graphene Nanoribbons and Occam's Razor

Aristides D. Zdetsis*

Molecular Engineering Laboratory, Department of Physics, University of Patras, Patras 26500
GR, Greece.

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#S1) supplementary information for the 5-AGNRs (or 2x AGNRs)

Comparison of Normal and Edge Modified 5-AGNRs at the Critical Length Region.

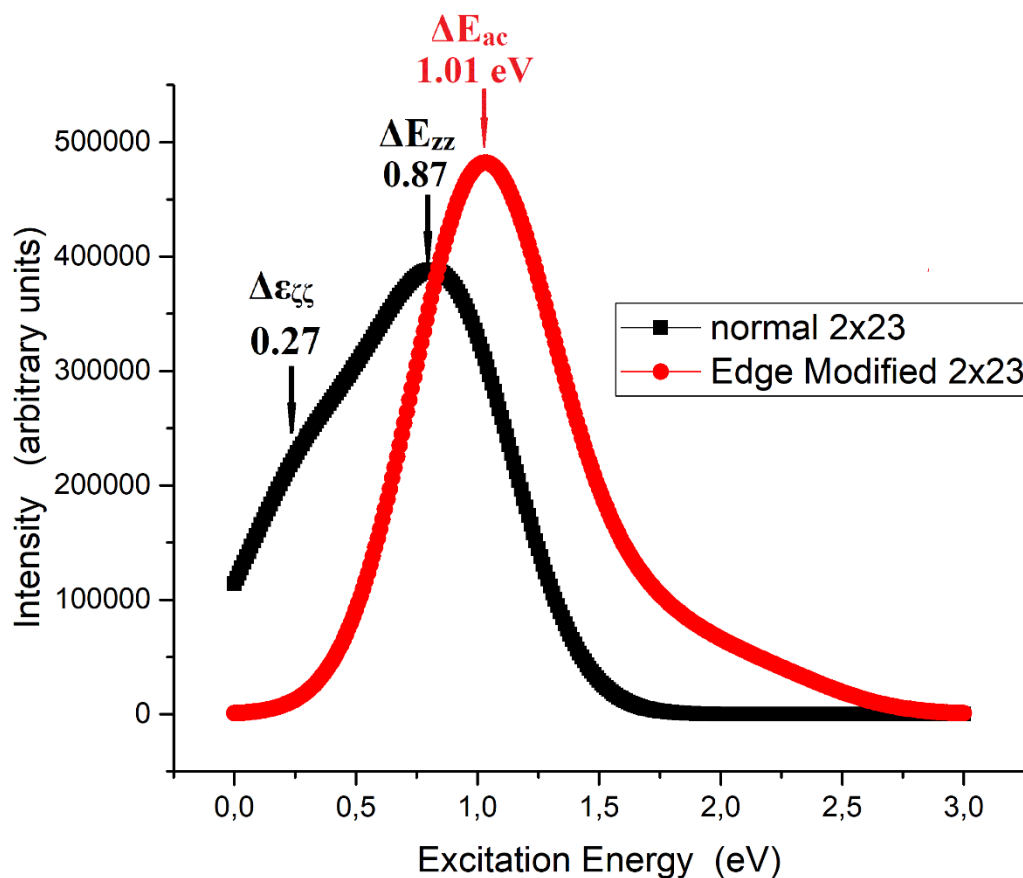


FIGURE S1. Spectrum of the 2x23 Normal and Edge Modified (in red) AGNRs, right after the end-states have appear at the critical length $L_c \sim 100 \text{ \AA}$.

These calculations have been performed with the Gaussian program package.¹

As we can see in the figure the spectrum of the normal 5-AGNR is dominated by the surface states through the ΔE_{zz} and $\Delta\epsilon_{\zeta\zeta}$ peaks, involving “mixt” transitions between edge and “bulk” states, and between pure edge states, respectively. The “bulk” ΔE_{ac} peak² is strongly suppressed in the normal 5x23 AGNR. In contrast, the spectrum of the corresponding edge modified AGNR, which have no zigzag ends and, therefore, no zigzag end states,³⁻⁴ is fully determined by the ΔE_{ac} peak.

#S2) 7-AGNRs (or 3x AGNRs)

Comparison of the spectra of 3x or 7-AGNR

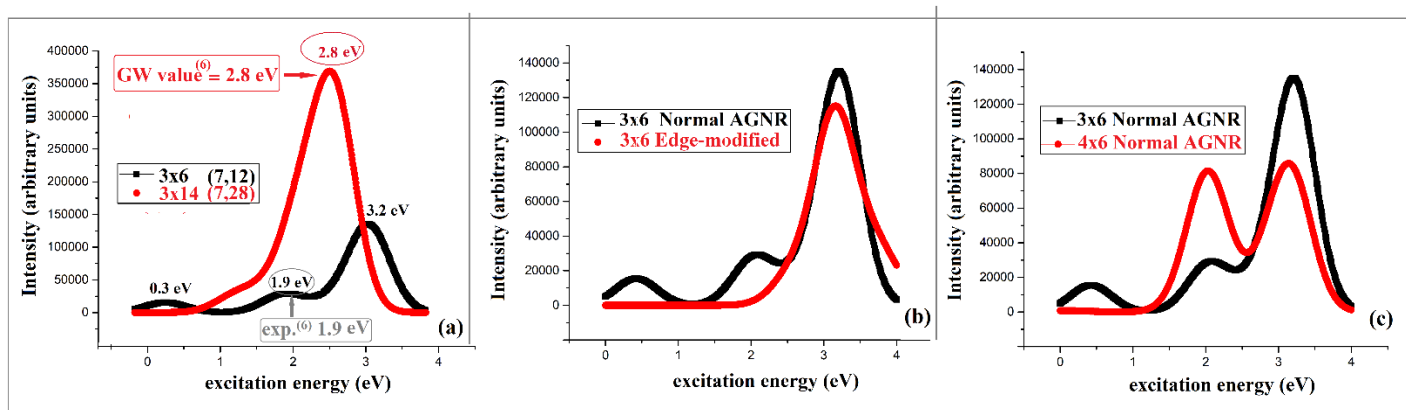


FIGURE S2. Comparisons of the spectra of 3x6 and 3x14 AGNRs and 4x6 AGNRs: (a) 3x6 and 3x14 normal AGNRs, (b) 3x6 normal and edge modified AGNRs, and (c) 3x6 and 4x6 (9,14) normal AGNRs.

In the spectrum of the 3x6 AGNR in Fig. S2(a) we can clearly see the $\Delta\epsilon_{zz}$ peak (at 0.3 eV), between pure end states; the ΔE_{zz} peak between mixt states at 1.9 eV ; and ΔE_{ac} peak at 3.2 eV, in excellent agreement with experimental measurements of Wang *et al.*² On the other hand the “bulk” peak ΔE_{ac} for the longer 3x14 AGNR has been shifted to 2.8 eV, which is in excellent agreement with the measurement and GW calculations of Wang *et al.*² for this AGNR. In Fig. S2(b) we can verify that the peak at 3.2 eV of the 3x6 AGNR is indeed a “bulk” peak since it dominates the spectrum of the corresponding edge modified AGNR,⁴ whereas the “surface” peaks have disappeared. Finally in Fig. S2(c) we emphasize the similarity between the spectra of 3x6 and 4x6 AGNRs, which have the same length different width.

#S3) 9-AGNRs (or 4x AGNRs)

In Fig. S3 we can observe the “bulk” ΔE_{ac} peak of the 4x (9-AGNRs), which starts (for short lengths 4x13) at 1.6 eV and stabilizes to the value 1.45 eV for larger lengths (4x18, 4x24). The corresponding experimental value⁵ is 1.4 eV.

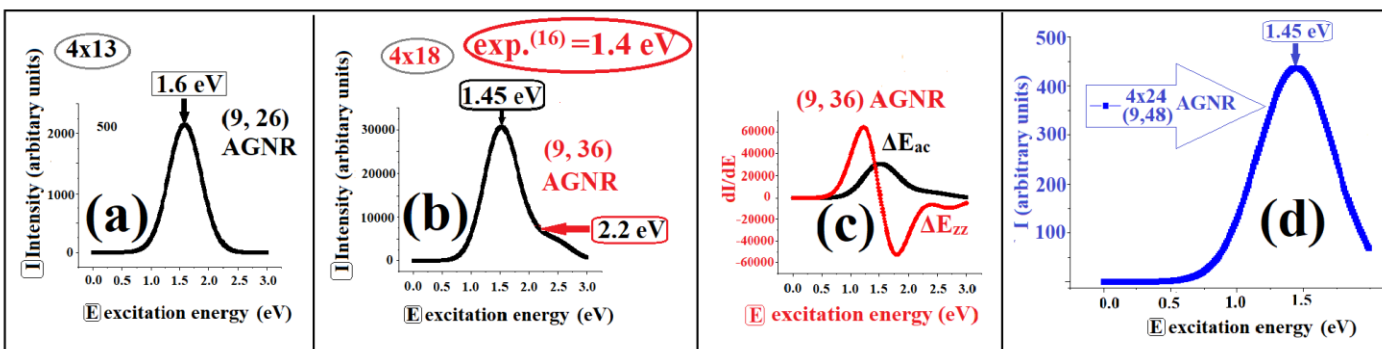


FIGURE S3. Comparison of the spectra of the 4x13, 4x18, and 4x24 AGNRs. (a) the 4x13 spectrum. (b) the 4x18 (b) AGNR spectrum. (c) the variation of intensity (I) with energy (E) for the 4x18 AGNR, i.e., the derivative dI/dE , which is given to emphasize the “surface” ΔE_{zz} peak at ~ 2.2 eV. (d) The corresponding spectrum of the 4x24 AGNR. The width of these three AGNRs is about 11.6 Å, and their lengths (including end-hydrogens) 56.4 Å, 77.8 Å, and 103.5 Å, respectively.

The edge modified 4x24 AGNR is described in Fig. S4.

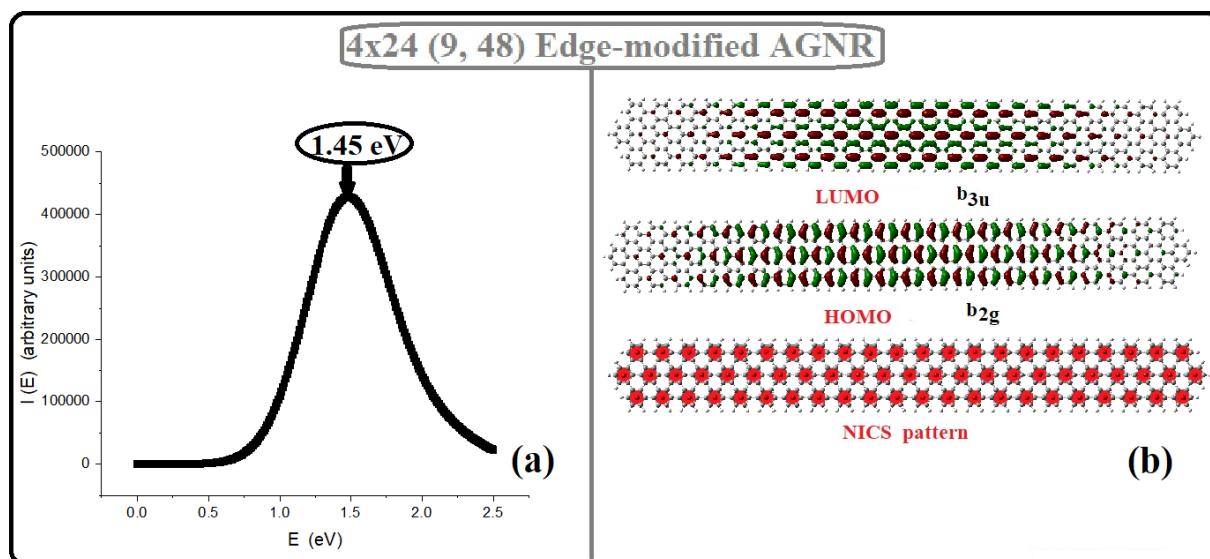


FIGURE S4. Edge-Modified 4x24 (9, 48) AGNR. (a) spectrum, and (b) HOMO, LUMO orbitals and aromaticity (NICS) pattern.

Observe that (by construction¹) there are no “empty” edge-, or end-rings, and that the HOMO is characterized by even parity² (and LUMO with odd parity) similarly to hexagonal PAHs with odd shell number³. In full analogy to such PAHs (benzene, circum-coronene, etc.), the aromaticity pattern (CIRCO)³ is fully compatible with Clar’s rules(s). In contrast, 3x AGNRs (as the 3x6, and 3x14 examined before) are characterized by odd parity HOMOs (and even parity LUMOs) associated with CO aromaticity pattern³ (like Coronene, circum-circum-coronene, etc.). All these calculations have been performed with the Gaussian program package.¹

§S4 Cartesian Coordinates of 2x- AGNR Key Structures (in Å):

2x22 closed singlet

C 0.00000000 2.41689400 46.02708200
C 0.00000000 1.22953100 46.71786900
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2x22 Open Singlet

open singlet 2x22 trying triplet

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2x23 open singlet

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Edge-modified closed singlet 2x23

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C 0.00000000 2.43434600 9.27383700
C 0.00000000 1.22994700 10.02723000
C 0.00000000 1.22995600 7.15809300
C 0.00000000 2.43436400 7.91147900
C 0.00000000 2.43434600 4.97751100
C 0.00000000 1.22995000 5.73090000
C 0.00000000 1.22995400 2.86176400
C 0.00000000 2.43435500 3.61514900

C 0.00000000 2.43435000 0.68118200
C 0.00000000 1.22995200 1.43456800
C 0.00000000 1.22995200 -1.43456800
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C 0.00000000 2.43435500 -3.61514900
C 0.00000000 1.22995400 -2.86176400
C 0.00000000 1.22995000 -5.73090000
C 0.00000000 2.43434600 -4.97751100
C 0.00000000 2.43436400 -7.91147900
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C 0.00000000 1.22994700 -10.02723000
C 0.00000000 2.43434600 -9.27383700
C 0.00000000 2.43437700 -12.20780300
C 0.00000000 1.22995800 -11.45441400
C 0.00000000 1.22994400 -14.32355500
C 0.00000000 2.43435100 -13.57015300
C 0.00000000 2.43440000 -16.50411800
C 0.00000000 1.22995900 -15.75072100
C 0.00000000 1.22993800 -18.61986900
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C 0.00000000 2.43444200 -20.80041400
C 0.00000000 1.22995800 -20.04699700
C 0.00000000 1.22993000 -22.91616100
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C 0.00000000 1.22995100 -24.34321200
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C 0.00000000 2.43448800 -26.45887600
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C 0.00000000 1.22987900 -31.50855000
C 0.00000000 2.43467800 -30.75487300
C 0.00000000 2.43490400 -33.68894000
C 0.00000000 1.22984900 -32.93507900
C 0.00000000 1.22953600 -35.80468100
C 0.00000000 2.43488700 -35.05056800
C 0.00000000 2.43646600 -37.98298900
C 0.00000000 1.22944600 -37.23043800
C 0.00000000 1.23258600 -40.10011300
C 0.00000000 2.43804400 -39.34333900
C 0.00000000 2.44743700 -42.28372400
C 0.00000000 1.23576500 -41.52340200
C 0.00000000 1.22532200 -44.38201700
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C 0.00000000 1.20423500 -45.78330200
C 0.00000000 -1.20423500 45.78330200

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C 0.00000000 -1.23576500 41.52340200
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C 0.00000000 -1.22993500 28.63929500
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C 0.00000000 0.00000000 26.49623600
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C 0.00000000 0.00000000 -3.57791900

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C 0.00000000 0.00000000 -16.46688500
C 0.00000000 -1.22995900 -15.75072100
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C 0.00000000 0.00000000 -17.90371800
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C 0.00000000 -1.22995800 -20.04699700
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C 0.00000000 0.00000000 -25.05938900
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C 0.00000000 0.00000000 -37.94776700
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C 0.00000000 -2.43435100 13.57015300
C 0.00000000 -2.43437700 12.20780300
C 0.00000000 -2.43434600 9.27383700
C 0.00000000 -2.43436400 7.91147900
C 0.00000000 -2.43434600 4.97751100
C 0.00000000 -2.43435500 3.61514900
C 0.00000000 -2.43435000 0.68118200
C 0.00000000 -2.43435000 -0.68118200
C 0.00000000 -2.43435500 -3.61514900
C 0.00000000 -2.43434600 -4.97751100
C 0.00000000 -2.43436400 -7.91147900
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C 0.00000000 -2.43490400 -33.68894000
C 0.00000000 -2.43488700 -35.05056800
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H 0.00000000 -3.38567000 44.19035200
H 0.00000000 -3.40211800 41.77094600
H 0.00000000 -3.39470200 39.85207800
H 0.00000000 -3.39222800 37.47261500
H 0.00000000 -3.39159800 35.55914700
H 0.00000000 -3.39155800 33.18016400
H 0.00000000 -3.39136100 31.26359300
H 0.00000000 -3.39137400 28.88412600
H 0.00000000 -3.39120800 26.96753100

H 0.00000000 -3.39125100 24.58803200
H 0.00000000 -3.39114000 22.67133200
H 0.00000000 -3.39118800 20.29181000
H 0.00000000 -3.39111100 18.37506200
H 0.00000000 -3.39115400 15.99552800
H 0.00000000 -3.39110000 14.07875700
H 0.00000000 -3.39113300 11.69921800
H 0.00000000 -3.39109700 9.78243500
H 0.00000000 -3.39112000 7.40289300
H 0.00000000 -3.39109900 5.48610500
H 0.00000000 -3.39111100 3.10656200
H 0.00000000 -3.39110400 1.18977200
H 0.00000000 -3.39110400 -1.18977200
H 0.00000000 -3.39111100 -3.10656200
H 0.00000000 -3.39109900 -5.48610500
H 0.00000000 -3.39112000 -7.40289300
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H 0.00000000 -3.39137400 -28.88412600
H 0.00000000 -3.39136100 -31.26359300
H 0.00000000 -3.39155800 -33.18016400
H 0.00000000 -3.39159800 -35.55914700
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H 0.00000000 3.38567000 44.19035200
H 0.00000000 3.40211800 41.77094600
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H 0.00000000 3.39159800 35.55914700
H 0.00000000 3.39155800 33.18016400
H 0.00000000 3.39136100 31.26359300
H 0.00000000 3.39137400 28.88412600
H 0.00000000 3.39120800 26.96753100
H 0.00000000 3.39125100 24.58803200
H 0.00000000 3.39114000 22.67133200
H 0.00000000 3.39118800 20.29181000
H 0.00000000 3.39111100 18.37506200

H 0.00000000 3.39115400 15.99552800
H 0.00000000 3.39110000 14.07875700
H 0.00000000 3.39113300 11.69921800
H 0.00000000 3.39109700 9.78243500
H 0.00000000 3.39112000 7.40289300
H 0.00000000 3.39109900 5.48610500
H 0.00000000 3.39111100 3.10656200
H 0.00000000 3.39110400 1.18977200
H 0.00000000 3.39110400 -1.18977200
H 0.00000000 3.39111100 -3.10656200
H 0.00000000 3.39109900 -5.48610500
H 0.00000000 3.39112000 -7.40289300
H 0.00000000 3.39109700 -9.78243500
H 0.00000000 3.39113300 -11.69921800
H 0.00000000 3.39110000 -14.07875700
H 0.00000000 3.39115400 -15.99552800
H 0.00000000 3.39111100 -18.37506200
H 0.00000000 3.39118800 -20.29181000
H 0.00000000 3.39114000 -22.67133200
H 0.00000000 3.39125100 -24.58803200
H 0.00000000 3.39120800 -26.96753100
H 0.00000000 3.39137400 -28.88412600
H 0.00000000 3.39136100 -31.26359300
H 0.00000000 3.39155800 -33.18016400
H 0.00000000 3.39159800 -35.55914700
H 0.00000000 3.39222800 -37.47261500
H 0.00000000 3.39470200 -39.85207800
H 0.00000000 3.40211800 -41.77094600
H 0.00000000 3.38567000 -44.19035200
H 0.00000000 2.14753100 -46.32409200
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H 0.00000000 -2.14753100 -46.32409200
H 0.00000000 2.14753100 46.32409200
H 0.00000000 0.00000000 47.56248000
H 0.00000000 -2.14753100 46.32409200

§S5 Cartesian coordinates of key 3x (7-AGNRs)

3x6 AGNR Closed Singlet

C 0.00000000 3.64294200 11.45432700
C 0.00000000 2.45005000 12.14130200
C 0.00000000 2.47081600 9.31146000
C 0.00000000 3.65629800 10.05762100
C 0.00000000 3.65719300 7.11969000
C 0.00000000 2.46326100 7.86114000
C 0.00000000 2.45808500 5.00968600
C 0.00000000 3.65732800 5.74934400
C 0.00000000 3.65721100 2.82743800
C 0.00000000 2.45677200 3.56899600
C 0.00000000 2.45611700 0.71975900
C 0.00000000 3.65736000 1.46081300
C 0.00000000 3.65736000 -1.46081300
C 0.00000000 2.45611700 -0.71975900
C 0.00000000 2.45677200 -3.56899600
C 0.00000000 3.65721100 -2.82743800
C 0.00000000 3.65732800 -5.74934400
C 0.00000000 2.45808500 -5.00968600
C 0.00000000 2.46326100 -7.86114000
C 0.00000000 3.65719300 -7.11969000
C 0.00000000 3.65629800 -10.05762100
C 0.00000000 2.47081600 -9.31146000
C 0.00000000 2.45005000 -12.14130200
C 0.00000000 3.64294200 -11.45432700
C 0.00000000 1.22142300 11.43933800
C 0.00000000 0.00000000 12.11944000
C 0.00000000 0.00000000 9.29026500
C 0.00000000 1.22967600 10.00430500
C 0.00000000 1.23386300 7.15238800
C 0.00000000 0.00000000 7.86385200
C 0.00000000 0.00000000 5.00019300
C 0.00000000 1.23316600 5.71918100
C 0.00000000 1.23224100 2.86124800
C 0.00000000 0.00000000 3.58159100
C 0.00000000 0.00000000 0.70830700
C 0.00000000 1.23233900 1.42867100
C 0.00000000 1.23233900 -1.42867100
C 0.00000000 0.00000000 -0.70830700
C 0.00000000 0.00000000 -3.58159100
C 0.00000000 1.23224100 -2.86124800
C 0.00000000 1.23316600 -5.71918100
C 0.00000000 0.00000000 -5.00019300

C 0.00000000 0.00000000 -7.86385200
C 0.00000000 1.23386300 -7.15238800
C 0.00000000 1.22967600 -10.00430500
C 0.00000000 0.00000000 -9.29026500
C 0.00000000 0.00000000 -12.11944000
C 0.00000000 1.22142300 -11.43933800
C 0.00000000 -1.22142300 11.43933800
C 0.00000000 -2.45005000 12.14130200
C 0.00000000 -2.47081600 9.31146000
C 0.00000000 -1.22967600 10.00430500
C 0.00000000 -1.23386300 7.15238800
C 0.00000000 -2.46326100 7.86114000
C 0.00000000 -2.45808500 5.00968600
C 0.00000000 -1.23316600 5.71918100
C 0.00000000 -1.23224100 2.86124800
C 0.00000000 -2.45677200 3.56899600
C 0.00000000 -2.45611700 0.71975900
C 0.00000000 -1.23233900 1.42867100
C 0.00000000 -1.23233900 -1.42867100
C 0.00000000 -2.45611700 -0.71975900
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C 0.00000000 -1.23224100 -2.86124800
C 0.00000000 -1.23316600 -5.71918100
C 0.00000000 -2.45808500 -5.00968600
C 0.00000000 -2.46326100 -7.86114000
C 0.00000000 -1.23386300 -7.15238800
C 0.00000000 -1.22967600 -10.00430500
C 0.00000000 -2.47081600 -9.31146000
C 0.00000000 -2.45005000 -12.14130200
C 0.00000000 -1.22142300 -11.43933800
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C 0.00000000 -3.65736000 -1.46081300
C 0.00000000 -3.65721100 -2.82743800
C 0.00000000 -3.65732800 -5.74934400
C 0.00000000 -3.65719300 -7.11969000
C 0.00000000 -3.65629800 -10.05762100
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H 0.00000000 -4.61761000 -9.55739600
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H 0.00000000 -4.61386600 -5.24096000

H 0.00000000 -4.61345800 -3.33648200
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H 0.00000000 4.58481300 -11.99598000
H 0.00000000 4.61761000 -9.55739600
H 0.00000000 4.61376000 -7.62920700
H 0.00000000 4.61386600 -5.24096000
H 0.00000000 4.61345800 -3.33648200
H 0.00000000 4.61352600 -0.95167000
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H 0.00000000 4.61345800 3.33648200
H 0.00000000 4.61386600 5.24096000
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H 0.00000000 0.00000000 -13.20724300
H 0.00000000 -2.43226200 -13.22810300
H 0.00000000 2.43226200 13.22810300
H 0.00000000 0.00000000 13.20724300
H 0.00000000 -2.43226200 13.22810300

3x6 open singlet

C 0.00000000 3.64975900 11.44029300
C 0.00000000 2.45053300 12.12850400
C 0.00000000 2.47046800 9.30099500
C 0.00000000 3.66372400 10.04946000
C 0.00000000 3.66312100 7.11231300
C 0.00000000 2.46344900 7.85537500
C 0.00000000 2.45832200 5.00550200
C 0.00000000 3.66224000 5.74604100
C 0.00000000 3.66069800 2.82483700
C 0.00000000 2.45702500 3.56718700
C 0.00000000 2.45631300 0.71891500
C 0.00000000 3.66057900 1.46054400
C 0.00000000 3.66057900 -1.46054400
C 0.00000000 2.45631300 -0.71891500
C 0.00000000 2.45702500 -3.56718700
C 0.00000000 3.66069800 -2.82483700
C 0.00000000 3.66224000 -5.74604100

C 0.00000000 2.45832200 -5.00550200
C 0.00000000 2.46344900 -7.85537500
C 0.00000000 3.66312100 -7.11231300
C 0.00000000 3.66372400 -10.04946000
C 0.00000000 2.47046800 -9.30099500
C 0.00000000 2.45053300 -12.12850400
C 0.00000000 3.64975900 -11.44029300
C 0.00000000 1.22620800 11.42753200
C 0.00000000 0.00000000 12.10953600
C 0.00000000 0.00000000 9.27833300
C 0.00000000 1.23398200 9.99406300
C 0.00000000 1.23733400 7.14704800
C 0.00000000 0.00000000 7.86079600
C 0.00000000 0.00000000 4.99511200
C 0.00000000 1.23580500 5.71477800
C 0.00000000 1.23416000 2.85973500
C 0.00000000 0.00000000 3.58109100
C 0.00000000 0.00000000 0.70666100
C 0.00000000 1.23406200 1.42763100
C 0.00000000 1.23406200 -1.42763100
C 0.00000000 0.00000000 -0.70666100
C 0.00000000 0.00000000 -3.58109100
C 0.00000000 1.23416000 -2.85973500
C 0.00000000 1.23580500 -5.71477800
C 0.00000000 0.00000000 -4.99511200
C 0.00000000 0.00000000 -7.86079600
C 0.00000000 1.23733400 -7.14704800
C 0.00000000 1.23398200 -9.99406300
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C 0.00000000 0.00000000 -12.10953600
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C 0.00000000 -1.22620800 11.42753200
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C 0.00000000 -2.47046800 9.30099500
C 0.00000000 -1.23398200 9.99406300
C 0.00000000 -1.23733400 7.14704800
C 0.00000000 -2.46344900 7.85537500
C 0.00000000 -2.45832200 5.00550200
C 0.00000000 -1.23580500 5.71477800
C 0.00000000 -1.23416000 2.85973500
C 0.00000000 -2.45702500 3.56718700
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C 0.00000000 -1.23406200 -1.42763100
C 0.00000000 -2.45631300 -0.71891500
C 0.00000000 -2.45702500 -3.56718700

C 0.00000000 -1.23416000 -2.85973500
C 0.00000000 -1.23580500 -5.71477800
C 0.00000000 -2.45832200 -5.00550200
C 0.00000000 -2.46344900 -7.85537500
C 0.00000000 -1.23733400 -7.14704800
C 0.00000000 -1.23398200 -9.99406300
C 0.00000000 -2.47046800 -9.30099500
C 0.00000000 -2.45053300 -12.12850400
C 0.00000000 -1.22620800 -11.42753200
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C 0.00000000 -3.66057900 -1.46054400
C 0.00000000 -3.66069800 -2.82483700
C 0.00000000 -3.66224000 -5.74604100
C 0.00000000 -3.66312100 -7.11231300
C 0.00000000 -3.66372400 -10.04946000
C 0.00000000 -3.64975900 -11.44029300
H 0.00000000 -4.59029000 -11.98428100
H 0.00000000 -4.62381300 -9.54712900
H 0.00000000 -4.61881000 -7.62313900
H 0.00000000 -4.61761200 -5.23552000
H 0.00000000 -4.61635300 -3.33484600
H 0.00000000 -4.61608400 -0.95027500
H 0.00000000 -4.61608400 0.95027500
H 0.00000000 -4.61635300 3.33484600
H 0.00000000 -4.61761200 5.23552000
H 0.00000000 -4.61881000 7.62313900
H 0.00000000 -4.62381300 9.54712900
H 0.00000000 -4.59029000 11.98428100
H 0.00000000 4.59029000 -11.98428100
H 0.00000000 4.62381300 -9.54712900
H 0.00000000 4.61881000 -7.62313900
H 0.00000000 4.61761200 -5.23552000
H 0.00000000 4.61635300 -3.33484600
H 0.00000000 4.61608400 -0.95027500
H 0.00000000 4.61608400 0.95027500
H 0.00000000 4.61635300 3.33484600
H 0.00000000 4.61761200 5.23552000
H 0.00000000 4.61881000 7.62313900
H 0.00000000 4.62381300 9.54712900
H 0.00000000 4.59029000 11.98428100
H 0.00000000 2.43326400 -13.21530400

H 0.00000000 0.00000000 -13.19714800
H 0.00000000 -2.43326400 -13.21530400
H 0.00000000 2.43326400 13.21530400
H 0.00000000 0.00000000 13.19714800
H 0.00000000 -2.43326400 13.21530400

3x6 Triplet

C 0.00000000 3.64975900 11.44029300
C 0.00000000 2.45053300 12.12850400
C 0.00000000 2.47046800 9.30099500
C 0.00000000 3.66372400 10.04946000
C 0.00000000 3.66312100 7.11231300
C 0.00000000 2.46344900 7.85537500
C 0.00000000 2.45832200 5.00550200
C 0.00000000 3.66224000 5.74604100
C 0.00000000 3.66069800 2.82483700
C 0.00000000 2.45702500 3.56718700
C 0.00000000 2.45631300 0.71891500
C 0.00000000 3.66057900 1.46054400
C 0.00000000 3.66057900 -1.46054400
C 0.00000000 2.45631300 -0.71891500
C 0.00000000 2.45702500 -3.56718700
C 0.00000000 3.66069800 -2.82483700
C 0.00000000 3.66224000 -5.74604100
C 0.00000000 2.45832200 -5.00550200
C 0.00000000 2.46344900 -7.85537500
C 0.00000000 3.66312100 -7.11231300
C 0.00000000 3.66372400 -10.04946000
C 0.00000000 2.47046800 -9.30099500
C 0.00000000 2.45053300 -12.12850400
C 0.00000000 3.64975900 -11.44029300
C 0.00000000 1.22620800 11.42753200
C 0.00000000 0.00000000 12.10953600
C 0.00000000 0.00000000 9.27833300
C 0.00000000 1.23398200 9.99406300
C 0.00000000 1.23733400 7.14704800
C 0.00000000 0.00000000 7.86079600
C 0.00000000 0.00000000 4.99511200
C 0.00000000 1.23580500 5.71477800
C 0.00000000 1.23416000 2.85973500
C 0.00000000 0.00000000 3.58109100
C 0.00000000 0.00000000 0.70666100
C 0.00000000 1.23406200 1.42763100
C 0.00000000 1.23406200 -1.42763100
C 0.00000000 0.00000000 -0.70666100

C 0.00000000 0.00000000 -3.58109100
C 0.00000000 1.23416000 -2.85973500
C 0.00000000 1.23580500 -5.71477800
C 0.00000000 0.00000000 -4.99511200
C 0.00000000 0.00000000 -7.86079600
C 0.00000000 1.23733400 -7.14704800
C 0.00000000 1.23398200 -9.99406300
C 0.00000000 0.00000000 -9.27833300
C 0.00000000 0.00000000 -12.10953600
C 0.00000000 1.22620800 -11.42753200
C 0.00000000 -1.22620800 11.42753200
C 0.00000000 -2.45053300 12.12850400
C 0.00000000 -2.47046800 9.30099500
C 0.00000000 -1.23398200 9.99406300
C 0.00000000 -1.23733400 7.14704800
C 0.00000000 -2.46344900 7.85537500
C 0.00000000 -2.45832200 5.00550200
C 0.00000000 -1.23580500 5.71477800
C 0.00000000 -1.23416000 2.85973500
C 0.00000000 -2.45702500 3.56718700
C 0.00000000 -2.45631300 0.71891500
C 0.00000000 -1.23406200 1.42763100
C 0.00000000 -1.23406200 -1.42763100
C 0.00000000 -2.45631300 -0.71891500
C 0.00000000 -2.45702500 -3.56718700
C 0.00000000 -1.23416000 -2.85973500
C 0.00000000 -1.23580500 -5.71477800
C 0.00000000 -2.45832200 -5.00550200
C 0.00000000 -2.46344900 -7.85537500
C 0.00000000 -1.23733400 -7.14704800
C 0.00000000 -1.23398200 -9.99406300
C 0.00000000 -2.47046800 -9.30099500
C 0.00000000 -2.45053300 -12.12850400
C 0.00000000 -1.22620800 -11.42753200
C 0.00000000 -3.64975900 11.44029300
C 0.00000000 -3.66372400 10.04946000
C 0.00000000 -3.66312100 7.11231300
C 0.00000000 -3.66224000 5.74604100
C 0.00000000 -3.66069800 2.82483700
C 0.00000000 -3.66057900 1.46054400
C 0.00000000 -3.66057900 -1.46054400
C 0.00000000 -3.66069800 -2.82483700
C 0.00000000 -3.66224000 -5.74604100
C 0.00000000 -3.66312100 -7.11231300
C 0.00000000 -3.66372400 -10.04946000
C 0.00000000 -3.64975900 -11.44029300

H 0.00000000 -4.59029000 -11.98428100
H 0.00000000 -4.62381300 -9.54712900
H 0.00000000 -4.61881000 -7.62313900
H 0.00000000 -4.61761200 -5.23552000
H 0.00000000 -4.61635300 -3.33484600
H 0.00000000 -4.61608400 -0.95027500
H 0.00000000 -4.61608400 0.95027500
H 0.00000000 -4.61635300 3.33484600
H 0.00000000 -4.61761200 5.23552000
H 0.00000000 -4.61881000 7.62313900
H 0.00000000 -4.62381300 9.54712900
H 0.00000000 -4.59029000 11.98428100
H 0.00000000 4.59029000 -11.98428100
H 0.00000000 4.62381300 -9.54712900
H 0.00000000 4.61881000 -7.62313900
H 0.00000000 4.61761200 -5.23552000
H 0.00000000 4.61635300 -3.33484600
H 0.00000000 4.61608400 -0.95027500
H 0.00000000 4.61608400 0.95027500
H 0.00000000 4.61635300 3.33484600
H 0.00000000 4.61761200 5.23552000
H 0.00000000 4.61881000 7.62313900
H 0.00000000 4.62381300 9.54712900
H 0.00000000 4.59029000 11.98428100
H 0.00000000 2.43326400 -13.21530400
H 0.00000000 0.00000000 -13.19714800
H 0.00000000 -2.43326400 -13.21530400
H 0.00000000 2.43326400 13.21530400
H 0.00000000 0.00000000 13.19714800
H 0.00000000 -2.43326400 13.21530400

Edge-modified 3x6

C 0.00000000 3.64294200 11.45432700
C 0.00000000 2.45005000 12.14130200
C 0.00000000 2.47081600 9.31146000
C 0.00000000 3.65629800 10.05762100
C 0.00000000 3.65719300 7.11969000
C 0.00000000 2.46326100 7.86114000
C 0.00000000 2.45808500 5.00968600
C 0.00000000 3.65732800 5.74934400
C 0.00000000 3.65721100 2.82743800
C 0.00000000 2.45677200 3.56899600
C 0.00000000 2.45611700 0.71975900
C 0.00000000 3.65736000 1.46081300

C 0.00000000 3.65736000 -1.46081300
C 0.00000000 2.45611700 -0.71975900
C 0.00000000 2.45677200 -3.56899600
C 0.00000000 3.65721100 -2.82743800
C 0.00000000 3.65732800 -5.74934400
C 0.00000000 2.45808500 -5.00968600
C 0.00000000 2.46326100 -7.86114000
C 0.00000000 3.65719300 -7.11969000
C 0.00000000 3.65629800 -10.05762100
C 0.00000000 2.47081600 -9.31146000
C 0.00000000 2.45005000 -12.14130200
C 0.00000000 3.64294200 -11.45432700
C 0.00000000 1.22142300 11.43933800
C 0.00000000 0.00000000 12.11944000
C 0.00000000 0.00000000 9.29026500
C 0.00000000 1.22967600 10.00430500
C 0.00000000 1.23386300 7.15238800
C 0.00000000 0.00000000 7.86385200
C 0.00000000 0.00000000 5.00019300
C 0.00000000 1.23316600 5.71918100
C 0.00000000 1.23224100 2.86124800
C 0.00000000 0.00000000 3.58159100
C 0.00000000 0.00000000 0.70830700
C 0.00000000 1.23233900 1.42867100
C 0.00000000 1.23233900 -1.42867100
C 0.00000000 0.00000000 -0.70830700
C 0.00000000 0.00000000 -3.58159100
C 0.00000000 1.23224100 -2.86124800
C 0.00000000 1.23316600 -5.71918100
C 0.00000000 0.00000000 -5.00019300
C 0.00000000 0.00000000 -7.86385200
C 0.00000000 1.23386300 -7.15238800
C 0.00000000 1.22967600 -10.00430500
C 0.00000000 0.00000000 -9.29026500
C 0.00000000 0.00000000 -12.11944000
C 0.00000000 1.22142300 -11.43933800
C 0.00000000 -1.22142300 11.43933800
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C 0.00000000 -2.47081600 9.31146000
C 0.00000000 -1.22967600 10.00430500
C 0.00000000 -1.23386300 7.15238800
C 0.00000000 -2.46326100 7.86114000
C 0.00000000 -2.45808500 5.00968600
C 0.00000000 -1.23316600 5.71918100
C 0.00000000 -1.23224100 2.86124800
C 0.00000000 -2.45677200 3.56899600

C 0.00000000 -2.45611700 0.71975900
C 0.00000000 -1.23233900 1.42867100
C 0.00000000 -1.23233900 -1.42867100
C 0.00000000 -2.45611700 -0.71975900
C 0.00000000 -2.45677200 -3.56899600
C 0.00000000 -1.23224100 -2.86124800
C 0.00000000 -1.23316600 -5.71918100
C 0.00000000 -2.45808500 -5.00968600
C 0.00000000 -2.46326100 -7.86114000
C 0.00000000 -1.23386300 -7.15238800
C 0.00000000 -1.22967600 -10.00430500
C 0.00000000 -2.47081600 -9.31146000
C 0.00000000 -2.45005000 -12.14130200
C 0.00000000 -1.22142300 -11.43933800
C 0.00000000 -3.64294200 11.45432700
C 0.00000000 -3.65629800 10.05762100
C 0.00000000 -3.65719300 7.11969000
C 0.00000000 -3.65732800 5.74934400
C 0.00000000 -3.65721100 2.82743800
C 0.00000000 -3.65736000 1.46081300
C 0.00000000 -3.65736000 -1.46081300
C 0.00000000 -3.65721100 -2.82743800
C 0.00000000 -3.65732800 -5.74934400
C 0.00000000 -3.65719300 -7.11969000
C 0.00000000 -3.65629800 -10.05762100
C 0.00000000 -3.64294200 -11.45432700
H 0.00000000 -4.58481300 -11.99598000
H 0.00000000 -4.61761000 -9.55739600
H 0.00000000 -4.61376000 -7.62920700
H 0.00000000 -4.61386600 -5.24096000
H 0.00000000 -4.61345800 -3.33648200
H 0.00000000 -4.61352600 -0.95167000
H 0.00000000 -4.61352600 0.95167000
H 0.00000000 -4.61345800 3.33648200
H 0.00000000 -4.61386600 5.24096000
H 0.00000000 -4.61376000 7.62920700
H 0.00000000 -4.61761000 9.55739600
H 0.00000000 -4.58481300 11.99598000
H 0.00000000 4.58481300 -11.99598000
H 0.00000000 4.61761000 -9.55739600
H 0.00000000 4.61376000 -7.62920700
H 0.00000000 4.61386600 -5.24096000
H 0.00000000 4.61345800 -3.33648200
H 0.00000000 4.61352600 -0.95167000
H 0.00000000 4.61352600 0.95167000
H 0.00000000 4.61345800 3.33648200

H 0.00000000 4.61386600 5.24096000
H 0.00000000 4.61376000 7.62920700
H 0.00000000 4.61761000 9.55739600
H 0.00000000 4.58481300 11.99598000
H 0.00000000 2.43226200 -13.22810300
H 0.00000000 0.00000000 -13.20724300
H 0.00000000 -2.43226200 -13.22810300
H 0.00000000 2.43226200 13.22810300
H 0.00000000 0.00000000 13.20724300
H 0.00000000 -2.43226200 13.22810300

3x14 AGNR

C 0.00000000 3.64412000 28.59535400
C 0.00000000 2.45006100 29.28262800
C 0.00000000 2.47068600 26.45318300
C 0.00000000 3.65798700 27.20000900
C 0.00000000 3.65948200 24.26219500
C 0.00000000 2.46319200 25.00417400
C 0.00000000 2.45809200 22.15339700
C 0.00000000 3.65968900 22.89367900
C 0.00000000 3.65966700 19.97199500
C 0.00000000 2.45680900 20.71407700
C 0.00000000 2.45635300 17.86547000
C 0.00000000 3.65999600 18.60717900
C 0.00000000 3.66022600 15.68527700
C 0.00000000 2.45633000 16.42748100
C 0.00000000 2.45653300 13.57861600
C 0.00000000 3.66043900 14.32095700
C 0.00000000 3.66052100 11.39853300
C 0.00000000 2.45651900 12.14085000
C 0.00000000 2.45656800 9.29198400
C 0.00000000 3.66058500 10.03431200
C 0.00000000 3.66056900 7.11193200
C 0.00000000 2.45654500 7.85426500
C 0.00000000 2.45655900 5.00541300
C 0.00000000 3.66059400 5.74773200
C 0.00000000 3.66058100 2.82537400
C 0.00000000 2.45654800 3.56770300
C 0.00000000 2.45655300 0.71885400
C 0.00000000 3.66058800 1.46117800
C 0.00000000 3.66058800 -1.46117800
C 0.00000000 2.45655300 -0.71885400
C 0.00000000 2.45654800 -3.56770300
C 0.00000000 3.66058100 -2.82537400
C 0.00000000 3.66059400 -5.74773200

C 0.00000000 2.45655900 -5.00541300
C 0.00000000 2.45654500 -7.85426500
C 0.00000000 3.66056900 -7.11193200
C 0.00000000 3.66058500 -10.03431200
C 0.00000000 2.45656800 -9.29198400
C 0.00000000 2.45651900 -12.14085000
C 0.00000000 3.66052100 -11.39853300
C 0.00000000 3.66043900 -14.32095700
C 0.00000000 2.45653300 -13.57861600
C 0.00000000 2.45633000 -16.42748100
C 0.00000000 3.66022600 -15.68527700
C 0.00000000 3.65999600 -18.60717900
C 0.00000000 2.45635300 -17.86547000
C 0.00000000 2.45680900 -20.71407700
C 0.00000000 3.65966700 -19.97199500
C 0.00000000 3.65968900 -22.89367900
C 0.00000000 2.45809200 -22.15339700
C 0.00000000 2.46319200 -25.00417400
C 0.00000000 3.65948200 -24.26219500
C 0.00000000 3.65798700 -27.20000900
C 0.00000000 2.47068600 -26.45318300
C 0.00000000 2.45006100 -29.28262800
C 0.00000000 3.64412000 -28.59535400
C 0.00000000 1.22211800 28.58084900
C 0.00000000 0.00000000 29.26079400
C 0.00000000 0.00000000 26.43135300
C 0.00000000 1.23069900 27.14590300
C 0.00000000 1.23514100 24.29559900
C 0.00000000 0.00000000 25.00744800
C 0.00000000 0.00000000 22.14318000
C 0.00000000 1.23446800 22.86263900
C 0.00000000 1.23358500 20.00648000
C 0.00000000 0.00000000 20.72721300
C 0.00000000 0.00000000 17.85341700
C 0.00000000 1.23377400 18.57418900
C 0.00000000 1.23395100 15.71902800
C 0.00000000 0.00000000 16.43968000
C 0.00000000 0.00000000 13.56634800
C 0.00000000 1.23406600 14.28704400
C 0.00000000 1.23411500 11.43237600
C 0.00000000 0.00000000 12.15299900
C 0.00000000 0.00000000 9.27976100
C 0.00000000 1.23414300 10.00043100
C 0.00000000 1.23413400 7.14580900
C 0.00000000 0.00000000 7.86646200
C 0.00000000 0.00000000 4.99320000

C 0.00000000 1.23414400 5.71386800
C 0.00000000 1.23413700 2.85924800
C 0.00000000 0.00000000 3.57991000
C 0.00000000 0.00000000 0.70664400
C 0.00000000 1.23414000 1.42730900
C 0.00000000 1.23414000 -1.42730900
C 0.00000000 0.00000000 -0.70664400
C 0.00000000 0.00000000 -3.57991000
C 0.00000000 1.23413700 -2.85924800
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C 0.00000000 0.00000000 -7.86646200
C 0.00000000 1.23413400 -7.14580900
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C 0.00000000 1.23411500 -11.43237600
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C 0.00000000 1.23395100 -15.71902800
C 0.00000000 1.23377400 -18.57418900
C 0.00000000 0.00000000 -17.85341700
C 0.00000000 0.00000000 -20.72721300
C 0.00000000 1.23358500 -20.00648000
C 0.00000000 1.23446800 -22.86263900
C 0.00000000 0.00000000 -22.14318000
C 0.00000000 0.00000000 -25.00744800
C 0.00000000 1.23514100 -24.29559900
C 0.00000000 1.23069900 -27.14590300
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C 0.00000000 0.00000000 -29.26079400
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C 0.00000000 -2.47068600 26.45318300
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C 0.00000000 -2.46319200 25.00417400
C 0.00000000 -2.45809200 22.15339700
C 0.00000000 -1.23446800 22.86263900
C 0.00000000 -1.23358500 20.00648000
C 0.00000000 -2.45680900 20.71407700
C 0.00000000 -2.45635300 17.86547000
C 0.00000000 -1.23377400 18.57418900
C 0.00000000 -1.23395100 15.71902800

C 0.00000000 -2.45633000 16.42748100
C 0.00000000 -2.45653300 13.57861600
C 0.00000000 -1.23406600 14.28704400
C 0.00000000 -1.23411500 11.43237600
C 0.00000000 -2.45651900 12.14085000
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C 0.00000000 -1.23414300 10.00043100
C 0.00000000 -1.23413400 7.14580900
C 0.00000000 -2.45654500 7.85426500
C 0.00000000 -2.45655900 5.00541300
C 0.00000000 -1.23414400 5.71386800
C 0.00000000 -1.23413700 2.85924800
C 0.00000000 -2.45654800 3.56770300
C 0.00000000 -2.45655300 0.71885400
C 0.00000000 -1.23414000 1.42730900
C 0.00000000 -1.23414000 -1.42730900
C 0.00000000 -2.45655300 -0.71885400
C 0.00000000 -2.45654800 -3.56770300
C 0.00000000 -1.23413700 -2.85924800
C 0.00000000 -1.23414400 -5.71386800
C 0.00000000 -2.45655900 -5.00541300
C 0.00000000 -2.45654500 -7.85426500
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C 0.00000000 -1.23414300 -10.00043100
C 0.00000000 -2.45656800 -9.29198400
C 0.00000000 -2.45651900 -12.14085000
C 0.00000000 -1.23411500 -11.43237600
C 0.00000000 -1.23406600 -14.28704400
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C 0.00000000 -2.45633000 -16.42748100
C 0.00000000 -1.23395100 -15.71902800
C 0.00000000 -1.23377400 -18.57418900
C 0.00000000 -2.45635300 -17.86547000
C 0.00000000 -2.45680900 -20.71407700
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C 0.00000000 -3.65798700 27.20000900
C 0.00000000 -3.65948200 24.26219500

C 0.00000000 -3.65968900 22.89367900
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C 0.00000000 -3.65999600 18.60717900
C 0.00000000 -3.66022600 15.68527700
C 0.00000000 -3.66043900 14.32095700
C 0.00000000 -3.66052100 11.39853300
C 0.00000000 -3.66058500 10.03431200
C 0.00000000 -3.66056900 7.11193200
C 0.00000000 -3.66059400 5.74773200
C 0.00000000 -3.66058100 2.82537400
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C 0.00000000 -3.66052100 -11.39853300
C 0.00000000 -3.66043900 -14.32095700
C 0.00000000 -3.66022600 -15.68527700
C 0.00000000 -3.65999600 -18.60717900
C 0.00000000 -3.65966700 -19.97199500
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C 0.00000000 -3.65798700 -27.20000900
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H 0.00000000 -4.58557100 29.13776400
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H 0.00000000 -4.61557100 24.77247300
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H 0.00000000 -4.61622900 3.33535000
H 0.00000000 -4.61624100 0.95121100
H 0.00000000 -4.61624100 -0.95121100
H 0.00000000 -4.61622900 -3.33535000
H 0.00000000 -4.61625300 -5.23777500
H 0.00000000 -4.61621100 -7.62192300
H 0.00000000 -4.61625900 -9.52438000
H 0.00000000 -4.61615100 -11.90855100
H 0.00000000 -4.61617400 -13.81113400

H 0.00000000 -4.61584700 -16.19531800
H 0.00000000 -4.61575800 -18.09742400
H 0.00000000 -4.61540700 -20.48184600
H 0.00000000 -4.61580200 -22.38464000
H 0.00000000 -4.61557100 -24.77247300
H 0.00000000 -4.61906100 -26.69950500
H 0.00000000 -4.58557100 -29.13776400
H 0.00000000 4.58557100 29.13776400
H 0.00000000 4.61906100 26.69950500
H 0.00000000 4.61557100 24.77247300
H 0.00000000 4.61580200 22.38464000
H 0.00000000 4.61540700 20.48184600
H 0.00000000 4.61575800 18.09742400
H 0.00000000 4.61584700 16.19531800
H 0.00000000 4.61617400 13.81113400
H 0.00000000 4.61615100 11.90855100
H 0.00000000 4.61625900 9.52438000
H 0.00000000 4.61621100 7.62192300
H 0.00000000 4.61625300 5.23777500
H 0.00000000 4.61622900 3.33535000
H 0.00000000 4.61624100 0.95121100
H 0.00000000 4.61624100 -0.95121100
H 0.00000000 4.61622900 -3.33535000
H 0.00000000 4.61625300 -5.23777500
H 0.00000000 4.61621100 -7.62192300
H 0.00000000 4.61625900 -9.52438000
H 0.00000000 4.61615100 -11.90855100
H 0.00000000 4.61617400 -13.81113400
H 0.00000000 4.61584700 -16.19531800
H 0.00000000 4.61575800 -18.09742400
H 0.00000000 4.61540700 -20.48184600
H 0.00000000 4.61580200 -22.38464000
H 0.00000000 4.61557100 -24.77247300
H 0.00000000 4.61906100 -26.69950500
H 0.00000000 4.58557100 -29.13776400
H 0.00000000 2.43253100 -30.36941400
H 0.00000000 0.00000000 -30.34859600
H 0.00000000 -2.43253100 -30.36941400
H 0.00000000 2.43253100 30.36941400
H 0.00000000 0.00000000 30.34859600
H 0.00000000 -2.43253100 30.36941400

§S5) Cartesian Coordinates of key 4x or 9-AGNRs

4x6 Closed Singlet

C 0.00000000 4.86668700 11.44905200
C 0.00000000 3.67102800 12.13344400
C 0.00000000 3.69782900 9.30617300
C 0.00000000 4.88354200 10.05341800
C 0.00000000 4.88613100 7.11546500
C 0.00000000 3.69216400 7.85306600
C 0.00000000 3.68729400 5.00783900
C 0.00000000 4.88497600 5.74376900
C 0.00000000 4.88313200 2.82661200
C 0.00000000 3.68534800 3.56282000
C 0.00000000 3.68394700 0.72198500
C 0.00000000 4.88259700 1.45718200
C 0.00000000 4.88259700 -1.45718200
C 0.00000000 3.68394700 -0.72198500
C 0.00000000 3.68534800 -3.56282000
C 0.00000000 4.88313200 -2.82661200
C 0.00000000 4.88497600 -5.74376900
C 0.00000000 3.68729400 -5.00783900
C 0.00000000 3.69216400 -7.85306600
C 0.00000000 4.88613100 -7.11546500
C 0.00000000 4.88354200 -10.05341800
C 0.00000000 3.69782900 -9.30617300
C 0.00000000 3.67102800 -12.13344400
C 0.00000000 4.86668700 -11.44905200
C 0.00000000 2.44554800 11.42870100
C 0.00000000 1.22050500 12.10441200
C 0.00000000 1.22705700 9.27557000
C 0.00000000 2.45964600 9.99451100
C 0.00000000 2.46673000 7.14250300
C 0.00000000 1.22554700 7.85167700
C 0.00000000 1.22482600 4.99620100
C 0.00000000 2.46436500 5.71501500
C 0.00000000 2.46185600 2.85603700
C 0.00000000 1.22378200 3.57436400
C 0.00000000 1.22293300 0.71095000
C 0.00000000 2.46114000 1.42929200
C 0.00000000 2.46114000 -1.42929200
C 0.00000000 1.22293300 -0.71095000
C 0.00000000 1.22378200 -3.57436400
C 0.00000000 2.46185600 -2.85603700
C 0.00000000 2.46436500 -5.71501500
C 0.00000000 1.22482600 -4.99620100

C 0.00000000 1.22554700 -7.85167700
C 0.00000000 2.46673000 -7.14250300
C 0.00000000 2.45964600 -9.99451100
C 0.00000000 1.22705700 -9.27557000
C 0.00000000 1.22050500 -12.10441200
C 0.00000000 2.44554800 -11.42870100
C 0.00000000 0.00000000 11.42033400
C 0.00000000 -1.22050500 12.10441200
C 0.00000000 -1.22705700 9.27557000
C 0.00000000 0.00000000 9.97862200
C 0.00000000 0.00000000 7.14317400
C 0.00000000 -1.22554700 7.85167700
C 0.00000000 -1.22482600 4.99620100
C 0.00000000 0.00000000 5.70568200
C 0.00000000 0.00000000 2.86239200
C 0.00000000 -1.22378200 3.57436400
C 0.00000000 -1.22293300 0.71095000
C 0.00000000 0.00000000 1.42372400
C 0.00000000 0.00000000 -1.42372400
C 0.00000000 -1.22293300 -0.71095000
C 0.00000000 -1.22378200 -3.57436400
C 0.00000000 0.00000000 -2.86239200
C 0.00000000 0.00000000 -5.70568200
C 0.00000000 -1.22482600 -4.99620100
C 0.00000000 -1.22554700 -7.85167700
C 0.00000000 0.00000000 -7.14317400
C 0.00000000 0.00000000 -9.97862200
C 0.00000000 -1.22705700 -9.27557000
C 0.00000000 -1.22050500 -12.10441200
C 0.00000000 0.00000000 -11.42033400
C 0.00000000 -2.44554800 11.42870100
C 0.00000000 -3.67102800 12.13344400
C 0.00000000 -3.69782900 9.30617300
C 0.00000000 -2.45964600 9.99451100
C 0.00000000 -2.46673000 7.14250300
C 0.00000000 -3.69216400 7.85306600
C 0.00000000 -3.68729400 5.00783900
C 0.00000000 -2.46436500 5.71501500
C 0.00000000 -2.46185600 2.85603700
C 0.00000000 -3.68534800 3.56282000
C 0.00000000 -3.68394700 0.72198500
C 0.00000000 -2.46114000 1.42929200
C 0.00000000 -2.46114000 -1.42929200
C 0.00000000 -3.68394700 -0.72198500
C 0.00000000 -3.68534800 -3.56282000
C 0.00000000 -2.46185600 -2.85603700

C 0.00000000 -2.46436500 -5.71501500
C 0.00000000 -3.68729400 -5.00783900
C 0.00000000 -3.69216400 -7.85306600
C 0.00000000 -2.46673000 -7.14250300
C 0.00000000 -2.45964600 -9.99451100
C 0.00000000 -3.69782900 -9.30617300
C 0.00000000 -3.67102800 -12.13344400
C 0.00000000 -2.44554800 -11.42870100
C 0.00000000 -4.86668700 11.44905200
C 0.00000000 -4.88354200 10.05341800
C 0.00000000 -4.88613100 7.11546500
C 0.00000000 -4.88497600 5.74376900
C 0.00000000 -4.88313200 2.82661200
C 0.00000000 -4.88259700 1.45718200
C 0.00000000 -4.88259700 -1.45718200
C 0.00000000 -4.88313200 -2.82661200
C 0.00000000 -4.88497600 -5.74376900
C 0.00000000 -4.88613100 -7.11546500
C 0.00000000 -4.88354200 -10.05341800
C 0.00000000 -4.86668700 -11.44905200
H 0.00000000 -5.80684400 -11.99365200
H 0.00000000 -5.84546700 -9.55449100
H 0.00000000 -5.84252600 -7.62513500
H 0.00000000 -5.84123000 -5.23490800
H 0.00000000 -5.83945900 -3.33529800
H 0.00000000 -5.83859400 -0.94795700
H 0.00000000 -5.83859400 0.94795700
H 0.00000000 -5.83945900 3.33529800
H 0.00000000 -5.84123000 5.23490800
H 0.00000000 -5.84252600 7.62513500
H 0.00000000 -5.84546700 9.55449100
H 0.00000000 -5.80684400 11.99365200
H 0.00000000 5.80684400 -11.99365200
H 0.00000000 5.84546700 -9.55449100
H 0.00000000 5.84252600 -7.62513500
H 0.00000000 5.84123000 -5.23490800
H 0.00000000 5.83945900 -3.33529800
H 0.00000000 5.83859400 -0.94795700
H 0.00000000 5.83859400 0.94795700
H 0.00000000 5.83945900 3.33529800
H 0.00000000 5.84123000 5.23490800
H 0.00000000 5.84252600 7.62513500
H 0.00000000 5.84546700 9.55449100
H 0.00000000 5.80684400 11.99365200
H 0.00000000 3.65110800 -13.22017300
H 0.00000000 1.21582000 -13.19209000

H 0.00000000 -1.21582000 -13.19209000
H 0.00000000 -3.65110800 -13.22017300
H 0.00000000 3.65110800 13.22017300
H 0.00000000 1.21582000 13.19209000
H 0.00000000 -1.21582000 13.19209000
H 0.00000000 -3.65110800 13.22017300

4x6 Open Singlet

C 0.00000000 4.87259500 11.44252000
C 0.00000000 3.67230800 12.12761800
C 0.00000000 3.69911400 9.30331200
C 0.00000000 4.88858000 10.05080300
C 0.00000000 4.88811200 7.11363300
C 0.00000000 3.69312900 7.85153500
C 0.00000000 3.68780900 5.00718900
C 0.00000000 4.88633100 5.74259200
C 0.00000000 4.88364600 2.82630400
C 0.00000000 3.68563200 3.56245400
C 0.00000000 3.68415200 0.72194400
C 0.00000000 4.88305200 1.45699700
C 0.00000000 4.88305200 -1.45699700
C 0.00000000 3.68415200 -0.72194400
C 0.00000000 3.68563200 -3.56245400
C 0.00000000 4.88364600 -2.82630400
C 0.00000000 4.88633100 -5.74259200
C 0.00000000 3.68780900 -5.00718900
C 0.00000000 3.69312900 -7.85153500
C 0.00000000 4.88811200 -7.11363300
C 0.00000000 4.88858000 -10.05080300
C 0.00000000 3.69911400 -9.30331200
C 0.00000000 3.67230800 -12.12761800
C 0.00000000 4.87259500 -11.44252000
C 0.00000000 2.45193700 11.42362300
C 0.00000000 1.22013900 12.10267900
C 0.00000000 1.22685800 9.27299400
C 0.00000000 2.46367400 9.99281400
C 0.00000000 2.46823500 7.14164000
C 0.00000000 1.22567400 7.85206800
C 0.00000000 1.22493100 4.99596300
C 0.00000000 2.46518900 5.71472300
C 0.00000000 2.46214100 2.85587200
C 0.00000000 1.22384600 3.57447400
C 0.00000000 1.22295800 0.71088100
C 0.00000000 2.46137600 1.42926500
C 0.00000000 2.46137600 -1.42926500
C 0.00000000 1.22295800 -0.71088100

C 0.00000000 1.22384600 -3.57447400
C 0.00000000 2.46214100 -2.85587200
C 0.00000000 2.46518900 -5.71472300
C 0.00000000 1.22493100 -4.99596300
C 0.00000000 1.22567400 -7.85206800
C 0.00000000 2.46823500 -7.14164000
C 0.00000000 2.46367400 -9.99281400
C 0.00000000 1.22685800 -9.27299400
C 0.00000000 1.22013900 -12.10267900
C 0.00000000 2.45193700 -11.42362300
C 0.00000000 0.00000000 11.41774600
C 0.00000000 -1.22013900 12.10267900
C 0.00000000 -1.22685800 9.27299400
C 0.00000000 0.00000000 9.97610200
C 0.00000000 0.00000000 7.14290100
C 0.00000000 -1.22567400 7.85206800
C 0.00000000 -1.22493100 4.99596300
C 0.00000000 0.00000000 5.70558700
C 0.00000000 0.00000000 2.86240700
C 0.00000000 -1.22384600 3.57447400
C 0.00000000 -1.22295800 0.71088100
C 0.00000000 0.00000000 1.42374400
C 0.00000000 0.00000000 -1.42374400
C 0.00000000 -1.22295800 -0.71088100
C 0.00000000 -1.22384600 -3.57447400
C 0.00000000 0.00000000 -2.86240700
C 0.00000000 0.00000000 -5.70558700
C 0.00000000 -1.22493100 -4.99596300
C 0.00000000 -1.22567400 -7.85206800
C 0.00000000 0.00000000 -7.14290100
C 0.00000000 0.00000000 -9.97610200
C 0.00000000 -1.22685800 -9.27299400
C 0.00000000 -1.22013900 -12.10267900
C 0.00000000 0.00000000 -11.41774600
C 0.00000000 -2.45193700 11.42362300
C 0.00000000 -3.67230800 12.12761800
C 0.00000000 -3.69911400 9.30331200
C 0.00000000 -2.46367400 9.99281400
C 0.00000000 -2.46823500 7.14164000
C 0.00000000 -3.69312900 7.85153500
C 0.00000000 -3.68780900 5.00718900
C 0.00000000 -2.46518900 5.71472300
C 0.00000000 -2.46214100 2.85587200
C 0.00000000 -3.68563200 3.56245400
C 0.00000000 -3.68415200 0.72194400
C 0.00000000 -2.46137600 1.42926500

C 0.00000000 -2.46137600 -1.42926500
C 0.00000000 -3.68415200 -0.72194400
C 0.00000000 -3.68563200 -3.56245400
C 0.00000000 -2.46214100 -2.85587200
C 0.00000000 -2.46518900 -5.71472300
C 0.00000000 -3.68780900 -5.00718900
C 0.00000000 -3.69312900 -7.85153500
C 0.00000000 -2.46823500 -7.14164000
C 0.00000000 -2.46367400 -9.99281400
C 0.00000000 -3.69911400 -9.30331200
C 0.00000000 -3.67230800 -12.12761800
C 0.00000000 -2.45193700 -11.42362300
C 0.00000000 -4.87259500 11.44252000
C 0.00000000 -4.88858000 10.05080300
C 0.00000000 -4.88811200 7.11363300
C 0.00000000 -4.88633100 5.74259200
C 0.00000000 -4.88364600 2.82630400
C 0.00000000 -4.88305200 1.45699700
C 0.00000000 -4.88305200 -1.45699700
C 0.00000000 -4.88364600 -2.82630400
C 0.00000000 -4.88633100 -5.74259200
C 0.00000000 -4.88811200 -7.11363300
C 0.00000000 -4.88858000 -10.05080300
C 0.00000000 -4.87259500 -11.44252000
H 0.00000000 -5.81211100 -11.98818900
H 0.00000000 -5.84965600 -9.55010500
H 0.00000000 -5.84440600 -7.62341500
H 0.00000000 -5.84218400 -5.23291200
H 0.00000000 -5.83988000 -3.33519000
H 0.00000000 -5.83893600 -0.94755500
H 0.00000000 -5.83893600 0.94755500
H 0.00000000 -5.83988000 3.33519000
H 0.00000000 -5.84218400 5.23291200
H 0.00000000 -5.84440600 7.62341500
H 0.00000000 -5.84965600 9.55010500
H 0.00000000 -5.81211100 11.98818900
H 0.00000000 5.81211100 -11.98818900
H 0.00000000 5.84965600 -9.55010500
H 0.00000000 5.84440600 -7.62341500
H 0.00000000 5.84218400 -5.23291200
H 0.00000000 5.83988000 -3.33519000
H 0.00000000 5.83893600 -0.94755500
H 0.00000000 5.83893600 0.94755500
H 0.00000000 5.83988000 3.33519000
H 0.00000000 5.84218400 5.23291200
H 0.00000000 5.84440600 7.62341500

H 0.00000000 5.84965600 9.55010500
H 0.00000000 5.81211100 11.98818900
H 0.00000000 3.65255600 -13.21441000
H 0.00000000 1.21621600 -13.19023900
H 0.00000000 -1.21621600 -13.19023900
H 0.00000000 -3.65255600 -13.21441000
H 0.00000000 3.65255600 13.21441000
H 0.00000000 1.21621600 13.19023900
H 0.00000000 -1.21621600 13.19023900
H 0.00000000 -3.65255600 13.21441000

4x6 Triplet

C 0.00000000 4.87259500 11.44252000
C 0.00000000 3.67230800 12.12761800
C 0.00000000 3.69911400 9.30331200
C 0.00000000 4.88858000 10.05080300
C 0.00000000 4.88811200 7.11363300
C 0.00000000 3.69312900 7.85153500
C 0.00000000 3.68780900 5.00718900
C 0.00000000 4.88633100 5.74259200
C 0.00000000 4.88364600 2.82630400
C 0.00000000 3.68563200 3.56245400
C 0.00000000 3.68415200 0.72194400
C 0.00000000 4.88305200 1.45699700
C 0.00000000 4.88305200 -1.45699700
C 0.00000000 3.68415200 -0.72194400
C 0.00000000 3.68563200 -3.56245400
C 0.00000000 4.88364600 -2.82630400
C 0.00000000 4.88633100 -5.74259200
C 0.00000000 3.68780900 -5.00718900
C 0.00000000 3.69312900 -7.85153500
C 0.00000000 4.88811200 -7.11363300
C 0.00000000 4.88858000 -10.05080300
C 0.00000000 3.69911400 -9.30331200
C 0.00000000 3.67230800 -12.12761800
C 0.00000000 4.87259500 -11.44252000
C 0.00000000 2.45193700 11.42362300
C 0.00000000 1.22013900 12.10267900
C 0.00000000 1.22685800 9.27299400
C 0.00000000 2.46367400 9.99281400
C 0.00000000 2.46823500 7.14164000
C 0.00000000 1.22567400 7.85206800
C 0.00000000 1.22493100 4.99596300
C 0.00000000 2.46518900 5.71472300
C 0.00000000 2.46214100 2.85587200
C 0.00000000 1.22384600 3.57447400

C 0.00000000 1.22295800 0.71088100
C 0.00000000 2.46137600 1.42926500
C 0.00000000 2.46137600 -1.42926500
C 0.00000000 1.22295800 -0.71088100
C 0.00000000 1.22384600 -3.57447400
C 0.00000000 2.46214100 -2.85587200
C 0.00000000 2.46518900 -5.71472300
C 0.00000000 1.22493100 -4.99596300
C 0.00000000 1.22567400 -7.85206800
C 0.00000000 2.46823500 -7.14164000
C 0.00000000 2.46367400 -9.99281400
C 0.00000000 1.22685800 -9.27299400
C 0.00000000 1.22013900 -12.10267900
C 0.00000000 2.45193700 -11.42362300
C 0.00000000 0.00000000 11.41774600
C 0.00000000 -1.22013900 12.10267900
C 0.00000000 -1.22685800 9.27299400
C 0.00000000 0.00000000 9.97610200
C 0.00000000 0.00000000 7.14290100
C 0.00000000 -1.22567400 7.85206800
C 0.00000000 -1.22493100 4.99596300
C 0.00000000 0.00000000 5.70558700
C 0.00000000 0.00000000 2.86240700
C 0.00000000 -1.22384600 3.57447400
C 0.00000000 -1.22295800 0.71088100
C 0.00000000 0.00000000 1.42374400
C 0.00000000 0.00000000 -1.42374400
C 0.00000000 -1.22295800 -0.71088100
C 0.00000000 -1.22384600 -3.57447400
C 0.00000000 0.00000000 -2.86240700
C 0.00000000 0.00000000 -5.70558700
C 0.00000000 -1.22493100 -4.99596300
C 0.00000000 -1.22567400 -7.85206800
C 0.00000000 0.00000000 -7.14290100
C 0.00000000 0.00000000 -9.97610200
C 0.00000000 -1.22685800 -9.27299400
C 0.00000000 -1.22013900 -12.10267900
C 0.00000000 0.00000000 -11.41774600
C 0.00000000 -2.45193700 11.42362300
C 0.00000000 -3.67230800 12.12761800
C 0.00000000 -3.69911400 9.30331200
C 0.00000000 -2.46367400 9.99281400
C 0.00000000 -2.46823500 7.14164000
C 0.00000000 -3.69312900 7.85153500
C 0.00000000 -3.68780900 5.00718900
C 0.00000000 -2.46518900 5.71472300

C 0.00000000 -2.46214100 2.85587200
C 0.00000000 -3.68563200 3.56245400
C 0.00000000 -3.68415200 0.72194400
C 0.00000000 -2.46137600 1.42926500
C 0.00000000 -2.46137600 -1.42926500
C 0.00000000 -3.68415200 -0.72194400
C 0.00000000 -3.68563200 -3.56245400
C 0.00000000 -2.46214100 -2.85587200
C 0.00000000 -2.46518900 -5.71472300
C 0.00000000 -3.68780900 -5.00718900
C 0.00000000 -3.69312900 -7.85153500
C 0.00000000 -2.46823500 -7.14164000
C 0.00000000 -2.46367400 -9.99281400
C 0.00000000 -3.69911400 -9.30331200
C 0.00000000 -3.67230800 -12.12761800
C 0.00000000 -2.45193700 -11.42362300
C 0.00000000 -4.87259500 11.44252000
C 0.00000000 -4.88858000 10.05080300
C 0.00000000 -4.88811200 7.11363300
C 0.00000000 -4.88633100 5.74259200
C 0.00000000 -4.88364600 2.82630400
C 0.00000000 -4.88305200 1.45699700
C 0.00000000 -4.88305200 -1.45699700
C 0.00000000 -4.88364600 -2.82630400
C 0.00000000 -4.88633100 -5.74259200
C 0.00000000 -4.88811200 -7.11363300
C 0.00000000 -4.88858000 -10.05080300
C 0.00000000 -4.87259500 -11.44252000
H 0.00000000 -5.81211100 -11.98818900
H 0.00000000 -5.84965600 -9.55010500
H 0.00000000 -5.84440600 -7.62341500
H 0.00000000 -5.84218400 -5.23291200
H 0.00000000 -5.83988000 -3.33519000
H 0.00000000 -5.83893600 -0.94755500
H 0.00000000 -5.83893600 0.94755500
H 0.00000000 -5.83988000 3.33519000
H 0.00000000 -5.84218400 5.23291200
H 0.00000000 -5.84440600 7.62341500
H 0.00000000 -5.84965600 9.55010500
H 0.00000000 -5.81211100 11.98818900
H 0.00000000 5.81211100 -11.98818900
H 0.00000000 5.84965600 -9.55010500
H 0.00000000 5.84440600 -7.62341500
H 0.00000000 5.84218400 -5.23291200
H 0.00000000 5.83988000 -3.33519000
H 0.00000000 5.83893600 -0.94755500

H 0.00000000 5.83893600 0.94755500
H 0.00000000 5.83988000 3.33519000
H 0.00000000 5.84218400 5.23291200
H 0.00000000 5.84440600 7.62341500
H 0.00000000 5.84965600 9.55010500
H 0.00000000 5.81211100 11.98818900
H 0.00000000 3.65255600 -13.21441000
H 0.00000000 1.21621600 -13.19023900
H 0.00000000 -1.21621600 -13.19023900
H 0.00000000 -3.65255600 -13.21441000
H 0.00000000 3.65255600 13.21441000
H 0.00000000 1.21621600 13.19023900
H 0.00000000 -1.21621600 13.19023900
H 0.00000000 -3.65255600 13.21441000

Partially Edge-modified 4x6 closed singlet

C 0.00000000 3.64427900 9.28123600
C 0.00000000 4.88304400 7.13684600
C 0.00000000 3.67340800 7.85344700
C 0.00000000 3.69503200 5.01339000
C 0.00000000 4.89148200 5.76342600
C 0.00000000 4.88882400 2.82895900
C 0.00000000 3.69185900 3.56733300
C 0.00000000 3.68885700 0.72215900
C 0.00000000 4.88741400 1.45917600
C 0.00000000 4.88741400 -1.45917600
C 0.00000000 3.68885700 -0.72215900
C 0.00000000 3.69185900 -3.56733300
C 0.00000000 4.88882400 -2.82895900
C 0.00000000 4.89148200 -5.76342600
C 0.00000000 3.69503200 -5.01339000
C 0.00000000 3.67340800 -7.85344700
C 0.00000000 4.88304400 -7.13684600
C 0.00000000 3.64427900 -9.28123600
C 0.00000000 1.21732200 9.26485700
C 0.00000000 2.46688600 9.95975300
C 0.00000000 2.45506500 7.13037600
C 0.00000000 1.22101300 7.83764600
C 0.00000000 1.22618200 4.98661000
C 0.00000000 2.46376200 5.70644400
C 0.00000000 2.46718200 2.85613200
C 0.00000000 1.22552000 3.56724100
C 0.00000000 1.22577400 0.71058300
C 0.00000000 2.46563600 1.42924700
C 0.00000000 2.46563600 -1.42924700

C 0.00000000 1.22577400 -0.71058300
C 0.00000000 1.22552000 -3.56724100
C 0.00000000 2.46718200 -2.85613200
C 0.00000000 2.46376200 -5.70644400
C 0.00000000 1.22618200 -4.98661000
C 0.00000000 1.22101300 -7.83764600
C 0.00000000 2.45506500 -7.13037600
C 0.00000000 2.46688600 -9.95975300
C 0.00000000 1.21732200 -9.26485700
C 0.00000000 -1.21732200 9.26485700
C 0.00000000 0.00000000 9.94545400
C 0.00000000 0.00000000 7.12733600
C 0.00000000 -1.22101300 7.83764600
C 0.00000000 -1.22618200 4.98661000
C 0.00000000 0.00000000 5.69398400
C 0.00000000 0.00000000 2.85677000
C 0.00000000 -1.22552000 3.56724100
C 0.00000000 -1.22577400 0.71058300
C 0.00000000 0.00000000 1.42024800
C 0.00000000 0.00000000 -1.42024800
C 0.00000000 -1.22577400 -0.71058300
C 0.00000000 -1.22552000 -3.56724100
C 0.00000000 0.00000000 -2.85677000
C 0.00000000 0.00000000 -5.69398400
C 0.00000000 -1.22618200 -4.98661000
C 0.00000000 -1.22101300 -7.83764600
C 0.00000000 0.00000000 -7.12733600
C 0.00000000 0.00000000 -9.94545400
C 0.00000000 -1.21732200 -9.26485700
C 0.00000000 -3.64427900 9.28123600
C 0.00000000 -2.46688600 9.95975300
C 0.00000000 -2.45506500 7.13037600
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C 0.00000000 -3.69185900 3.56733300
C 0.00000000 -3.68885700 0.72215900
C 0.00000000 -2.46563600 1.42924700
C 0.00000000 -2.46563600 -1.42924700
C 0.00000000 -3.68885700 -0.72215900
C 0.00000000 -3.69185900 -3.56733300
C 0.00000000 -2.46718200 -2.85613200
C 0.00000000 -2.46376200 -5.70644400
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C 0.00000000 -3.67340800 -7.85344700

C 0.00000000 -2.45506500 -7.13037600
 C 0.00000000 -2.46688600 -9.95975300
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 C 0.00000000 -4.88741400 1.45917600
 C 0.00000000 -4.88741400 -1.45917600
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 C 0.00000000 -4.89148200 -5.76342600
 C 0.00000000 -4.88304400 -7.13684600
 H 0.00000000 -5.82171200 -7.68567500
 H 0.00000000 -5.84989900 -5.25762900
 H 0.00000000 -5.84500700 -3.33863100
 H 0.00000000 -5.84335300 -0.94965500
 H 0.00000000 -5.84335300 0.94965500
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 H 0.00000000 5.84500700 3.33863100
 H 0.00000000 5.84989900 5.25762900
 H 0.00000000 5.82171200 7.68567500
 H 0.00000000 4.59064200 -9.81672600
 H 0.00000000 2.45381500 -11.04690300
 H 0.00000000 0.00000000 -11.03359000
 H 0.00000000 -2.45381500 -11.04690300
 H 0.00000000 -4.59064200 -9.81672600
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 H 0.00000000 -4.59064200 9.81672600

Edge-modified 4x6 closed singlet

C 0.00000000 3.64427900 9.28123600
 C 0.00000000 4.88304400 7.13684600
 C 0.00000000 3.67340800 7.85344700
 C 0.00000000 3.69503200 5.01339000
 C 0.00000000 4.89148200 5.76342600
 C 0.00000000 4.88882400 2.82895900
 C 0.00000000 3.69185900 3.56733300

C 0.00000000 3.68885700 0.72215900
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C 0.00000000 4.88741400 -1.45917600
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C 0.00000000 3.69185900 -3.56733300
C 0.00000000 4.88882400 -2.82895900
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C 0.00000000 4.88304400 -7.13684600
C 0.00000000 3.64427900 -9.28123600
C 0.00000000 1.21732200 9.26485700
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C 0.00000000 1.22552000 3.56724100
C 0.00000000 1.22577400 0.71058300
C 0.00000000 2.46563600 1.42924700
C 0.00000000 2.46563600 -1.42924700
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H 0.00000000 5.84500700 3.33863100
H 0.00000000 5.84989900 5.25762900
H 0.00000000 5.82171200 7.68567500
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