

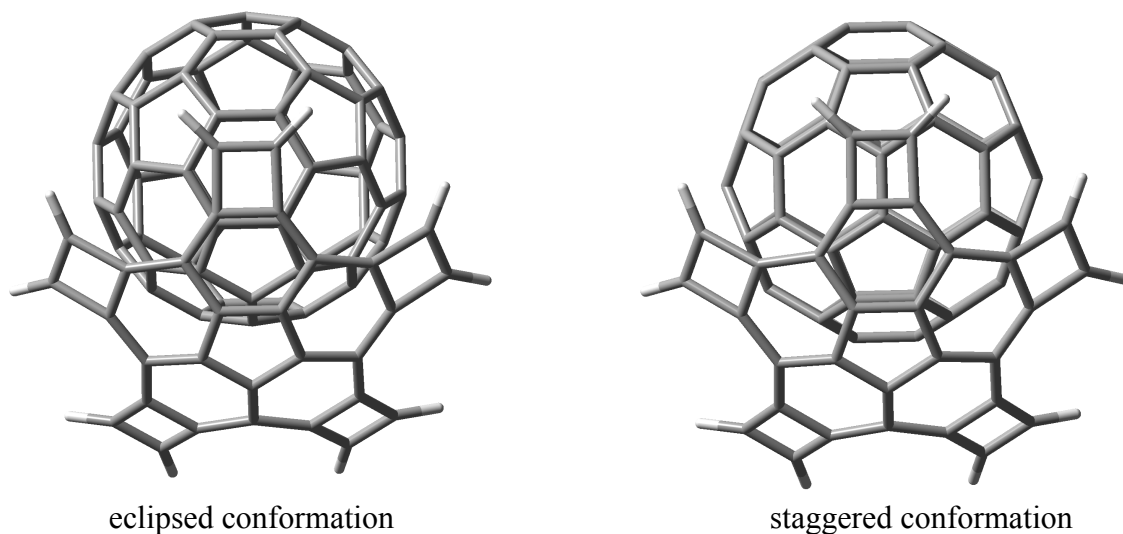
Ring-annelated corannulenes as fullerene receptors. A DFT-D study.

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Teodorico de Castro Ramalho**

Supplementary Information

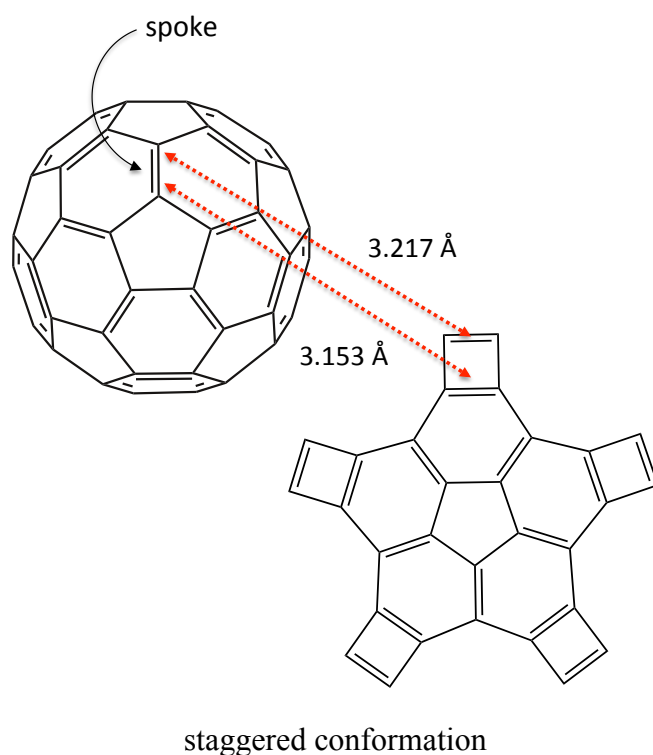
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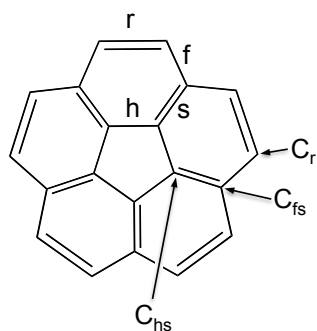
Why $4 \cdots C_{60}$ is more stable in the staggered conformation?



In the staggered conformation of complex $4 \cdots X$ both π bonds of the cyclobutadiene (which owns an extremely localized π clouds) are directly facing the *spoke* bond of fullerene, which is precisely the bond with the largest π character of fullerene (the largest bond order, the shortest bond length, the largest double-bond character). Thus, this additional $\pi \cdots \pi$ interaction, that takes place in the staggered conformation in a more appropriate way, not only offsets the advantage of the general trend favouring the eclipsed conformation, but it also overcomes it.

To support the above explanation, QTAIM calculations and NCI plots were performed. Both methodologies make clear the interaction between the π bonds of the cyclobutadiene and the *spoke* bonds of fullerene that takes place in the staggered conformation of the complex.





bonds:
 h = hub
 s = spoke
 f = flank
 r = rim

C atom types:
 hs = hub-spoke
 fs = flank-spoke
 r = rim

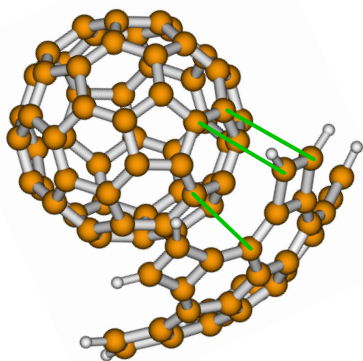
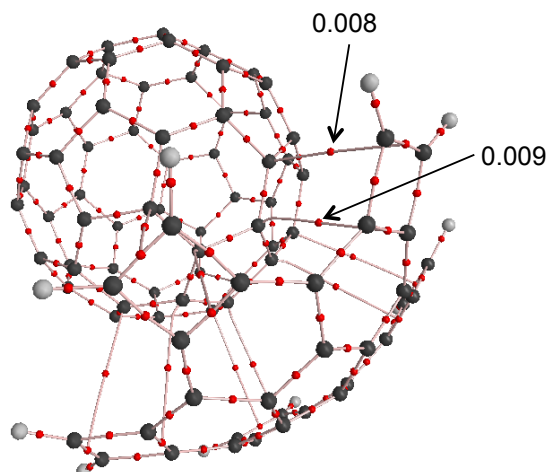
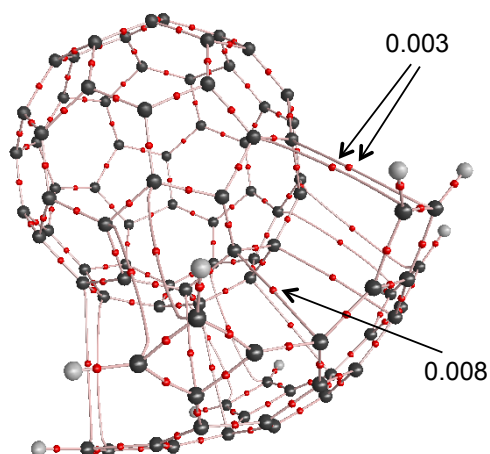
QTAIM: BCP=Bond Critical Point, BP=Bond Path

Eclipsed conformation: there are two types of BP between corannulene 4 and fullerene.

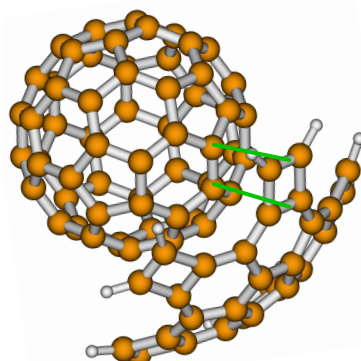
- 1) From each of the external carbons of cyclobutadiene to a C_r of fullerene (density of the BCP, 0.003). A total of 10 BPs.
- 2) From the C_{fs} of corannulene to a C_{hs} of fullerene (0.008). A total of 5 BPs.

Staggered conformation: there are two types of BP between corannulene 4 and fullerene.

- 1) From the BCP between the external carbons of cyclobutadiene to a C_{fs} of fullerene (0.008): A total of 5 BPs.
- 2) From the BCP between the internal carbons of cyclobutadiene to a C_{hs} of fullerene (0.009): A total of 5 BPs.



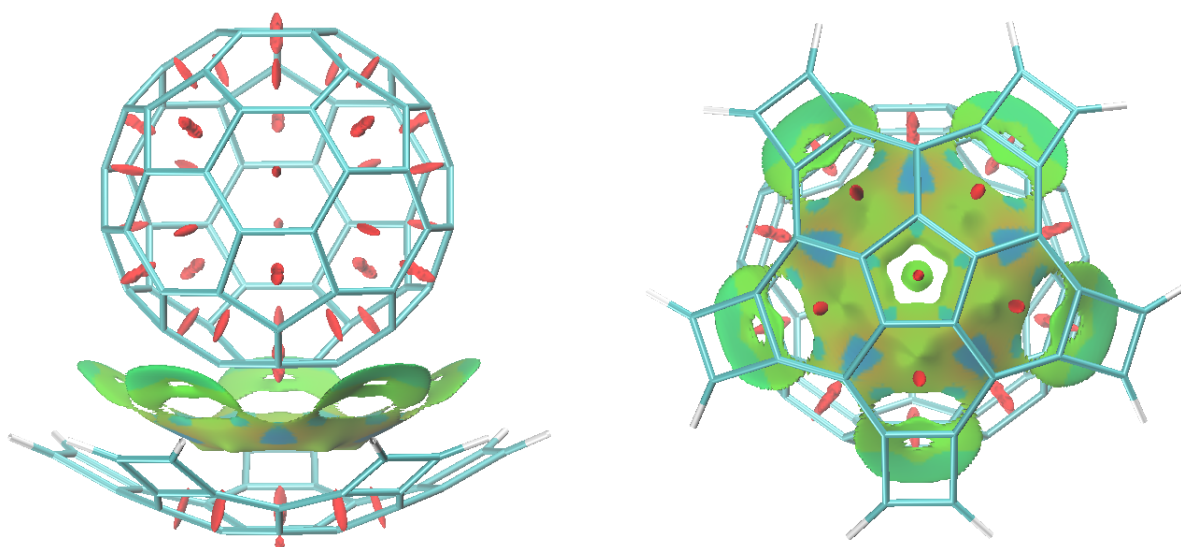
eclipsed



staggered

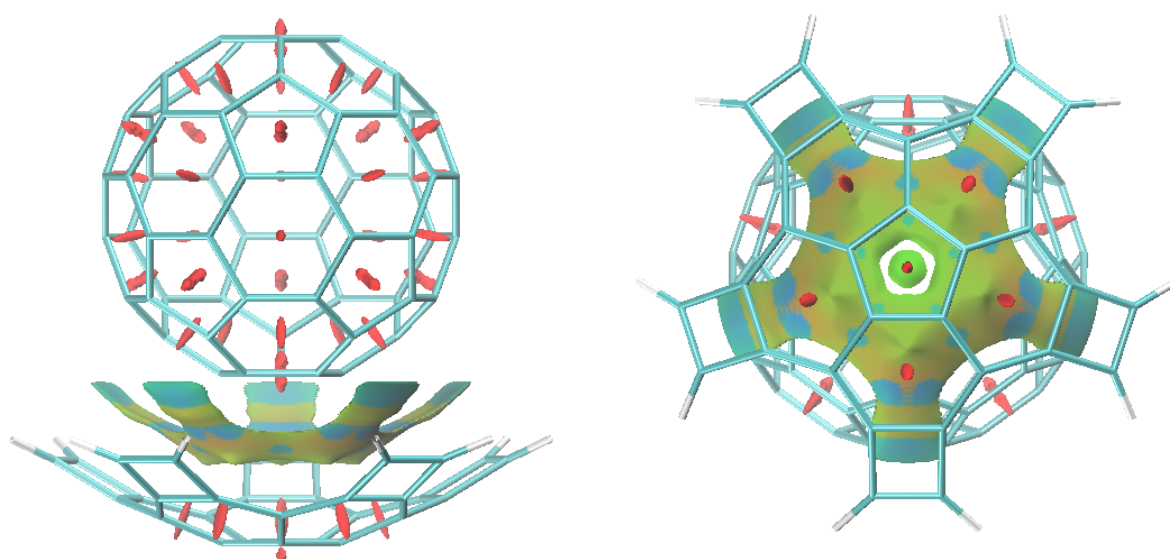
Thus, in the staggered conformation the density of the BCPs is significantly larger than in the eclipsed conformation (0.085 vs. 0.070)

NCIPLOT, eclipsed conformation:



The largest interaction (blue) takes place between the spoke of corannulene and the *spoke* of fullerene (which is clearly related to BP type 2, above commented).

NCIPLOT, staggered conformation:

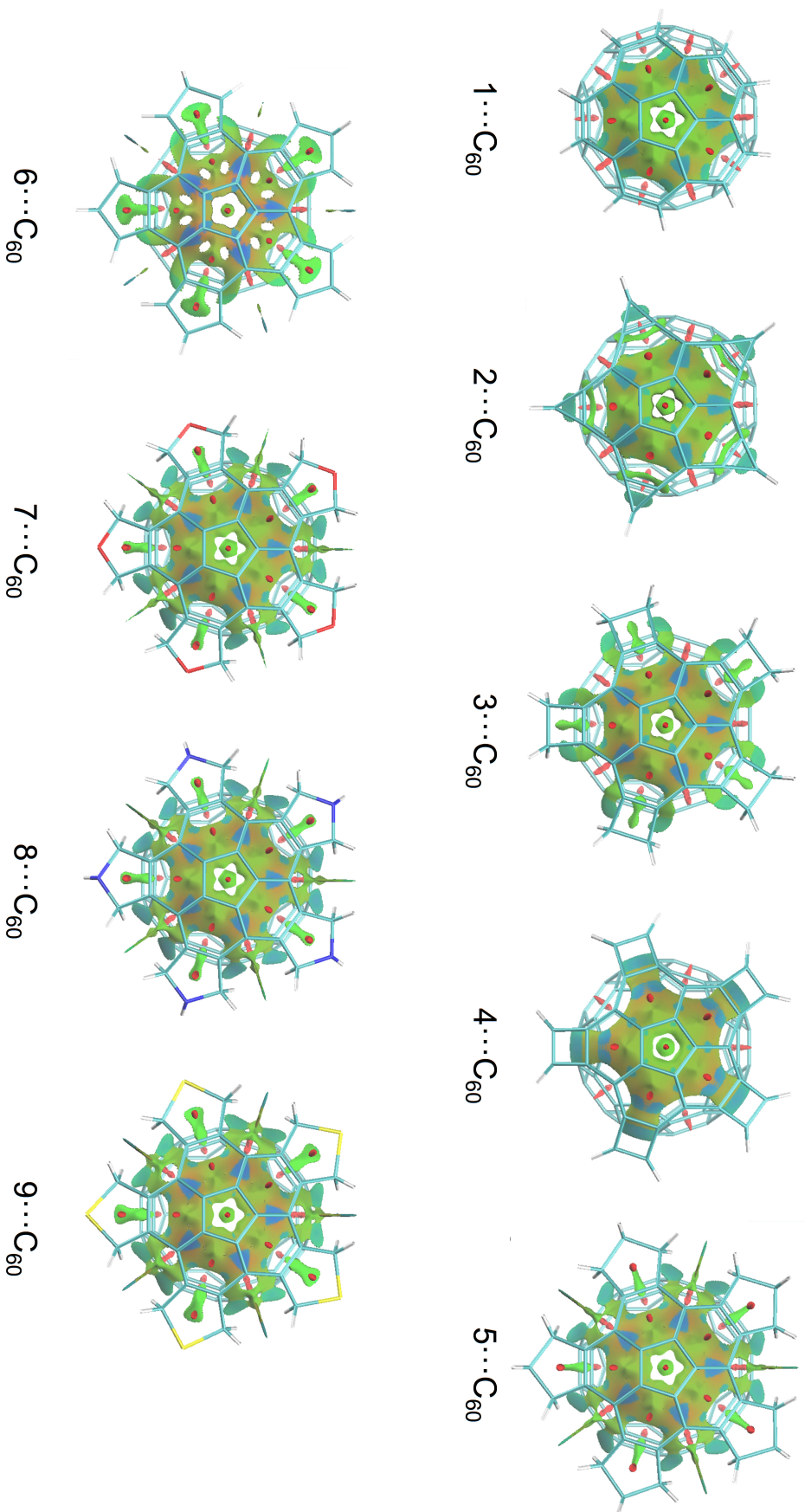


An important portion of *spoke-spoke* interaction is lost. However, this is not only offset, but it also overcome by the emergence of two new strong $p \cdots p$ interactions which correspond to those that takes place between the two double bonds of cyclobutadiene (external and internal) and the *spoke* of fullerene (which are clearly related to BP types 1 and 2, respectively, above commented).

Isosurface: 0.40

Colour scale: from -0.15 to 0.15

NCIPLoTs



NBO calculations

Second order perturbation analysis as the energies of delocalization of electrons from filled NBOs into empty NBOs—so that they do not finish up quite filled or quite empty.

Stabilization energies (kcal/mol), E(2):

Donor	Acceptor	1···C ₆₀	2···C ₆₀	3···C ₆₀	4···C ₆₀	5···C ₆₀	6···C ₆₀	7···C ₆₀	8···C ₆₀	9···C ₆₀
π(spoke) corannulene	π*(spoke) C ₆₀	0.86	1.05	1.46	-	1.28	1.71	1.07	1.18	1.32
σ(spoke) corannulene	Ry*(C _{hs}) C ₆₀	0.45	0.55	0.62	-	0.51	0.77	0.48	0.48	0.55
π(external ^a) corannulene	π*(spoke) C ₆₀	-	-	-	1.05	-	-	-	-	-
σ(external ^a) corannulene	Ry*(C _{fs}) C ₆₀	-	-	-	0.52	-	-	-	-	-

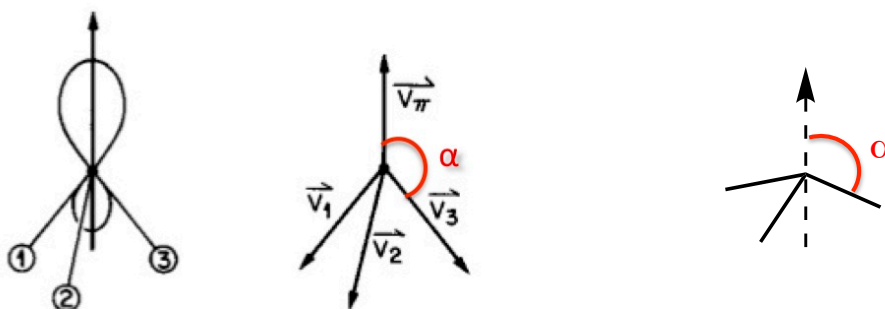
^a external bond of cyclobutadiene.

Only values larger than 0.45 are shown.

Eclipsed disposition, except for complex 4···C₆₀, which is staggered.

- Except for 4···C₆₀: the main contribution comes from the interaction between the π orbital of the *spokes* of both monomers. The second most important contribution is that which takes place between the σ orbital of the *spokes* of corannulene and the Rydberg orbital of the C_{hs} of C₆₀.
- Only for 4···C₆₀: the main contribution comes from the interaction between the π orbital of the external bond of cyclobutadienes of 4 and the π orbital of the *spokes* of C₆₀. The second most important contribution is that which takes place between the σ orbital of the external bond of cyclobutadienes of 4 and the Rydberg orbital of the C_{fs} of C₆₀.

POAV angle



$$\text{POAV} = \alpha - 90^\circ$$

B97-D2/TZVP optimized geometries of complexes included in this work.

1...C₆₀(eclip.):

C	-0.99954700	-0.72621300	5.33621100
C	-0.99954700	0.72621300	5.33621100
C	-1.96156400	1.42516000	4.59953700
C	-2.96073900	0.69916600	3.83561100
C	-2.96073900	-0.69916600	3.83561100
C	-1.96156400	-1.42516000	4.59953700
C	0.38179300	-1.17503700	5.33621100
C	1.23550700	0.00000000	5.33621100
C	0.38179300	1.17503700	5.33621100
C	0.74925100	2.30595700	4.59953700
C	-1.57986500	2.59977600	3.83561100
C	-3.19687800	1.42522600	2.60016900
C	-3.42486600	0.72634800	1.41011500
C	-3.42486600	-0.72634800	1.41011500
C	-3.19687800	-1.42522600	2.60016900
C	-2.34336000	-2.59999200	2.60016900
C	-1.57986500	-2.59977600	3.83561100
C	-0.24997300	-3.03188400	3.83561100
C	0.74925100	-2.30595700	4.59953700
C	2.42462700	0.00000000	4.59953700
C	2.80624800	-1.17464200	3.83561100
C	1.98432900	-2.30591600	3.83561100
C	1.74860100	-3.03211000	2.60016900
C	0.36758100	-3.48083000	2.60016900
C	-0.36754400	-3.48169500	1.41011500
C	-1.74914000	-3.03278800	1.41011500
C	-1.98519600	-2.30710700	0.17434900
C	-2.80764800	-1.17509800	0.17434900
C	-2.34336000	2.59999200	2.60016900
C	-0.38074600	1.17181400	-1.31409000
C	-0.74894200	2.30500700	-0.58590500
C	0.24997400	3.03335800	0.17434900
C	1.58073000	2.60096900	0.17434900
C	1.96075600	1.42457300	-0.58590500
C	0.99680500	-0.72422100	-1.31409000
C	-0.38074600	-1.17181400	-1.31409000
C	-1.23211900	0.00000000	-1.31409000
C	-2.42362800	0.00000000	-0.58590500
C	-2.80764800	1.17509800	0.17434900
C	-1.98519600	2.30710700	0.17434900
C	-0.36754400	3.48169500	1.41011500
C	0.36758100	3.48083000	2.60016900
C	1.74860100	3.03211000	2.60016900
C	2.34338300	2.60071400	1.41011500
C	3.19771200	1.42545800	1.41011500
C	2.96214100	0.69962000	0.17434900
C	2.96214100	-0.69962000	0.17434900
C	1.96075600	-1.42457300	-0.58590500
C	-0.74894200	-2.30500700	-0.58590500
C	0.24997400	-3.03335800	0.17434900
C	1.58073000	-2.60096900	0.17434900
C	2.34338300	-2.60071400	1.41011500
C	3.19771200	-1.42545800	1.41011500
C	3.42405500	-0.72604500	2.60016900
C	3.42405500	0.72604500	2.60016900
C	2.80624800	1.17464200	3.83561100
C	1.98432900	2.30591600	3.83561100
C	-1.74914000	3.03278800	1.41011500
C	-0.24997300	3.03188400	3.83561100
C	0.99680500	0.72422100	-1.31409000
C	0.32236500	-3.24439700	-3.86752700
C	-0.76840700	-2.36491200	-4.23282500
C	-0.37250400	-1.14644900	-4.76978800
C	0.97522700	-0.70854400	-4.76978800
C	2.01171400	-1.46159600	-4.23282500
C	1.64621100	-2.81425400	-3.86752700
C	-2.16780700	-2.43529100	-3.86752700
C	-2.98598900	-1.30916100	-3.86752700
C	-1.20544700	0.00000000	-4.76978800
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C	2.01171400	1.46159600	-4.23282500
C	3.18522100	0.69598700	-3.86752700
C	3.18522100	-0.69598700	-3.86752700

C	-0.37250400	1.14644900	-4.76978800
C	1.64621100	2.81425400	-3.86752700
C	0.32236500	3.24439700	-3.86752700
C	-2.16780700	2.43529100	-3.86752700
C	-2.98598900	1.30916100	-3.86752700
C	-0.76840700	2.36491200	-4.23282500
C	-2.48661600	0.00000000	-4.23282500
H	4.06121100	1.21435300	-3.48023000
H	4.06121100	-1.21435300	-3.48023000
H	2.40990100	-3.48718500	-3.48023000
H	0.10006500	-4.23769600	-3.48023000
H	-2.57181000	-3.36955200	-3.48023000
H	-3.99936700	-1.40468800	-3.48023000
H	-3.99936700	1.40468800	-3.48023000
H	-2.57181000	3.36955200	-3.48023000
H	0.10006500	4.23769600	-3.48023000
H	2.40990100	3.48718500	-3.48023000

1...C₆₀(stagg.):

C	-0.99935600	-0.72607500	5.34824300
C	-0.99935600	0.72607500	5.34824300
C	-1.96242500	1.42578600	4.61431700
C	-2.96265100	0.69949200	3.85166800
C	-2.96265100	-0.69949200	3.85166800
C	-1.96242500	-1.42578600	4.61431700
C	0.38172000	-1.17481400	5.34824300
C	1.23527200	0.00000000	5.34824300
C	0.38172000	1.17481400	5.34824300
C	0.74958000	2.30696900	4.61431700
C	-1.58076600	2.60149400	3.85166800
C	-3.19890100	1.42622500	2.61661800
C	-3.42592500	0.72641800	1.42693700
C	-3.42592500	-0.72641800	1.42693700
C	-3.19890100	-1.42622500	2.61661800
C	-2.34493500	-2.60160800	2.61661800
C	-1.58076600	-2.60149400	3.85166800
C	-0.25025300	-3.03380400	3.85166800
C	0.74958000	-2.30696900	4.61431700
C	2.42569100	0.00000000	4.61431700
C	2.80798600	-1.17550200	3.85166800
C	1.98568400	-2.30730400	3.85166800
C	1.74965200	-3.03410700	2.61661800
C	0.36790600	-3.48306400	2.61661800
C	-0.36780500	-3.48272400	1.42693700
C	-1.74953300	-3.03377300	1.42693700
C	-1.98482300	-2.30689300	0.19167300
C	-2.80732900	-1.17481000	0.19167300
C	-2.34493500	2.60160800	2.61661800
C	-0.38054400	1.17119300	-1.29583200
C	-0.74866100	2.30414300	-0.56775800
C	0.24979800	3.03296500	0.19167300
C	1.58064100	2.60054800	0.19167300
C	1.96002100	1.42403900	-0.56775800
C	0.99627600	-0.72383700	-1.29583200
C	-0.38054400	-1.17119300	-1.29583200
C	-1.23146500	0.00000000	-1.29583200
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C	-2.80732900	1.17481000	0.19167300
C	-1.98482300	2.30689300	0.19167300
C	-0.36780500	3.48272400	1.42693700
C	0.36790600	3.48306400	2.61661800
C	1.74965200	3.03410700	2.61661800
C	2.34465400	2.60139200	1.42693700
C	3.19860900	1.42602400	1.42693700
C	2.96171300	0.69966600	0.19167300
C	2.96171300	-0.69966600	0.19167300
C	1.96002100	-1.42403900	-0.56775800
C	-0.74866100	-2.30414300	-0.56775800
C	0.24979800	-3.03296500	0.19167300
C	1.58064100	-2.60054800	0.19167300
C	2.34465400	-2.60139200	1.42693700
C	3.19860900	-1.42602400	1.42693700
C	3.42627900	-0.72642700	2.61661800
C	3.42627900	0.72642700	2.61661800
C	2.80798600	1.17550200	3.85166800
C	1.98568400	2.30730400	3.85166800
C	-1.74953300	3.03377300	1.42693700
C	-0.25025300	3.03380400	3.85166800
C	0.99627600	0.72383700	-1.29583200

C	-1.64947500	-2.82142300	-3.96272100	C	1.95975200	-1.42384300	-0.49424200
C	-2.01594600	-1.46467100	-4.31208200	C	-0.74855900	-2.30382600	-0.49424200
C	-0.97396000	-0.70762400	-4.83129000	C	0.24952700	-3.03095500	0.26791500
C	0.37202000	-1.14495900	-4.83129000	C	1.57967900	-2.59876200	0.26791500
C	0.77002300	-2.36988700	-4.31208200	C	2.34370100	-2.60037100	1.50256200
C	-0.32393800	-3.25211600	-3.96272100	C	3.19734400	-1.42543300	1.50256200
C	-3.19304800	-0.69687600	-3.96272100	C	3.42478300	-0.72612600	2.69248100
C	-3.19304800	0.69687600	-3.96272100	C	3.42478300	0.72612600	2.69248100
C	-0.97396000	0.70762400	-4.83129000	C	2.80723800	1.17515700	3.92797700
C	1.20388100	0.00000000	-4.83129000	C	1.98512500	2.30669800	3.92797700
C	2.49184700	0.00000000	-4.31208200	C	-1.74885700	3.03255100	1.50256200
C	2.99284400	-1.31304200	-3.96272100	C	-0.25015700	3.03298500	3.92797700
C	2.17361700	-2.44061100	-3.96272100	C	0.99746800	0.72470300	-1.22697500
C	0.37202000	1.14495900	-4.83129000	C	-1.21560100	0.00000000	-4.59116500
C	2.99284400	1.31304200	-3.96272100	C	-0.37564100	-1.15610500	-4.59116500
C	2.17361700	2.44061100	-3.96272100	C	-0.78892900	-2.42807500	-4.11056800
C	-0.32393800	3.25211600	-3.96272100	C	-2.18883300	-2.41999900	-3.83797600
C	-1.64947500	2.82142300	-3.96272100	C	-2.97794300	-1.33388300	-3.83797600
C	0.77002300	2.36988700	-4.31208200	C	-2.55302900	0.00000000	-4.11056800
C	-2.01594600	1.46467100	-4.31208200	C	-0.37564100	1.15610500	-4.59116500
H	4.01032800	-1.41510200	-3.58792600	C	0.98344200	0.71451200	-4.59116500
H	2.58510100	-3.37675800	-3.58792600	C	0.98344200	-0.71451200	-4.59116500
H	-0.10658200	-4.25133900	-3.58792600	C	2.06544400	-1.50063300	-4.11056800
H	-2.41264700	-3.50205300	-3.58792600	C	0.34836300	-3.24438400	-3.83797600
H	-4.07619900	-1.21237000	-3.58792600	C	-2.97794300	1.33388300	-3.83797600
H	-4.07619900	1.21237000	-3.58792600	C	-2.18883300	2.41999900	-3.83797600
H	-2.41264700	3.50205300	-3.58792600	C	-0.78892900	2.42807500	-4.11056800
H	-0.10658200	4.25133900	-3.58792600	C	2.06544400	1.50063300	-4.11056800
H	2.58510100	3.37675800	-3.58792600	C	1.62516900	2.82952500	-3.83797600
H	4.01032800	1.41510200	-3.58792600	C	0.34836300	3.24438400	-3.83797600

2...C₆₀(eclip.):

C	-0.99942500	-0.72612500	5.42629800	C	1.34647800	0.00000000	-3.15224900
C	-0.99942500	0.72612500	5.42629800	C	1.34647800	4.14403300	-3.15224900
C	-1.96220500	1.42562500	4.69143700	C	-3.52512500	2.56115300	-3.15224900
C	-2.96184300	0.69933100	3.92797700	C	-3.52512500	-2.56115300	-3.15224900
C	-2.96184300	-0.69933100	3.92797700	H	1.36664400	-4.20609800	-2.05716000
C	-1.96220500	-1.42562500	4.69143700	H	-3.57792100	-2.59951200	-2.05716000
C	0.38174600	-1.17489400	5.42629800	H	-4.31788800	-3.13712900	-3.64383700
C	1.23535700	0.00000000	5.42629800	H	1.64928600	-5.07598100	-3.64383700
C	0.38174600	1.17489400	5.42629800	H	-3.57792100	2.59951200	-2.05716000
C	0.74949600	2.30671000	4.69143700	H	-4.31788800	3.13712900	-3.64383700
C	-1.58036300	2.60077500	3.92797700	H	1.64928600	5.07598100	-3.64383700
C	-3.19751400	1.42558900	2.69248100	H	1.36664400	4.20609800	-2.05716000
C	-3.42455400	0.72615200	1.50256200	H	5.33720300	0.00000000	-3.64383700
C	-3.42455400	-0.72615200	1.50256200	H	4.42255300	0.00000000	-2.05716000
C	-3.19751400	-1.42558900	2.69248100				
C	-2.34390200	-2.60048600	2.69248100				
C	-1.58036300	-2.60077500	3.92797700				
C	-0.25015700	-3.03298500	3.92797700				
C	0.74949600	-2.30671000	4.69143700				
C	2.42541900	0.00000000	4.69143700				
C	2.80723800	-1.17515700	3.92797700				
C	1.98512500	-2.30669800	3.92797700				
C	1.74890300	-3.03277700	2.69248100				
C	0.36772900	-3.48154800	2.69248100				
C	-0.36763400	-3.48133800	1.50256200				
C	-1.74885700	-3.03255100	1.50256200				
C	-1.98342200	-2.30542600	0.26791500				
C	-2.80550100	-1.17393000	0.26791500				
C	-2.34390200	2.60048600	2.69248100				
C	-0.38099900	1.17259400	-1.22697500				
C	-0.74855900	2.30382600	-0.49424200				
C	0.24952700	3.03095500	0.26791500				
C	1.57967900	2.59876200	0.26791500				
C	1.95975200	1.42384300	-0.49424200				
C	0.99746800	-0.72470300	-1.22697500				
C	-0.38099900	-1.17259400	-1.22697500				
C	-1.23293800	0.00000000	-1.22697500				
C	-2.42238600	0.00000000	-0.49424200				
C	-2.80550100	1.17393000	0.26791500				
C	-1.98342200	2.30542600	0.26791500				
C	-0.36763400	3.48133800	1.50256200				
C	0.36772900	3.48154800	2.69248100				
C	1.74890300	3.03277700	2.69248100				
C	2.34370100	2.60037100	1.50256200				
C	3.19734400	1.42543300	1.50256200				
C	2.95971700	0.69930300	0.26791500				
C	2.95971700	-0.69930300	0.26791500				

2...C₆₀(stagg.):

C	-0.99943600	-0.72613300	5.45192800	C	-1.96221300	1.42563100	4.71703600
C	-0.99943600	0.72613300	5.45192800	C	-2.96189400	0.69937600	3.95360900
C	-1.96221300	1.42563100	4.71703600	C	-2.96189400	-0.69937600	3.95360900
C	-2.96189400	0.69937600	3.95360900	C	-1.96221300	-1.42563100	4.71703600
C	-2.96189400	-0.69937600	3.95360900	C	0.38175100	-1.17490700	5.45192800
C	-1.96221300	-1.42563100	4.71703600	C	1.23537000	0.00000000	5.45192800
C	0.38175100	-1.17490700	5.45192800	C	0.38175100	1.17490700	5.45192800
C	1.23537000	0.00000000	5.45192800	C	0.74949900	2.30671900	4.71703600
C	0.38175100	1.17490700	5.45192800	C	-1.58042200	2.60081000	3.95360900
C	0.74949900	2.30671900	4.71703600	C	-3.19780200	1.42569200	2.71824800
C	-1.58042200	2.60081000	3.95360900	C	-3.42493700	0.72628300	1.52816900
C	-3.19780200	1.42569200	2.71824800	C	-3.42493700	-0.72628300	1.52816900
C	-3.42493700	0.72628300	1.52816900	C	-3.19780200	-1.42569200	2.71824800
C	-3.42493700	-0.72628300	1.52816900	C	-2.34408900	-2.60072700	2.71824800
C	-3.19780200	-1.42569200	2.71824800	C	-1.58042200	-2.60081000	3.95360900
C	-2.34408900	-2.60072700	2.71824800	C	-0.25012900	-3.03304800	3.95360900
C	-1.58042200	-2.60081000	3.95360900	C	0.74949900	-2.30671900	4.71703600
C	-0.25012900	-3.03304800	3.95360900	C	2.42542800	0.00000000	4.71703600
C	0.74949900	-2.30671900	4.71703600	C	2.80730600	-1.17515100	3.95360900
C	2.42542800	0.00000000	4.71703600	C	1.98514000	-2.30676500	3.95360900
C	2.80730600	-1.17515100	3.95360900	C	1.74907500	-3.03303000	2.71824800
C	1.98514000	-2.30676500	3.95360900	C	0.36773900	-3.48185400	2.71824800
C	1.74907500	-3.03303000	2.71824800	C	-0.36762800	-3.48174200	1.52816900
C	0.36773900	-3.48185400	2.71824800	C	-1.74910000	-3.03287500	1.52816900
C	-0.36762800	-3.48174200	1.52816900	C	-1.98434000	-2.30587300	0.29356200
C	-1.74910000	-3.03287500	1.52816900	C	-2.80621100	-1.17466600	0.29356200
C	-1.98434000	-2.30587300	0.29356200	C	-2.34408900	2.60072700	2.71824800
C	-2.80621100	-1.17466600	0.29356200				
C	-2.34408900	2.60072700	2.71824800				

C	-0.38104600	1.17273700	-1.20060700	C	-4.59417600	-0.79194000	-2.65059700
C	-0.74798200	2.30205100	-0.46653400	C	-4.59417600	0.79194000	-2.65059700
C	0.25000700	3.03185600	0.29356200	C	-1.65367600	2.83592900	-3.26792000
C	1.57982100	2.59977400	0.29356200	C	-0.32906600	3.26632100	-3.26792000
C	1.95824200	1.42274600	-0.46653400	C	0.78635400	2.42015000	-3.58040100
C	0.99759000	-0.72479200	-1.20060700	C	2.54469600	0.00000000	-3.58040100
C	-0.38104600	-1.17273700	-1.20060700	C	3.00476900	1.32230900	-3.26792000
C	-1.23308900	0.00000000	-1.20060700	C	2.18611500	2.44908900	-3.26792000
C	-2.42052000	0.00000000	-0.46653400	C	-0.66649900	4.61404300	-2.65059700
C	-2.80621100	1.17466600	0.29356200	C	-2.17285800	4.12459800	-2.65059700
C	-1.98434000	2.30587300	0.29356200	C	-0.66649900	-4.61404300	-2.65059700
C	-0.36762800	3.48174200	1.52816900	C	3.25127600	-3.34108100	-2.65059700
C	0.36773900	3.48185400	2.71824800	C	4.18225700	-2.05969600	-2.65059700
C	1.74907500	3.03303000	2.71824800	C	3.25127600	3.34108100	-2.65059700
C	2.34393400	2.60070300	1.52816900	C	4.18225700	2.05969600	-2.65059700
C	3.19773100	1.42555200	1.52816900	C	3.00476900	-1.32230900	-3.26792000
C	2.96072300	0.69912500	0.29356200	C	2.18611500	-2.44908900	-3.26792000
C	2.96072300	-0.69912500	0.29356200	C	-2.17285800	-4.12459800	-2.65059700
C	1.95824200	-1.42274600	-0.46653400	C	-0.32906600	-3.26632100	-3.26792000
C	-0.74798200	-2.30205100	-0.46653400	H	-0.24874400	4.78361200	-1.64921900
C	0.25000700	-3.03185600	0.29356200	H	-2.61049900	4.01623100	-1.64921900
C	1.57982100	-2.59977400	0.29356200	H	-0.46755600	5.49453500	-3.27638700
C	2.34393400	-2.60070300	1.52816900	H	-2.85134600	4.71999500	-3.27638700
C	3.19773100	-1.42555200	1.52816900	H	3.60786800	4.17035000	-3.27638700
C	3.42507700	-0.72621100	2.71824800	H	3.01297400	3.72381600	-1.64921900
C	3.42507700	0.72621100	2.71824800	H	5.08113100	2.14257700	-3.27638700
C	2.80730600	1.17515100	3.95360900	H	4.47261900	1.71478700	-1.64921900
C	1.98514000	2.30676500	3.95360900	H	5.08113100	-2.14257700	-3.27638700
C	-1.74910000	3.03287500	1.52816900	H	4.47261900	-1.71478700	-1.64921900
C	-0.25012900	3.03304800	3.95360900	H	3.60786800	-4.17035000	-3.27638700
C	0.99759000	0.72479200	-1.20060700	H	3.01297400	-3.72381600	-1.64921900
C	-0.98303600	0.71421800	-4.59698500	H	-0.24874400	-4.78361200	-1.64921900
C	-0.98303600	-0.71421800	-4.59698500	H	-0.46755600	-5.49453500	-3.27638700
C	-2.06731200	-1.50199000	-4.12339200	H	-2.61049900	-4.01623100	-1.64921900
C	-3.19583900	-0.67153700	-3.85669500	H	-2.85134600	-4.71999500	-3.27638700
C	-3.19583900	0.67153700	-3.85669500	H	-4.62635100	-1.24164800	-1.64921900
C	-2.06731200	1.50199000	-4.12339200	H	-5.37009600	-1.25323300	-3.27638700
C	0.37548700	1.15562900	-4.59698500	H	-4.62635100	1.24164800	-1.64921900
C	1.21510000	0.00000000	-4.59698500	H	-5.37009600	1.25323300	-3.27638700
C	0.37548700	-1.15562900	-4.59698500	C	-0.38176300	-1.17494500	5.85271000
C	0.78964300	-2.43027100	-4.12339200	C	-1.23541000	0.00000000	5.85271000
C	-1.62623800	-2.83190700	-3.85669500	C	-2.42520900	0.00000000	5.11790100
C	-1.62623800	2.83190700	-3.85669500	C	-2.80738100	-1.17522800	4.35503000
C	-0.34889900	3.24694000	-3.85669500	C	-1.98523700	-2.30681200	4.35503000
C	0.78964300	2.43027100	-4.12339200	C	-0.74943100	-2.30651100	5.11790100
C	2.55533900	0.00000000	-4.12339200	C	0.99946800	-0.72615600	5.85271000
C	2.98020700	1.33518200	-3.85669500	C	0.99946800	0.72615600	5.85271000
C	2.19076900	2.42175200	-3.85669500	C	-0.38176300	1.17494500	5.85271000
C	2.98020700	-1.33518200	-3.85669500	C	-0.74943100	2.30651100	5.11790100
C	2.19076900	-2.42175200	-3.85669500	C	-2.80738100	1.17522800	4.35503000
C	-0.34889900	-3.24694000	-3.85669500	C	-3.42573000	-0.72616900	3.11984400
C	-1.35283200	-4.16359000	-3.20551100	C	-3.19852400	-1.42568800	1.92972600
C	3.54176100	-2.57324000	-3.20551100	C	-2.34430800	-2.60141500	1.92972600
C	3.54176100	2.57324000	-3.20551100	C	-1.74923600	-3.03366500	3.11984400
C	-1.35283200	4.16359000	-3.20551100	C	-0.36798200	-3.48246200	3.11984400
C	-4.37785800	0.00000000	-3.20551100	C	0.25018000	-3.03314300	4.35503000
H	-1.38191100	-4.25308600	-2.11135500	C	1.58043700	-2.60091700	4.35503000
H	-4.47195900	0.00000000	-2.11135500	C	1.96203600	-1.42550200	5.11790100
H	-5.34479100	0.00000000	-3.72242800	C	1.96203600	1.42550200	5.11790100
H	-1.65163100	-5.08319900	-3.72242800	C	2.96200100	0.69935700	4.35503000
H	-1.38191100	4.25308600	-2.11135500	C	2.96200100	-0.69935700	4.35503000
H	-1.65163100	5.08319900	-3.72242800	C	3.19830500	-1.42611100	3.11984400
H	4.32402700	3.14159000	-3.72242800	C	2.34464300	-2.60107600	3.11984400
H	3.61789100	2.62855200	-2.11135500	C	1.74966200	-3.03345100	1.92972600
H	4.32402700	-3.14159000	-3.72242800	C	0.36751200	-3.48253900	1.92972600
H	3.61789100	-2.62855200	-2.11135500	C	-0.24988400	-3.03347200	0.69491100
				C	-1.58086900	-2.60100800	0.69491100
				C	-3.42573000	0.72616900	3.11984400
				C	-0.99609700	0.72370700	-0.78990300
				C	-1.96030600	1.42424600	-0.06436000
				C	-1.58086900	2.60100800	0.69491100
				C	-0.24988400	3.03347200	0.69491100
				C	0.74877000	2.30447800	-0.06436000
				C	1.23124300	0.00000000	-0.78990300
				C	0.38047500	-1.17098200	-0.78990300
				C	-0.99609700	-0.72370700	-0.78990300
				C	-1.96030600	-1.42424600	-0.06436000
				C	-2.96222100	-0.69974000	0.69491100
				C	-2.96222100	0.69974000	0.69491100
				C	-2.34430800	2.60141500	1.92972600
				C	-1.74923600	3.03366500	3.11984400

3...C₆₀(eclip.):

C	-0.36798200	3.48246200	3.11984400
C	0.36751200	3.48253900	1.92972600
C	1.74966200	3.03345100	1.92972600
C	1.98519000	2.30725200	0.69491100
C	2.80778400	1.17504800	0.69491100
C	2.42307200	0.00000000	-0.06436000
C	0.74877000	-2.30447800	-0.06436000
C	1.98519000	-2.30725200	0.69491100
C	2.80778400	-1.17504800	0.69491100
C	3.42565900	-0.72663900	1.92972600
C	3.42565900	0.72663900	1.92972600
C	3.19830500	1.42611100	3.11984400
C	2.34464300	2.60107600	3.11984400
C	1.58043700	2.60091700	4.35503000
C	0.25018000	3.03314300	4.35503000
C	-3.19852400	1.42568800	1.92972600
C	-1.98523700	2.30681200	4.35503000
C	0.38047500	1.17098200	-0.78990300

3...C₆₀(stagg.):

C	-0.97993800	0.71196600	-4.12579500
C	-0.97993800	-0.71196600	-4.12579500
C	-2.05882500	-1.49582400	-3.67439200
C	-3.20770200	-0.69683400	-3.36256100
C	-3.20770200	0.69683400	-3.36256100
C	-2.05882500	1.49582400	-3.67439200
C	0.37430300	1.15198600	-4.12579500
C	1.21126900	0.00000000	-4.12579500
C	0.37430300	-1.15198600	-4.12579500
C	0.78640100	-2.42029400	-3.67439200
C	-1.65396300	-2.83537200	-3.36256100
C	-4.59015000	-0.79182400	-2.73823500
C	-4.59015000	0.79182400	-2.73823500
C	-1.65396300	2.83537200	-3.36256100
C	-0.32850600	3.26603900	-3.36256100
C	0.78640100	2.42029400	-3.67439200
C	2.54484800	0.00000000	-3.67439200
C	3.00467400	1.32169000	-3.36256100
C	2.18549700	2.44919000	-3.36256100
C	-0.66536500	4.61017900	-2.73823500
C	-2.17150400	4.12080500	-2.73823500
C	-0.66536500	-4.61017900	-2.73823500
C	3.24808700	-3.33862100	-2.73823500
C	4.17893100	-2.05742300	-2.73823500
C	3.24808700	3.33862100	-2.73823500
C	4.17893100	2.05742300	-2.73823500
C	3.00467400	-1.32169000	-3.36256100
C	2.18549700	-2.44919000	-3.36256100
C	-2.17150400	-4.12080500	-2.73823500
C	-0.32850600	-3.26603900	-3.36256100
H	-0.24623800	4.77421100	-1.73650900
H	-2.60700100	4.00715300	-1.73650900
H	-0.46647900	5.49435500	-3.35892100
H	-2.85211100	4.71921600	-3.35892100
H	3.60689000	4.17083700	-3.35892100
H	3.00542100	3.71768300	-1.73650900
H	5.08129200	2.14149700	-3.35892100
H	4.46445300	1.70949800	-1.73650900
H	5.08129200	-2.14149700	-3.35892100
H	4.46445300	-1.70949800	-1.73650900
H	3.60689000	-4.17083700	-3.35892100
H	3.00542100	-3.71768300	-1.73650900
H	-0.24623800	-4.77421100	-1.73650900
H	-0.46647900	-5.49435500	-3.35892100
H	-2.60700100	-4.00715300	-1.73650900
H	-2.85211100	-4.71921600	-3.35892100
H	-4.61663600	-1.24112700	-1.73650900
H	-5.36959200	-1.25420100	-3.35892100
H	-4.61663600	1.24112700	-1.73650900
H	-5.36959200	1.25420100	-3.35892100
C	0.38182000	-1.17512200	5.83506800
C	-0.99961900	-0.72626600	5.83506800
C	-1.96216400	-1.42559500	5.09974800
C	-1.58026400	-2.60064300	4.33614200
C	-0.25015900	-3.03282100	4.33614200
C	0.74948000	-2.30666200	5.09974800
C	1.23559700	0.00000000	5.83506800
C	0.38182000	1.17512200	5.83506800
C	-0.99961900	0.72626600	5.83506800

C	-1.96216400	1.42559500	5.09974800
C	-2.96168700	-0.69927800	4.33614200
C	-2.34423600	-2.60075300	3.10066200
C	-1.74945500	-3.03345900	1.91064400
C	-0.36768400	-3.48242400	1.91064400
C	0.36784300	-3.48196100	3.10066200
C	1.74905500	-3.03317800	3.10066200
C	1.98503000	-2.30656400	4.33614200
C	2.80708100	-1.17510900	4.33614200
C	2.42536800	0.00000000	5.09974800
C	0.74948000	2.30666200	5.09974800
C	1.98503000	2.30656400	4.33614200
C	2.80708100	1.17510900	4.33614200
C	3.42521100	0.72614600	3.10066200
C	3.42521100	-0.72614600	3.10066200
C	3.19836200	-1.42581600	1.91064400
C	2.34438000	-2.60122100	1.91064400
C	1.58072900	-2.60086900	0.67552000
C	0.24991600	-3.03327600	0.67552000
C	-3.19787200	-1.42582400	3.10066200
C	-1.23161800	0.00000000	-0.81063900
C	-2.42191500	0.00000000	-0.83349000
C	-2.80758900	1.17501800	0.67552000
C	-1.98510100	2.30707500	0.67552000
C	-0.74841300	2.30337800	-0.83349000
C	0.99640000	0.72392700	-0.81063900
C	0.99640000	-0.72392700	-0.81063900
C	-0.38059100	-1.17133800	-0.81063900
C	-0.74841300	-2.30337800	-0.83349000
C	-1.98510100	-2.30707500	0.67552000
C	-2.80758900	-1.17501800	0.67552000
C	-3.42560300	0.72644000	1.91064400
C	-3.19787200	1.42582400	3.10066200
C	-2.34423600	2.60075300	3.10066200
C	-1.74945500	3.03345900	1.91064400
C	-0.36768400	3.48242400	1.91064400
C	0.24991600	3.03327600	0.67552000
C	1.58072900	2.60086900	0.67552000
C	1.95937000	1.42356600	-0.83349000
C	1.95937000	-1.42356600	-0.83349000
C	2.96204600	-0.69965000	0.67552000
C	2.96204600	0.69965000	0.67552000
C	3.19836200	1.42581600	1.91064400
C	2.34438000	2.60122100	1.91064400
C	1.74905500	3.03317800	3.10066200
C	0.36784300	3.48196100	3.10066200
C	-0.25015900	3.03282100	4.33614200
C	-1.58026400	2.60064300	4.33614200
C	-3.42560300	-0.72644000	1.91064400
C	-2.96168700	0.69927800	4.33614200
C	-0.38059100	1.17133800	-0.81063900

4...C₆₀(eclip.):

C	-0.97345700	-0.70725800	4.30667600
C	-0.97345700	0.70725800	4.30667600
C	-2.06203500	1.49815600	3.81529500
C	-3.19219600	0.70363500	3.49875600
C	-3.19219600	-0.70363500	3.49875600
C	-2.06203500	-1.49815600	3.81529500
C	0.37182700	-1.14436700	4.30667600
C	1.20325900	0.00000000	4.30667600
C	0.37182700	1.14436700	4.30667600
C	0.78762700	2.42406800	3.81529500
C	-1.65563900	2.81852400	3.49875600
C	-4.56060900	0.67467300	2.78195900
C	-4.56060900	-0.67467300	2.78195900
C	-1.65563900	-2.81852400	3.49875600
C	-0.31724700	-3.25339400	3.49875600
C	0.78762700	-2.42406800	3.81529500
C	2.54881600	0.00000000	3.81529500
C	2.99612700	-1.30707300	3.49875600
C	2.16895500	-2.44557900	3.49875600
C	-0.76765400	-4.54588200	2.78195900
C	-2.05095800	-4.12891100	2.78195900
C	-0.76765400	4.54588200	2.78195900
C	3.29304700	3.22648000	2.78195900
C	4.08617300	2.13483700	2.78195900
C	3.29304700	-3.22648000	2.78195900
C	4.08617300	-2.13483700	2.78195900

C	2.99612700	1.30707300	3.49875600	C	-3.17621900	0.70329500	3.44050100
C	2.16895500	2.44557900	3.49875600	C	-3.17621900	-0.70329500	3.44050100
C	-2.05095800	4.12891100	2.78195900	C	-2.05309300	-1.49165900	3.78522800
C	-0.31724700	3.25339400	3.49875600	C	0.37246600	-1.14633100	4.32071900
H	-0.25305600	5.42399700	2.40569900	C	1.20532400	0.00000000	4.32071900
H	-2.98341800	4.53684800	2.40569900	C	0.37246600	1.14633100	4.32071900
H	-5.23672600	1.43543600	2.40569900	C	0.78421200	2.41355600	3.78522800
H	-5.23672600	-1.43543600	2.40569900	C	-1.65037900	2.80343300	3.44050100
H	-2.98341800	-4.53684800	2.40569900	C	-4.50942200	0.67578800	2.67070500
H	-0.25305600	-5.42399700	2.40569900	C	-4.50942200	-0.67578800	2.67070500
H	3.39287200	-4.23936300	2.40569900	C	-1.65037900	-2.80343300	3.44050100
H	5.08032900	-1.91677800	2.40569900	C	-0.31263200	-3.23809400	3.44050100
H	5.08032900	1.91677800	2.40569900	C	0.78421200	-2.41355600	3.78522800
H	3.39287200	4.23936300	2.40569900	C	2.53776300	0.00000000	3.78522800
C	0.38066800	-1.17157600	0.95686200	C	2.98300100	-1.29795700	3.44050100
C	-0.99660200	-0.72407400	0.95686200	C	2.15622900	-2.43591200	3.44050100
C	-1.96064600	-1.42449300	0.22809400	C	-0.75077500	-4.49754600	2.67070500
C	-1.57970600	-2.59941300	-0.53366600	C	-2.03620100	-4.07988500	2.67070500
C	-0.24988700	-3.03149700	-0.53366600	C	-0.75077500	4.49754600	2.67070500
C	0.74890000	-2.30487700	0.22809400	C	3.25098100	3.19729600	2.67070500
C	1.23186800	0.00000000	0.95686200	C	4.04541800	2.10384800	2.67070500
C	0.38066800	1.17157600	0.95686200	C	3.25098100	-3.19729600	2.67070500
C	-0.99660200	0.72407400	0.95686200	C	4.04541800	-2.10384800	2.67070500
C	-1.96064600	1.42449300	0.22809400	C	2.98300100	1.29795700	3.44050100
C	-2.96034400	-0.69912700	-0.53366600	C	2.15622900	2.43591200	3.44050100
C	-2.34274200	-2.60000000	-1.76846100	C	-2.03620100	4.07988500	2.67070500
C	-1.74877600	-3.03307500	-2.95873200	C	-0.31263200	3.23809400	3.44050100
C	-0.36800700	-3.48171400	-2.95873200	H	-0.23060900	5.35760000	2.26184300
C	0.36707600	-3.48047300	-1.76846100	H	-2.96255200	4.46993800	2.26184300
C	1.74880000	-3.03152400	-1.76846100	H	-5.16664200	1.43626700	2.26184300
C	1.98403200	-2.30565200	-0.53366600	H	-5.16664200	-1.43626700	2.26184300
C	2.80590600	-1.17444100	-0.53366600	H	-2.96255200	-4.46993800	2.26184300
C	2.42349100	0.00000000	0.22809400	H	-0.23060900	-5.35760000	2.26184300
C	0.74890000	2.30487700	0.22809400	H	3.33568500	-4.19884100	2.26184300
C	1.98403200	2.30565200	-0.53366600	H	5.02411800	-1.87491200	2.26184300
C	2.80590600	1.17444100	-0.53366600	H	5.02411800	1.87491200	2.26184300
C	3.42355900	0.72641500	-1.76846100	H	3.33568500	4.19884100	2.26184300
C	3.42355900	-0.72641500	-1.76846100	C	-0.38119100	-1.17318400	0.95574600
C	3.19758600	-1.42590400	-2.95873200	C	-1.23355900	0.00000000	0.95574600
C	2.34422400	-2.60045700	-2.95873200	C	-2.42132100	0.00000000	0.22349000
C	1.58030700	-2.60063100	-4.19427300	C	-2.80801700	-1.17482100	-0.53307400
C	0.25011700	-3.03283600	-4.19427300	C	-1.98504600	-2.30754300	-0.53307400
C	-3.19669400	-1.42463500	-1.76846100	C	-0.74822900	-2.30281300	0.22349000
C	-1.23552200	0.00000000	-5.69331600	C	0.99797000	-0.72506800	0.95574600
C	-2.42511600	0.00000000	-4.95770000	C	0.99797000	0.72506800	0.95574600
C	-2.80710800	1.17507300	-4.19427300	C	-0.38119100	1.17318400	0.95574600
C	-1.98500500	2.30660100	-4.19427300	C	-0.74822900	2.30281300	0.22349000
C	-0.74940200	2.30642200	-4.95770000	C	-2.80801700	1.17482100	-0.53307400
C	0.99955800	0.72622100	-5.69331600	C	-3.42586900	-0.72674400	-1.76811400
C	0.99955800	-0.72622100	-5.69331600	C	-3.19862100	-1.42617600	-2.95877300
C	-0.38179700	-1.17505100	-5.69331600	C	-2.34480200	-2.60135700	-2.95877300
C	-0.74940200	-2.30642200	-4.95770000	C	-1.74982600	-3.03361900	-1.76811400
C	-1.98500500	-2.30660100	-4.19427300	C	-0.36747800	-3.48277100	-1.76811400
C	-2.80710800	-1.17507300	-4.19427300	C	0.24959600	-3.03362200	-0.53307400
C	-3.42502700	0.72591300	-2.95873200	C	1.58119100	-2.60096100	-0.53307400
C	-3.19669400	1.42463500	-1.76846100	C	1.95888900	-1.42321700	0.22349000
C	-2.34274200	2.60000000	-1.76846100	C	1.95888900	1.42321700	0.22349000
C	-1.74877600	3.03307500	-2.95873200	C	2.96227600	0.70006100	-0.53307400
C	-0.36800700	3.48171400	-2.95873200	C	2.96227600	-0.70006100	-0.53307400
C	0.25011700	3.03283600	-4.19427300	C	3.19875600	-1.42572800	-1.76811400
C	1.58030700	2.60063100	-4.19427300	C	2.34441700	-2.60162300	-1.76811400
C	1.96196000	1.42544700	-4.95770000	C	1.74945400	-3.03390300	-2.95877300
C	1.96196000	-1.42544700	-4.95770000	C	0.36794600	-3.48278200	-2.95877300
C	2.96168900	-0.69932300	-4.19427300	C	-0.25002700	-3.03354400	-4.19355000
C	2.96168900	0.69932300	-4.19427300	C	-1.58079600	-2.60115100	-4.19355000
C	3.19758600	1.42590400	-2.95873200	C	-3.42586900	0.72674400	-1.76811400
C	2.34422400	2.60045700	-2.95873200	C	-0.99945700	0.72614800	-5.69184400
C	1.74880000	3.03152400	-1.76846100	C	-1.96245100	1.42580400	-4.95680100
C	0.36707600	3.48047300	-1.76846100	C	-1.58079600	2.60115100	-4.19355000
C	-0.24988700	3.03149700	-0.53366600	C	-0.25002700	3.03354400	-4.19355000
C	-1.57970600	2.59941300	-0.53366600	C	0.74959000	2.30700000	-4.95680100
C	-3.42502700	-0.72591300	-2.95873200	C	1.23539700	0.00000000	-5.69184400
C	-2.96034400	0.69912700	-0.53366600	C	0.38175900	-1.17493300	-5.69184400
C	-0.38179700	1.17505100	-5.69331600	C	-0.99945700	-0.72614800	-5.69184400
				C	-1.96245100	-1.42580400	-4.95680100
				C	-2.96233400	-0.69962700	-4.19355000
				C	-2.96233400	0.69962700	-4.19355000
				C	-2.34480200	2.60135700	-2.95877300
				C	-1.74982600	3.03361900	-1.76811400
				C	-0.36747800	3.48277100	-1.76811400
				C	0.36794600	3.48278200	-2.95877300

4...C₆₀(stagg.):

C	-0.97512800	-0.70847200	4.32071900
C	-0.97512800	0.70847200	4.32071900
C	-2.05309300	1.49165900	3.78522800

C	1.74945400	3.03390300	-2.95877300
C	1.98534900	2.30722600	-4.19355000
C	2.80780900	1.17520700	-4.19355000
C	2.42572300	0.00000000	-4.95680100
C	0.74959000	-2.30700000	-4.95680100
C	1.98534900	-2.30722600	-4.19355000
C	2.80780900	-1.17520700	-4.19355000
C	3.42602400	-0.72630200	-2.95877300
C	3.42602400	0.72630200	-2.95877300
C	3.19875600	1.42572800	-1.76811400
C	2.34441700	2.60162300	-1.76811400
C	1.58119100	2.60096100	-0.53307400
C	0.24959600	3.03362200	-0.53307400
C	-3.19862100	1.42617600	-2.95877300
C	-1.98504600	2.30754300	-0.53307400
C	0.38175900	1.17493300	-5.69184400

H	2.85516100	-3.58434000	-1.28425500
H	-2.52661700	-3.82304100	-1.28425500
H	-4.41669600	1.22157100	-1.28425500
H	-0.20305100	4.57801300	-1.28425500
C	-0.99943500	-0.72613200	6.21004000
C	-0.99943500	0.72613200	6.21004000
C	-1.96226800	1.42567100	5.47536300
C	-2.96209500	0.69939300	4.71212200
C	-2.96209500	-0.69939300	4.71212200
C	-1.96226800	-1.42567100	5.47536300
C	0.38175000	-1.17490600	6.21004000
C	1.23537000	0.00000000	6.21004000
C	0.38175000	1.17490600	6.21004000
C	0.74952000	2.30678500	5.47536300
C	-1.58050100	2.60099600	4.71212200
C	-3.19818100	1.42611500	3.47695900
C	-3.42480000	0.72645600	2.28672000
C	-3.42480000	-0.72645600	2.28672000
C	-3.19818100	-1.42611500	3.47695900
C	-2.34460800	-2.60095800	3.47695900
C	-1.58050100	-2.60099600	4.71212200
C	-0.25017500	-3.03324500	4.71212200
C	0.74952000	-2.30678500	5.47536300
C	2.42549700	0.00000000	5.47536300
C	2.80747900	-1.17525500	4.71212200
C	1.98529300	-2.30689700	4.71212200
C	1.74913400	-3.03359500	3.47695900
C	0.36802300	-3.48234500	3.47695900
C	-0.36742100	-3.48166500	2.28672000
C	-1.74922200	-3.03269100	2.28672000
C	-1.98392600	-2.30570200	1.05254700
C	-2.80592000	-1.17432400	1.05254700
C	-2.34460800	2.60095800	3.47695900
C	-0.38080300	1.17199200	-0.43797700
C	-0.74806900	2.30231800	0.29307100
C	0.24977200	3.03147400	1.05254700
C	1.57978600	2.59932700	1.05254700
C	1.95846900	1.42291100	0.29307100
C	0.99695600	-0.72433100	-0.43797700
C	-0.38080300	-1.17199200	-0.43797700
C	-1.23230500	0.00000000	-0.43797700
C	-2.42080000	0.00000000	0.29307100
C	-2.80592000	1.17432400	1.05254700
C	-1.98392600	2.30570200	1.05254700
C	-0.36742100	3.48166500	2.28672000
C	0.36802300	3.48234500	3.47695900
C	1.74913400	3.03359500	3.47695900
C	2.34372100	2.60076200	2.28672000
C	3.19772100	1.42533200	2.28672000
C	2.96028700	0.69923000	1.05254700
C	2.96028700	-0.69923000	1.05254700
C	1.95846900	-1.42291100	0.29307100
C	-0.74806900	-2.30231800	0.29307100
C	0.24977200	-3.03147400	1.05254700
C	1.57978600	-2.59932700	1.05254700
C	2.34372100	-2.60076200	2.28672000
C	3.19772100	-1.42533200	2.28672000
C	3.42563200	-0.72609300	3.47695900
C	3.42563200	0.72609300	3.47695900
C	2.80747900	1.17525500	4.71212200
C	1.98529300	2.30689700	4.71212200
C	-1.74922200	3.03269100	2.28672000
C	-0.25017500	3.03324500	4.71212200
C	0.99695600	0.72433100	-0.43797700

5...C₆₀(eclip.):

C	0.97589800	-0.70903100	-3.76712100
C	0.97589800	0.70903100	-3.76712100
C	2.02213100	1.46916400	-3.24518300
C	3.19342900	0.69955000	-2.89566400
C	3.19342900	-0.69955000	-2.89566400
C	2.02213100	-1.46916400	-3.24518300
C	-0.37276000	-1.14723700	-3.76712100
C	-1.20627600	0.00000000	-3.76712100
C	-0.37276000	1.14723700	-3.76712100
C	-0.77238500	2.37715800	-3.24518300
C	1.65213500	2.82095800	-2.89566400
C	4.47928300	1.23261300	-2.30163300
C	4.47928300	-1.23261300	-2.30163300
C	2.55646000	-3.87915300	-2.30163300
C	1.65213500	-2.82095800	-2.89566400
C	0.32151200	-3.25330400	-2.89566400
C	-0.77238500	-2.37715800	-3.24518300
C	-2.49949100	0.00000000	-3.24518300
C	-2.99472300	-1.31110300	-2.89566400
C	-2.17235300	-2.44299800	-2.89566400
C	-2.89930500	-3.63006200	-2.30163300
C	0.21189000	-4.64095000	-2.30163300
C	2.55646000	3.87915300	-2.30163300
C	0.21189000	4.64095000	-2.30163300
C	-2.89930500	3.63006200	-2.30163300
C	-4.34832800	-1.63565200	-2.30163300
C	-4.34832800	1.63565200	-2.30163300
C	-2.99472300	1.31110300	-2.89566400
C	-2.17235300	2.44299800	-2.89566400
C	0.32151200	3.25330400	-2.89566400
C	1.67453200	5.15368000	-2.28296900
C	-4.38398200	3.18514900	-2.28296900
C	-4.38398200	-3.18514900	-2.28296900
C	1.67453200	-5.15368000	-2.28296900
C	5.41890000	0.00000000	-2.28296900
H	3.48139600	4.01664500	-2.87519300
H	-0.45558400	5.29584700	-2.87519300
H	-2.74424600	4.55221600	-2.87519300
H	-5.17743300	1.20322100	-2.87519300
H	-5.17743300	-1.20322100	-2.87519300
H	-2.74424600	-4.55221600	-2.87519300
H	-0.45558400	-5.29584700	-2.87519300
H	3.48139600	-4.01664500	-2.87519300
H	4.89586700	-2.06979300	-2.87519300
H	4.89586700	2.06979300	-2.87519300
H	1.88334300	5.79633300	-1.42002200
H	1.86450800	5.73836500	-3.19164200
H	-4.88134500	3.54650500	-3.19164200
H	-4.93065500	3.58233100	-1.42002200
H	-4.88134500	-3.54650500	-3.19164200
H	-4.93065500	-3.58233100	-1.42002200
H	1.88334300	-5.79633300	-1.42002200
H	1.86450800	-5.73836500	-3.19164200
H	6.09462500	0.00000000	-1.42002200
H	6.03367400	0.00000000	-3.19164200
H	-2.52661700	3.82304100	-1.28425500
H	-4.41669600	-1.22157100	-1.28425500
H	-0.20305100	-4.57801300	-1.28425500
H	4.29120300	-1.60779700	-1.28425500
H	2.85516100	3.58434000	-1.28425500
H	4.29120300	1.60779700	-1.28425500

5...C₆₀(stagg.):

C	0.97629000	-0.70931600	-3.83516200
C	0.97629000	0.70931600	-3.83516200
C	2.02252300	1.46944900	-3.31148500
C	3.19071800	0.70026500	-2.95525800
C	3.19071800	-0.70026500	-2.95525800
C	2.02252300	-1.46944900	-3.31148500
C	-0.37291000	-1.14769800	-3.83516200
C	-1.20676100	0.00000000	-3.83516200
C	-0.37291000	1.14769800	-3.83516200
C	-0.77253500	2.37761800	-3.31148500
C	1.65197800	2.81815900	-2.95525800
C	4.46792600	1.22919600	-2.33926700
C	4.46792600	-1.22919600	-2.33926700

H	-1.94850300	-5.99687500	-3.00736000	C	0.37837800	-1.16452700	-3.74475100
H	5.10124700	-3.70627300	-3.00736000	C	0.78762300	-2.42405400	-3.37818100
H	4.64078300	-3.37172600	-1.34257000	C	-1.73710200	-2.89202400	-3.10751400
H	5.10124700	3.70627300	-3.00736000	C	-4.52798500	-1.18488600	-2.73989200
H	4.64078300	3.37172600	-1.34257000	C	-4.52798500	1.18488600	-2.73989200
H	-1.77262100	5.45556700	-1.34257000	C	-2.52611800	3.94022000	-2.73989200
H	-1.94850300	5.99687500	-3.00736000	C	-1.73710200	2.89202400	-3.10751400
H	-5.73632300	0.00000000	-1.34257000	C	-0.29454400	3.36073900	-3.10751400
H	-6.30548800	0.00000000	-3.00736000	C	0.78762300	2.42405400	-3.37818100
C	0.99939400	-0.72610200	6.02444900	C	2.54880200	0.00000000	-3.37818100
C	-0.38173500	-1.17485800	6.02444900	C	3.10523400	1.31865300	-3.10751400
C	-0.74941700	-2.30646800	5.28913500	C	2.21368400	2.54576600	-3.10751400
C	0.25011600	-3.03317300	4.52591800	C	2.96675800	3.62007600	-2.73989200
C	1.58050600	-2.60090300	4.52591800	C	-0.27233100	4.67252000	-2.73989200
C	1.96199900	-1.42547600	5.28913500	C	-2.52611800	-3.94022000	-2.73989200
C	0.99939400	0.72610200	6.02444900	C	-0.27233100	-4.67252000	-2.73989200
C	-0.38173500	1.17485800	6.02444900	C	2.96675800	-3.62007600	-2.73989200
C	-1.23531900	0.00000000	6.02444900	C	4.35967500	1.70289000	-2.73989200
C	-2.42516400	0.00000000	5.28913500	C	4.35967500	-1.70289000	-2.73989200
C	-1.98520300	-2.30687400	4.52591800	C	3.10523400	-1.31865300	-3.10751400
C	-0.36811700	-3.48337500	3.29110800	C	2.21368400	-2.54576600	-3.10751400
C	0.36748200	-3.48380400	2.10070000	C	-0.29454400	-3.36073900	-3.10751400
C	1.75043000	-3.03445700	2.10070000	C	-1.67097800	-5.14274000	-2.47255000
C	2.34529000	-2.60173600	3.29110800	C	4.37467600	-3.17838800	-2.47255000
C	3.19913200	-1.42652300	3.29110800	C	4.37467600	3.17838800	-2.47255000
C	2.96200900	-0.69942700	4.52591800	C	-1.67097800	5.14274000	-2.47255000
C	2.96200900	0.69942700	4.52591800	C	-5.40739700	0.00000000	-2.47255000
C	1.96199900	1.42547600	5.28913500	H	-3.60410500	-3.93702000	-2.63796700
C	-0.74941700	2.30646800	5.28913500	H	0.60166000	-5.30355600	-2.63796700
C	0.25011600	3.03317300	4.52591800	H	2.63059900	-4.64431300	-2.63796700
C	1.58050600	2.60090300	4.52591800	H	5.22990400	-1.06667600	-2.63796700
C	2.34529000	2.60173600	3.29110800	H	5.22990400	1.06667600	-2.63796700
C	3.19913200	1.42652300	3.29110800	H	2.63059900	4.64431300	-2.63796700
C	3.42685200	0.72705900	2.10070000	H	0.60166000	5.30355600	-2.63796700
C	3.42685200	-0.72705900	2.10070000	H	-3.60410500	3.93702000	-2.63796700
C	2.81017600	-1.17614000	0.86496100	H	-4.85805800	2.21110100	-2.63796700
C	1.98696800	-2.30918900	0.86496100	H	-4.85805800	-2.21110100	-2.63796700
C	-1.74966300	-3.03448400	3.29110800	H	-1.78369700	-5.48965400	-1.42937800
C	-0.99677600	-0.72420000	-0.61282400	H	-1.95111100	-6.00490300	-3.10248600
C	-1.96255700	-1.42588100	0.10791900	H	5.10807600	-3.71123400	-3.10248600
C	-2.96479800	-0.70026200	0.86496100	H	4.66977900	-3.39279300	-1.42937800
C	-2.96479800	0.70026200	0.86496100	H	5.10807600	3.71123400	-3.10248600
C	-1.96255700	1.42588100	0.10791900	H	4.66977900	3.39279300	-1.42937800
C	0.38073400	1.17178000	-0.61282400	H	-1.78369700	5.48965400	-1.42937800
C	1.23208200	0.00000000	-0.61282400	H	-1.95111100	6.00490300	-3.10248600
C	0.38073400	-1.17178000	-0.61282400	H	-5.77216400	0.00000000	-1.42937800
C	0.74963000	-2.30712500	0.10791900	H	-6.31392900	0.00000000	-3.10248600
C	-0.25018400	-3.03608300	0.86496100	C	0.38180700	-1.17508000	6.07102400
C	-1.58216200	-2.60329700	0.86496100	C	-0.99958300	-0.72623900	6.07102400
C	-3.19973600	-1.42605000	2.10070000	C	-1.96198400	-1.42546500	5.33525600
C	-3.42664100	-0.72632200	3.29110800	C	-1.58031000	-2.60057600	4.57166900
C	-3.42664100	0.72632200	3.29110800	C	-0.25008200	-3.03279300	4.57166900
C	-3.19973600	1.42605000	2.10070000	C	0.74941100	-2.30645100	5.33525600
C	-2.34502700	2.60245600	2.10070000	C	1.23555200	0.00000000	6.07102400
C	-1.58216200	2.60329700	0.86496100	C	0.38180700	1.17508000	6.07102400
C	-0.25018400	3.03608300	0.86496100	C	-0.99958300	0.72623900	6.07102400
C	0.74963000	2.30712500	0.10791900	C	-1.96198400	1.42546500	5.33525600
C	2.42585400	0.00000000	0.10791900	C	-2.96163700	-0.69934300	4.57166900
C	2.81017600	1.17614000	0.86496100	C	-2.34499900	-2.60137500	3.33657400
C	1.98696800	2.30918900	0.86496100	C	-1.75034000	-3.03429200	2.14629100
C	1.75043000	3.03445700	2.10070000	C	-0.36745700	-3.48361800	2.14629100
C	0.36748200	3.48380400	2.10070000	C	0.36809500	-3.48291200	3.33657400
C	-0.36811700	3.48337500	3.29110800	C	1.74941000	-3.03409600	3.33657400
C	-1.74966300	3.03448400	3.29110800	C	1.98495200	-2.30658600	4.57166900
C	-1.98520300	2.30687400	4.52591800	C	2.80707800	-1.17502700	4.57166900
C	-2.80742800	1.17517700	4.52591800	C	2.42514600	0.00000000	5.33525600
C	-2.34502700	-2.60245600	2.10070000	C	0.74941100	2.30645100	5.33525600
C	-2.80742800	-1.17517700	4.52591800	C	1.98495200	2.30658600	4.57166900
C	-0.99677600	0.72420000	-0.61282400	C	2.80707800	1.17502700	4.57166900
				C	3.42619400	0.72620000	3.33657400
				C	3.42619400	-0.72620000	3.33657400
				C	3.19956700	-1.42596900	2.14629100
				C	2.34489800	-2.60232000	2.14629100
				C	1.58185100	-2.60339900	0.91103500
				C	0.25049500	-3.03598200	0.91103500
				C	-3.19869900	-1.42635800	3.33657400
				C	-1.23069700	0.00000000	-0.56351000
				C	-2.42674500	0.00000000	0.15241100
				C	-2.80998400	1.17640500	0.91103500
				C	-1.98716000	2.30892400	0.91103500
				C	-0.74990500	2.30797100	0.15241100

6...C₆₀(stagg.):

C	-0.99060600	0.71971700	-3.74475100	C	0.37837800	-1.16452700	-3.74475100
C	-0.99060600	-0.71971700	-3.74475100	C	0.78762300	-2.42405400	-3.37818100
C	-2.06202400	-1.49814800	-3.37818100	C	-1.73710200	-2.89202400	-3.10751400
C	-3.28727200	-0.75839800	-3.10751400	C	-4.52798500	-1.18488600	-2.73989200
C	-3.28727200	0.75839800	-3.10751400	C	-4.52798500	1.18488600	-2.73989200
C	-2.06202400	1.49814800	-3.37818100	C	-2.52611800	3.94022000	-2.73989200
C	0.37837800	1.16452700	-3.74475100	C	-1.73710200	2.89202400	-3.10751400
C	1.22445600	0.00000000	-3.74475100	C	-0.29454400	3.36073900	-3.10751400

C	0.99565500	0.72338600	-0.56351000	C	-0.99943500	0.72613200	6.01092900
C	0.99565500	-0.72338600	-0.56351000	C	-1.96213800	1.42557700	5.27603200
C	-0.38030600	-1.17046200	-0.56351000	C	-2.96175200	0.69933900	4.51259800
C	-0.74990500	-2.30797100	0.15241100	C	-2.96175200	-0.69933900	4.51259800
C	-1.98716000	-2.30892400	0.91103500	C	-1.96213800	-1.42557700	5.27603200
C	-2.80998400	-1.17640500	0.91103500	C	0.38175000	-1.17490700	6.01092900
C	-3.42666800	0.72702500	2.14629100	C	1.23537000	0.00000000	6.01092900
C	-3.19869900	1.42635800	3.33657400	C	0.38175000	1.17490700	6.01092900
C	-2.34499900	2.60137500	3.33657400	C	0.74947000	2.30663200	5.27603200
C	-1.75034000	3.03429200	2.14629100	C	-1.58034200	2.60068600	4.51259800
C	-0.36745700	3.48361800	2.14629100	C	-3.19787800	1.42589400	3.27738200
C	0.25049500	3.03598200	0.91103500	C	-3.42567800	0.72642800	2.08750700
C	1.58185100	2.60339900	0.91103500	C	-3.42567800	-0.72642800	2.08750700
C	1.96327800	1.42640500	0.15241100	C	-3.19787800	-1.42589400	3.27738200
C	1.96327800	-1.42640500	0.15241100	C	-2.34430400	-2.60073700	3.27738200
C	2.96479800	-0.69993600	0.91103500	C	-1.58034200	-2.60068600	4.51259800
C	2.96479800	0.69993600	0.91103500	C	-0.25012100	-3.03290100	4.51259800
C	3.19956700	1.42596900	2.14629100	C	0.74947000	-2.30663200	5.27603200
C	2.34489800	2.60232000	2.14629100	C	2.42533600	0.00000000	5.27603200
C	1.74941000	3.03409600	3.33657400	C	2.80716900	-1.17509700	4.51259800
C	0.36809500	3.48291200	3.33657400	C	1.98504600	-2.30665100	4.51259800
C	-0.25008200	3.03279300	4.57166900	C	1.74901800	-3.03323800	3.27738200
C	-1.58031000	2.60057600	4.57166900	C	0.36790700	-3.48198800	3.27738200
C	-3.42666800	-0.72702500	2.14629100	C	-0.36771900	-3.48249200	2.08750700
C	-2.96163700	0.69934300	4.57166900	C	-1.74946700	-3.03353500	2.08750700
C	-0.38030600	1.17046200	-0.56351000	C	-1.98487200	-2.30627000	0.85384300

7...C₆₀(eclip.):

C	0.97679300	-0.70968200	-3.99864400	C	-0.99943500	0.72613200	6.01092900
C	0.97679300	0.70968200	-3.99864400	C	-1.96213800	1.42557700	5.27603200
C	2.02038900	1.46789900	-3.46536500	C	-2.96175200	0.69933900	4.51259800
C	3.18028700	0.69484700	-3.10392500	C	-2.96175200	-0.69933900	4.51259800
C	3.18028700	-0.69484700	-3.10392500	C	-1.96213800	-1.42557700	5.27603200
C	2.02038900	-1.46789900	-3.46536500	C	0.38175000	-1.17490700	6.01092900
C	-0.37310200	-1.14828900	-3.99864400	C	1.23537000	0.00000000	6.01092900
C	-1.20738200	0.00000000	-3.99864400	C	0.38175000	1.17490700	6.01092900
C	-0.37310200	1.14828900	-3.99864400	C	0.74947000	2.30663200	5.27603200
C	-0.77172000	2.37511000	-3.46536500	C	-1.58034200	2.60068600	4.51259800
C	1.64360200	2.80991400	-3.10392500	C	-3.19787800	1.42589400	3.27738200
C	4.46400400	1.17754600	-2.48382700	C	-3.42567800	0.72642800	2.08750700
C	4.46400400	-1.17754600	-2.48382700	C	-3.42567800	-0.72642800	2.08750700
C	2.49936600	-3.88163800	-2.48382700	C	-3.19787800	-1.42589400	3.27738200
C	1.64360200	-2.80991400	-3.10392500	C	-2.34430400	-2.60073700	3.27738200
C	0.32192400	-3.23935300	-3.10392500	C	-1.58034200	-2.60068600	4.51259800
C	-0.77172000	-2.37511000	-3.46536500	C	-0.25012100	-3.03290100	4.51259800
C	-2.49733800	0.00000000	-3.46536500	C	0.74947000	-2.30663200	5.27603200
C	-2.98132800	-1.30718300	-3.10392500	C	2.42533600	0.00000000	5.27603200
C	-2.16448600	-2.43146900	-3.10392500	C	2.80716900	-1.17509700	4.51259800
C	-2.91931100	-3.57653000	-2.48382700	C	1.98504600	-2.30665100	4.51259800
C	0.25954000	-4.60940200	-2.48382700	C	1.74901800	-3.03323800	3.27738200
C	2.49936600	3.88163800	-2.48382700	C	0.36790700	-3.48198800	3.27738200
C	0.25954000	4.60940200	-2.48382700	C	-0.36771900	-3.48249200	2.08750700
C	-2.91931100	3.57653000	-2.48382700	C	-1.74946700	-3.03353500	2.08750700
C	-4.30359900	-1.67122100	-2.48382700	C	-1.98487200	-2.30627000	0.85384300
C	-4.30359900	1.67122100	-2.48382700	C	-2.30627000	2.30627000	0.85384300
C	-2.98132800	1.30718300	-3.10392500	C	-0.36771900	3.48249200	2.08750700
C	-2.16448600	2.43146900	-3.10392500	C	0.36790700	3.48198800	3.27738200
C	0.32192400	3.23935300	-3.10392500	C	1.74901800	3.03323800	3.27738200
H	3.33140100	4.19917300	-3.13092600	C	2.34444800	2.60125600	2.08750700
H	-0.22694800	5.35535100	-3.13092600	C	2.34444800	2.60125600	2.08750700
H	-2.96419100	4.46596600	-3.13092600	C	3.19841500	1.42587100	2.08750700
H	-5.16337200	1.43905400	-3.13092600	C	2.96138700	0.69913300	0.85384300
H	-5.16337200	-1.43905400	-3.13092600	C	2.96138700	-0.69913300	0.85384300
H	-2.96419100	-4.46596600	-3.13092600	C	1.96019600	-1.42416600	0.09345500
H	-0.22694800	-5.35535100	-3.13092600	C	-0.74872800	-2.30434900	0.09345500
H	3.33140100	-4.19917300	-3.13092600	C	0.25020400	-3.03249000	0.85384300
H	5.02311000	-1.87073500	-3.13092600	C	1.58003400	-2.60040200	0.85384300
H	5.02311000	1.87073500	-3.13092600	C	2.34444800	-2.60125600	2.08750700
H	-2.46348800	3.87358500	-1.52245200	C	2.34444800	-2.60125600	2.08750700
H	-4.44525800	-1.14591300	-1.52245200	C	3.19841500	1.42587100	2.08750700
H	-0.28383300	-4.58179800	-1.52245200	C	2.96138700	0.69913300	0.85384300
H	4.26984000	-1.68579400	-1.52245200	C	2.96138700	-0.69913300	0.85384300
H	2.92273900	3.53992000	-1.52245200	C	1.96019600	-1.42416600	0.09345500
H	4.26984000	1.68579400	-1.52245200	C	-0.74872800	-2.30434900	0.09345500
H	2.92273900	-3.53992000	-1.52245200	C	0.25020400	-3.03249000	0.85384300
H	-2.46348800	-3.87358500	-1.52245200	C	1.58003400	-2.60040200	0.85384300
H	-4.44525800	-1.14591300	-1.52245200	C	2.34444800	-2.60125600	2.08750700
H	-0.28383300	4.58179800	-1.52245200	C	2.34444800	-2.60125600	2.08750700
C	-0.99943500	-0.72613200	6.01092900	C	3.19841500	-1.42587100	2.08750700

7...C₆₀(stagg.):

C	0.97668500	-0.70960300	-4.06085400	C	-0.99943500	0.72613200	6.01092900
C	0.97668500	0.70960300	-4.06085400	C	-1.96213800	1.42557700	5.27603200
C	2.02185500	1.46896300	-3.53151100	C	-2.96175200	0.69933900	4.51259800
C	3.18080300	0.69559800	-3.16969100	C	-2.96175200	-0.69933900	4.51259800
C	3.18080300	-0.69559800	-3.16969100	C	-1.96213800	-1.42557700	5.27603200
C	2.02185500	-1.46896300	-3.53151100	C	0.38175000	-1.17490700	6.01092900
C	-0.37306100	-1.14816200	-4.06085400	C	1.23537000	0.00000000	6.01092900
C	-1.20725000	0.00000000	-4.06085400	C	0.38175000	1.17490700	6.01092900
C	-0.37306100	1.14816200	-4.06085400	C	0.74947000	2.30663200	5.27603200
C	-0.77228000	2.37683300	-3.53151100	C	-1.58034200	2.60068600	4.51259800
C	1.64447500	2.81017200	-3.16969100	C	-3.19787800	1.42589400	3.27738200
C	4.45912800	1.17487500	-2.53418000	C	-3.42567800	0.72642800	2.08750700
C	4.45912800	-1.17487500	-2.53418000	C	-3.42567800	-0.72642800	2.08750700

C	0.38172100	-1.17481600	5.89247600	C	2.51863000	-3.86209000	-2.63046800
C	1.23527500	0.00000000	5.89247600	C	1.64619100	-2.81023300	-3.26559000
C	0.38172100	1.17481600	5.89247600	C	0.32001700	-3.24113300	-3.26559000
C	0.74956300	2.30691800	5.15824600	C	-0.77234700	-2.37704000	-3.63271000
C	-1.58051000	2.60101200	4.39501600	C	-2.49936800	0.00000000	-3.63271000
C	-3.19794900	1.42609100	3.15982100	C	-2.98361000	-1.30591900	-3.26559000
C	-3.42453900	0.72647300	1.96933100	C	-2.16398900	-2.43403000	-3.26559000
C	-3.42453900	-0.72647300	1.96933100	C	-2.89476600	-3.58881100	-2.63046800
C	-3.19794900	-1.42609100	3.15982100	C	0.23246500	-4.60491000	-2.63046800
C	-2.34451400	-2.60074400	3.15982100	C	2.51863000	3.86209000	-2.63046800
C	-1.58051000	-2.60101200	4.39501600	C	0.23246500	4.60491000	-2.63046800
C	-0.25017700	-3.03326300	4.39501600	C	-2.89476600	3.58881100	-2.63046800
C	0.74956300	-2.30691800	5.15824600	C	-4.30769400	-1.64408300	-2.63046800
C	2.42563700	0.00000000	5.15824600	C	-4.30769400	1.64408300	-2.63046800
C	2.80749600	-1.17526300	4.39501600	C	-2.98361000	1.30591900	-3.26559000
C	1.98530500	-2.30691100	4.39501600	C	-2.16398900	2.43403000	-3.26559000
C	1.74896000	-3.03344000	3.15982100	C	0.32001700	3.24113300	-3.26559000
C	0.36807300	-3.48211700	3.15982100	H	3.42356700	4.07232900	-3.22010500
C	-0.36732400	-3.48142300	1.96933100	H	-0.37606900	5.30690600	-3.22010500
C	-1.74915800	-3.03243700	1.96933100	H	-2.81507500	4.51442400	-3.22010500
C	-1.98442800	-2.30618200	0.73511000	H	-5.16337900	1.28226200	-3.22010500
C	-2.80653200	-1.17465400	0.73511000	H	-5.16337900	-1.28226200	-3.22010500
C	-2.34451400	2.60074400	3.15982100	H	-2.81507500	-4.51442400	-3.22010500
C	-0.38075900	1.17185500	-0.75381600	H	-0.37606900	-5.30690600	-3.22010500
C	-0.74903400	2.30528900	-0.02669100	H	3.42356700	-4.07232900	-3.22010500
C	0.24989600	3.03215800	0.73511000	H	4.93095600	-1.99758600	-3.22010500
C	1.58008800	2.59995300	0.73511000	H	4.93095600	1.99758600	-3.22010500
C	1.96099600	1.42474700	-0.02669100	H	-2.46000200	3.79794800	-1.63287500
C	0.99683900	-0.72424600	-0.75381600	H	-4.37224600	-1.16597100	-1.63287500
C	-0.38075900	-1.17185500	-0.75381600	H	-0.24219400	-4.51855800	-1.63287500
C	-1.23216100	0.00000000	-0.75381600	H	4.22256200	-1.62665200	-1.63287500
C	-2.42392500	0.00000000	-0.02669100	H	2.85188100	3.51323200	-1.63287500
C	-2.80653200	1.17465400	0.73511000	H	4.22256200	1.62665200	-1.63287500
C	-1.98442800	2.30618200	0.73511000	H	2.85188100	-3.51323200	-1.63287500
C	-0.36732400	3.48142300	1.96933100	H	-2.46000200	-3.79794800	-1.63287500
C	0.36807300	3.48211700	3.15982100	H	-4.37224600	1.16597100	-1.63287500
C	1.74896000	3.03344000	3.15982100	H	-0.24219400	4.51855800	-1.63287500
C	2.34350000	2.60062300	1.96933100	C	-0.38177500	-1.17498100	5.89348400
C	3.19752000	1.42516400	1.96933100	C	-1.23544900	0.00000000	5.89348400
C	2.96097600	0.69932300	0.73511000	C	-2.42513200	0.00000000	5.15829500
C	2.96097600	-0.69932300	0.73511000	C	-2.80718500	-1.17511200	4.39519100
C	1.96099600	-1.42474700	-0.02669100	C	-1.98506600	-2.30666200	4.39519100
C	-0.74903400	-2.30528900	-0.02669100	C	-0.74940700	-2.30643800	5.15829500
C	0.24989600	-3.03215800	0.73511000	C	0.99949900	-0.72617900	5.89348400
C	1.58008800	-2.59995300	0.73511000	C	0.99949900	0.72617900	5.89348400
C	2.34350000	-2.60062300	1.96933100	C	-0.38177500	1.17498100	5.89348400
C	3.19752000	-1.42516400	1.96933100	C	-0.74940700	2.30643800	5.15829500
C	3.42543100	-0.72597500	3.15982100	C	-2.80718500	1.17511200	4.39519100
C	3.42543100	0.72597500	3.15982100	C	-3.42556000	-0.72602700	3.15990000
C	2.80749600	1.17526300	4.39501600	C	-3.19893100	-1.42599800	1.96967200
C	1.98530500	2.30691100	4.39501600	C	-2.34472800	-2.60170600	1.96967200
C	-1.74915800	3.03243700	1.96933100	C	-1.74904900	-3.03354600	3.15990000
C	-0.25017700	3.03326300	4.39501600	C	-0.36806400	-3.48225600	3.15990000
C	0.99683900	0.72424600	-0.75381600	C	0.25013000	-3.03292100	4.39519100
N	-4.28801600	3.11542600	-2.47023800	C	1.58034700	-2.60070800	4.39519100
N	1.63787600	5.04086500	-2.47023800	C	1.96197300	-1.42545700	5.15829500
N	5.30027900	0.00000000	-2.47023800	C	1.96197300	1.42545700	5.15829500
N	1.63787600	-5.04086500	-2.47023800	C	2.96177400	0.69933700	4.39519100
N	-4.28801600	-3.11542600	-2.47023800	C	2.96177400	-0.69933700	4.39519100
H	-4.72590500	3.43357100	-1.61364300	C	3.19808400	-1.42612600	3.15990000
H	-4.72590500	-3.43357100	-1.61364300	C	2.34458800	-2.60086200	3.15990000
H	1.80513500	5.55563500	-1.61364300	C	1.74980900	-3.03394100	1.96967200
H	5.84154000	0.00000000	-1.61364300	C	0.36768100	-3.48302200	1.96967200
H	1.80513500	-5.55563500	-1.61364300	C	-0.24971100	-3.03327800	0.73553700

8...C₆₀(stagg.):

C	0.97682800	-0.70970700	-4.16139400	C	-1.58089600	2.60075000	0.73553700
C	0.97682800	0.70970700	-4.16139400	C	-0.24971100	3.03327800	0.73553700
C	2.02203100	1.46909200	-3.63271000	C	0.74809400	2.30239700	-0.02234200
C	3.18139100	0.69721100	-3.26559000	C	1.23177800	0.00000000	-0.75159400
C	3.18139100	-0.69721100	-3.26559000	C	0.38064000	-1.17149100	-0.75159400
C	2.02203100	-1.46909200	-3.63271000	C	-0.99653000	-0.72402100	-0.75159400
C	-0.37311500	-1.14833000	-4.16139400	C	-1.95853600	-1.42296000	-0.02234200
C	-1.20742600	0.00000000	-4.16139400	C	-2.96198400	-0.69984500	0.73553700
C	-0.37311500	1.14833000	-4.16139400	C	-2.96198400	0.69984500	0.73553700
C	-0.77234700	2.37704000	-3.63271000	C	-2.34472800	2.60170600	1.96967200
C	1.64619100	2.81023300	-3.26559000	C	-1.74904900	3.03354600	3.15990000
C	4.45136500	1.20190800	-2.63046800	C	-0.36806400	3.48225600	3.15990000
C	4.45136500	-1.20190800	-2.63046800	C	0.36768100	3.48302200	1.96967200

C	1.74980900	3.03394100	1.96967200	C	-0.99940400	0.72611000	5.88992600
C	1.98493700	2.30719700	0.73553700	C	-1.96210000	1.42554900	5.15515400
C	2.80765400	1.17482400	0.73553700	C	-2.96176300	0.69933300	4.39182600
C	2.42088300	0.00000000	-0.02234200	C	-2.96176300	-0.69933300	4.39182600
C	0.74809400	-2.30239700	-0.02234200	C	-1.96210000	-1.42554900	5.15515400
C	1.98493700	-2.30719700	0.73553700	C	0.38173800	-1.17487000	5.88992600
C	2.80765400	-1.17482400	0.73553700	C	1.23533100	0.00000000	5.88992600
C	3.42617000	-0.72662800	1.96967200	C	0.38173800	1.17487000	5.88992600
C	3.42617000	0.72662800	1.96967200	C	0.74945600	2.30658700	5.15515400
C	3.19808400	1.42612600	3.15990000	C	-1.58034100	2.60069900	4.39182600
C	2.34458800	2.60086200	3.15990000	C	-3.19817000	1.42599200	3.15668800
C	1.58034700	2.60070800	4.39519100	C	-3.42691700	0.72666200	1.96692100
C	0.25013000	3.03292100	4.39519100	C	-3.42691700	-0.72666200	1.96692100
C	-3.19893100	1.42599800	1.96967200	C	-3.19817000	-1.42599200	3.15668800
C	-1.98506600	2.30666200	4.39519100	C	-2.34448800	-2.60098500	3.15668800
C	0.38064000	1.17149100	-0.75159400	C	-1.58034100	-2.60069900	4.39182600
N	-4.29483400	3.12037900	-2.57113100	C	-0.25013000	-3.03291000	4.39182600
N	1.64048100	5.04888000	-2.57113100	C	0.74945600	-2.30658700	5.15515400
N	5.30870700	0.00000000	-2.57113100	C	2.42528900	0.00000000	5.15515400
N	1.64048100	-5.04888000	-2.57113100	C	2.80717500	-1.17510900	4.39182600
N	-4.29483400	-3.12037900	-2.57113100	C	1.98505900	-2.30665300	4.39182600
H	1.82188200	-5.60717600	-1.74467700	C	1.74919700	-3.03348900	3.15668800
H	-4.76974900	-3.46542500	-1.74467700	C	0.36791000	-3.48229600	3.15668800
H	5.89573400	0.00000000	-1.74467700	C	-0.36787900	-3.48374300	1.96692100
H	1.82188200	5.60717600	-1.74467700	C	-1.75007200	-3.03464100	1.96692100
H	-4.76974900	3.46542500	-1.74467700	C	-1.98630100	-2.30786200	0.73281500

9...C₆₀(eclip.):

C	0.97476000	-0.70820500	-4.03739300	C	-0.38049700	1.17105100	-0.75088600
C	0.97476000	0.70820500	-4.03739300	C	-0.74913600	2.30560300	-0.02608600
C	2.02032800	1.46785400	-3.52681500	C	0.25042400	3.03461800	0.73281500
C	3.20400900	0.69882000	-3.19135300	C	1.58110700	2.60225300	0.73281500
C	3.20400900	-0.69882000	-3.19135300	C	1.96126300	1.42494100	-0.02608600
C	2.02032800	-1.46785400	-3.52681500	C	0.99615500	-0.72374900	-0.75088600
C	-0.37232500	-1.14589900	-4.03739300	C	-0.38049700	-1.17105100	-0.75088600
C	-1.20487000	0.00000000	-4.03739300	C	-1.23131600	0.00000000	-0.75088600
C	-0.37232500	1.14589900	-4.03739300	C	-2.42425400	0.00000000	-0.02608600
C	-0.77169700	2.37503800	-3.52681500	C	-2.80870800	1.17591600	0.73281500
C	1.65471100	2.83124700	-3.19135300	C	-1.98630100	2.30786200	0.73281500
C	4.46757900	1.33830000	-2.66659400	C	-0.36787900	3.48374300	1.96692100
C	4.46757900	-1.33830000	-2.66659400	C	0.36791000	3.48229600	3.15668800
C	2.65335600	-3.83536300	-2.66659400	C	1.74919700	3.03348900	3.15668800
C	1.65471100	-2.83124700	-3.19135300	C	2.34531300	2.60217300	1.96692100
C	0.32547600	-3.26314100	-3.19135300	C	3.19955500	1.42641000	1.96692100
C	-0.77169700	-2.37503800	-3.52681500	C	2.96347900	0.69958100	0.73281500
C	-2.49726300	0.00000000	-3.52681500	C	2.96347900	-0.69958100	0.73281500
C	-3.00285400	-1.31791200	-3.19135300	C	1.96126300	-1.42494100	-0.02608600
C	-2.18134200	-2.44862700	-3.19135300	C	-0.74913600	-2.30560300	-0.02608600
C	-2.82771400	-3.70868400	-2.66659400	C	0.25042400	-3.03461800	0.73281500
C	0.10775900	-4.66247700	-2.66659400	C	1.58110700	-2.60225300	0.73281500
C	2.65335600	3.83536300	-2.66659400	C	2.34531300	-2.60217300	1.96692100
C	0.10775900	4.66247700	-2.66659400	C	3.19955500	-1.42641000	1.96692100
C	-2.82771400	3.70868400	-2.66659400	C	3.42555100	-0.72618500	3.15668800
C	-4.40098000	-1.54327000	-2.66659400	C	3.42555100	0.72618500	3.15668800
C	-4.40098000	1.54327000	-2.66659400	C	2.80717500	1.17510900	4.39182600
C	-3.00285400	1.31791200	-3.19135300	C	1.98505900	2.30665300	4.39182600
C	-2.18134200	2.44862700	-3.19135300	C	-1.75007200	3.03464100	1.96692100
C	0.32547600	3.26314100	-3.19135300	C	-0.25013000	3.03291000	4.39182600
H	3.50989700	3.95605200	-3.33886500	S	1.77209600	5.45395100	-2.52639500
H	-0.51425700	5.26357900	-3.33886500	S	-4.63940800	3.37072700	-2.52639500
H	-2.67781100	4.56059800	-3.33886500	S	-4.63940800	-3.37072700	-2.52639500
H	-5.16487600	1.13744800	-3.33886500	S	1.77209600	-5.45395100	-2.52639500
H	-5.16487600	-1.13744800	-3.33886500	S	5.73462300	0.00000000	-2.52639500
H	-2.67781100	-4.56059800	-3.33886500				
H	-0.51425700	-5.26357900	-3.33886500				
H	3.50989700	-3.95605200	-3.33886500				
H	4.84704700	-2.11562300	-3.33886500				
H	4.84704700	2.11562300	-3.33886500				
H	-2.41688600	3.97002300	-1.68259900				
H	-4.52257500	-1.07179100	-1.68259900				
H	-0.37821900	-4.63242600	-1.68259900				
H	4.28882300	-1.79120600	-1.68259900				
H	3.02885800	3.52540000	-1.68259900				
H	4.28882300	1.79120600	-1.68259900				
H	3.02885800	-3.52540000	-1.68259900				
H	-2.41688600	-3.97002300	-1.68259900				
H	-4.52257500	1.07179100	-1.68259900				
H	-0.37821900	4.63242600	-1.68259900				
C	-0.99940400	-0.72611000	5.88992600				

9...C₆₀(stagg.):

C	0.97413900	-0.70775300	-4.00246100				
C	0.97413900	0.70775300	-4.00246100				
C	2.02389800	1.47044800	-3.50664400				
C	3.20809500	0.69976900	-3.17779400				
C	3.20809500	-0.69976900	-3.17779400				
C	2.02389800	-1.47044800	-3.50664400				
C	-0.37208800	-1.14516900	-4.00246100				
C	-1.20410200	0.00000000	-4.00246100				
C	-0.37208800	1.14516900	-4.00246100				
C	-0.77306000	2.37923500	-3.50664400				
C	1.65687600	2.83483900	-3.17779400				
C	4.47171900	1.33850400	-2.65221400				
C	4.47171900	-1.33850400	-2.65221400				

C	-1.98798500	-2.31144400	0.64453500	C	-2.14597800	2.42916300	-3.21640600
C	-2.81263500	-1.17641100	0.64453500	C	0.30830700	3.22660900	-3.21640600
C	-2.34448900	2.60101100	3.07010400	H	-2.35543800	3.78603500	-1.70525300
C	-0.38103500	1.17270600	-0.84265600	H	-4.32860400	-1.07020500	-1.70525300
C	-0.75078000	2.31066200	-0.11664100	H	-0.31978600	-4.44745800	-1.70525300
C	0.24968100	3.03850600	0.64453500	H	4.13096500	-1.67847500	-1.70525300
C	1.58399300	2.60496100	0.64453500	H	2.87286300	3.41010400	-1.70525300
C	1.96556700	1.42806800	-0.11664100	H	4.13096500	1.67847500	-1.70525300
C	0.99756300	-0.72477200	-0.84265600	H	2.87286300	-3.41010400	-1.70525300
C	-0.38103500	-1.17270600	-0.84265600	H	-2.35543800	-3.78603500	-1.70525300
C	-1.23305600	0.00000000	-0.84265600	H	-4.32860400	1.07020500	-1.70525300
C	-2.42957400	0.00000000	-0.11664100	H	-0.31978600	4.44745800	-1.70525300
C	-2.81263500	1.17641100	0.64453500	C	-0.38172300	-1.17482400	5.80147100
C	-1.98798500	2.31144400	0.64453500	C	-1.23528300	0.00000000	5.80147100
C	-0.36708000	3.48347800	1.87800400	C	-2.42672300	0.00000000	5.06865800
C	0.36789600	3.48231800	3.07010400	C	-2.80973000	-1.17586200	4.30752600
C	1.74922100	3.03349800	3.07010400	C	-1.98656500	-2.30885100	4.30752600
C	2.34451100	2.60242900	1.87800400	C	-0.74989900	-2.30795100	5.06865800
C	3.19955100	1.42556700	1.87800400	C	0.99936500	-0.72608100	5.80147100
C	2.96694600	0.70148900	0.64453500	C	0.99936500	0.72608100	5.80147100
C	2.96694600	-0.70148900	0.64453500	C	-0.38172300	1.17482400	5.80147100
C	1.96556700	-1.42806800	-0.11664100	C	-0.74989900	2.30795100	5.06865800
C	-0.75078000	-2.31066200	-0.11664100	C	-2.80973000	-1.17586200	4.30752600
C	0.24968100	-3.03850600	0.64453500	C	-3.42686000	-0.72655000	3.07345000
C	1.58399300	-2.60496100	0.64453500	C	-3.20247500	-1.42737300	1.88205300
C	2.34451100	-2.60242900	1.87800400	C	-2.34713100	-2.60465200	1.88205300
C	3.19955100	-1.42556700	1.87800400	C	-1.74994900	-3.03462200	3.07345000
C	3.42556700	-0.72620600	3.07010400	C	-0.36796800	-3.48365400	3.07345000
C	3.42556700	0.72620600	3.07010400	C	0.25005700	-3.03557300	4.30752600
C	2.80952400	1.17573200	4.30432900	C	1.58196500	-2.60281000	4.30752600
C	1.98637800	2.30869500	4.30432900	C	1.96326000	-1.42639200	5.06865800
C	-1.75056400	3.03395700	1.87800400	C	1.96326000	1.42639200	5.06865800
C	-0.24999700	3.03533700	4.30432900	C	2.96427300	0.70022600	4.30752600
C	0.99756300	0.72477200	-0.84265600	C	2.96427300	-0.70022600	4.30752600
H	-4.52546300	3.28794200	-1.33666400	C	3.19944400	-1.42646600	3.07345000
H	-4.52546300	-3.28794200	-1.33666400	C	2.34533300	-2.60205000	3.07345000
H	1.72857300	5.32000100	-1.33666400	C	1.75186800	-3.03713600	1.88205300
H	5.59378000	0.00000000	-1.33666400	C	0.36789300	-3.48681700	1.88205300
H	1.72857300	-5.32000100	-1.33666400	C	-0.24918900	-3.04085200	0.64804300
C	1.60002800	-4.92437900	-2.35007400	C	-1.58577000	-2.60657000	0.64804300
C	-4.18892700	-3.04343300	-2.35007400	C	-3.42686000	0.72655000	3.07345000
C	-4.18892700	3.04343300	-2.35007400	C	-0.99779400	0.72494000	-0.83366200
C	5.17779800	0.00000000	-2.35007400	C	-1.96070100	1.42453200	-0.10473600
C	1.60002800	4.92437900	-2.35007400	C	-1.58577000	2.60657000	0.64804300
N	2.46998000	-3.75038600	-2.59193800	C	-0.24918900	3.04085200	0.64804300
N	0.20616600	-4.48594400	-2.59193800	C	0.74892100	2.30494200	-0.10473600
N	-2.80356300	-3.50802400	-2.59193800	C	1.23334100	0.00000000	-0.83366200
N	-4.20267800	-1.58230800	-2.59193800	C	0.38112300	-1.17297700	-0.83366200
N	-4.20267800	1.58230800	-2.59193800	C	-0.99779400	-0.72494000	-0.83366200
N	-2.80356300	3.50802400	-2.59193800	C	-1.96070100	-1.42453200	-0.10473600
N	0.20616600	4.48594400	-2.59193800	C	-2.96902500	-0.70268200	0.64804300
N	2.46998000	3.75038600	-2.59193800	C	-2.96902500	0.70268200	0.64804300
N	4.33009500	1.19015800	-2.59193800	C	-2.34713100	2.60465200	1.88205300
N	4.33009500	-1.19015800	-2.59193800	C	-1.74994900	3.03462200	3.07345000
H	1.85337400	5.70409800	-3.08140100	C	-0.36796800	3.48365400	3.07345000
H	5.99764400	0.00000000	-3.08140100	C	0.36789300	3.48681700	1.88205300
H	1.85337400	-5.70409800	-3.08140100	C	1.75186800	3.03713600	0.64804300
H	-4.85219600	-3.52532700	-3.08140100	C	1.98896600	2.31363100	0.64804300
H	-4.85219600	3.52532700	-3.08140100	C	2.81501800	1.17666700	0.64804300
10...C ₆₀ (stagg.):				C	2.42355900	0.00000000	-0.10473600
C	0.97841600	-0.71086100	-4.16789400	C	0.74892100	-2.30494200	-0.10473600
C	0.97841600	0.71086100	-4.16789400	C	1.98896600	-2.31363100	0.64804300
C	2.02607200	1.47202700	-3.62003500	C	2.81501800	-1.17666700	0.64804300
C	3.16395900	0.70386000	-3.21640600	C	3.42984500	-0.72759800	1.88205300
C	3.16395900	-0.70386000	-3.21640600	C	3.42984500	0.72759800	1.88205300
C	2.02607200	-1.47202700	-3.62003500	C	3.19944400	1.42646600	3.07345000
C	-0.37372200	-1.15019700	-4.16789400	C	2.34533300	2.60205000	3.07345000
C	-1.20938800	0.00000000	-4.16789400	C	1.58196500	2.60281000	4.30752600
C	-0.37372200	1.15019700	-4.16789400	C	0.25005700	3.03557300	4.30752600
C	-0.77389100	2.38179000	-3.62003500	C	-3.20247500	1.42737300	1.88205300
C	1.64712800	2.79159900	-3.21640600	C	-1.98656500	2.30885100	4.30752600
C	1.64712800	-2.79159900	-3.21640600	C	0.38112300	1.17297700	-0.83366200
C	0.30830700	-3.22660900	-3.21640600	H	1.75308500	-5.39544100	-1.40625500
C	-0.77389100	-2.38179000	-3.62003500	H	-4.58963600	-3.33456600	-1.40625500
C	-2.50436200	0.00000000	-3.62003500	H	5.67310300	0.00000000	-1.40625500
C	-2.97341500	-1.29029400	-3.21640600	H	1.75308500	5.39544100	-1.40625500
C	-2.14597800	-2.42916300	-3.21640600	H	-4.58963600	3.33456600	-1.40625500
C	-2.97341500	1.29029400	-3.21640600	C	-4.19856800	3.05043800	-2.38810300
				C	1.60371000	4.93571200	-2.38810300
				C	5.18971500	0.00000000	-2.38810300
				C	1.60371000	-4.93571200	-2.38810300

C	-4.19856800	-3.05043800	-2.38810300
N	-4.20189800	1.58247900	-2.57600400
N	-2.80348500	3.50723000	-2.57600400
N	0.20656800	4.48525600	-2.57600400
N	2.46925000	3.75006600	-2.57600400
N	4.32956500	1.18956200	-2.57600400
N	4.32956500	-1.18956200	-2.57600400
N	2.46925000	-3.75006600	-2.57600400
N	0.20656800	-4.48525600	-2.57600400
N	-2.80348500	-3.50723000	-2.57600400
N	-4.20189800	-1.58247900	-2.57600400
H	1.84025200	5.66371200	-3.17626300
H	5.95517900	0.00000000	-3.17626300
H	1.84025200	-5.66371200	-3.17626300
H	-4.81784100	-3.50036700	-3.17626300
H	-4.81784100	3.50036700	-3.17626300

1...C₇₀(eclip.):

C	0.99566800	0.72339500	1.98469800
C	0.99566800	-0.72339500	1.98469800
C	1.95436900	-1.41993300	1.24332000
C	2.93889900	-0.69691500	0.46913600
C	2.93889900	0.69691500	0.46913600
C	1.95436900	1.41993300	1.24332000
C	-0.38031100	1.17047800	1.98469800
C	-1.23071300	0.00000000	1.98469800
C	-0.38031100	-1.17047800	1.98469800
C	-0.74650300	-2.29749900	1.24332000
C	1.57097500	-2.57970100	0.46913600
C	3.17118500	-1.41506000	-0.76390400
C	3.48911800	-0.73541400	-1.97255000
C	3.48911800	0.73541400	-1.97255000
C	3.17118500	1.41506000	-0.76390400
C	2.32575200	2.57869900	-0.76390400
C	1.57097500	2.57970100	0.46913600
C	0.24536500	3.01041800	0.46913600
C	-0.74650300	2.29749900	1.24332000
C	-2.41573300	0.00000000	1.24332000
C	-2.78725600	1.16362600	0.46913600
C	-1.96798300	2.29125700	0.46913600
C	-1.73379200	3.00878400	-0.76390400
C	-0.36585200	3.45325400	-0.76390400
C	0.37877700	3.54560400	-1.97255000
C	1.77761700	3.09109300	-1.97255000
C	2.32575200	-2.57869900	-0.76390400
C	0.37877700	-3.54560400	-1.97255000
C	-0.36585200	-3.45325400	-0.76390400
C	-1.73379200	-3.00878400	-0.76390400
C	-2.39049100	-2.64581400	-1.97255000
C	-3.25502100	-1.45589000	-1.97255000
C	-2.39049100	2.64581400	-1.97255000
C	-3.25502100	1.45589000	-1.97255000
C	-3.39729400	0.71916800	-0.76390400
C	-3.39729400	-0.71916800	-0.76390400
C	-2.78725600	-1.16362600	0.46913600
C	-1.96798300	-2.29125700	0.46913600
C	1.77761700	-3.09109300	-1.97255000
C	0.24536500	-3.01041800	0.46913600
C	-3.39683400	0.71893000	-3.18132900
C	-3.39683400	-0.71893000	-3.18132900
C	-1.73342200	3.00841900	-3.18132900
C	-1.96809800	2.29104100	-4.41420200
C	-2.78708500	1.16380200	-4.41420200
C	-2.41776000	0.00000000	-5.19178300
C	-2.78708500	-1.16380200	-4.41420200
C	-1.96809800	-2.29104100	-4.41420200
C	-1.73342200	-3.00841900	-3.18132900
C	-0.36593600	-3.45274200	-3.18132900
C	0.24558500	-3.01031000	-4.41420200
C	-0.74712900	-2.29942700	-5.19178300
C	-0.38140200	-1.17383500	-5.93952300
C	-1.23424300	0.00000000	-5.93952300
C	-0.38140200	1.17383500	-5.93952300
C	-0.74712900	2.29942700	-5.19178300
C	2.32552000	2.57823500	-3.18132900
C	2.93886500	0.69667200	-4.41420200
C	1.95600900	1.42112400	-5.19178300
C	1.57073400	2.57974300	-4.41420200
C	0.24558500	3.01031000	-4.41420200

C	-0.36593600	3.45274200	-3.18132900
C	3.17067300	-1.41498200	-3.18132900
C	2.93886500	-0.69667200	-4.41420200
C	0.99852300	0.72547000	-5.93952300
C	0.99852300	-0.72547000	-5.93952300
C	1.95600900	-1.42112400	-5.19178300
C	1.57073400	-2.57974300	-4.41420200
C	2.32552000	-2.57823500	-3.18132900
C	3.17067300	1.41498200	-3.18132900
C	-0.37256200	1.14662700	5.43181800
C	-1.20563500	0.00000000	5.43181800
C	-0.37256200	-1.14662700	5.43181800
C	0.97538000	-0.70865500	5.43181800
C	0.97538000	0.70865500	5.43181800
C	-0.76824900	2.36442800	4.89213300
C	-2.48610700	0.00000000	4.89213300
C	-0.76824900	-2.36442800	4.89213300
C	2.01130300	-1.46129700	4.89213300
C	2.01130300	1.46129700	4.89213300
C	3.18363900	0.69589700	4.52331000
C	3.18363900	-0.69589700	4.52331000
C	1.64563600	-2.81277700	4.52331000
C	0.32196100	-3.24286500	4.52331000
C	-2.98465700	-1.30830400	4.52331000
C	-2.16658000	-2.43428900	4.52331000
C	-2.98465700	1.30830400	4.52331000
C	-2.16658000	2.43428900	4.52331000
C	0.32196100	3.24286500	4.52331000
C	1.64563600	2.81277700	4.52331000
H	4.05729500	1.21411600	4.13028300
H	4.05729500	-1.21411600	4.13028300
H	2.40846600	-3.48353400	4.13028300
H	0.09908000	-4.23389900	4.13028300
H	-3.99606000	-1.40257800	4.13028300
H	-2.56878100	-3.36705900	4.13028300
H	-3.99606000	1.40257800	4.13028300
H	-2.56878100	3.36705900	4.13028300
H	0.09908000	4.23389900	4.13028300
H	2.40846600	3.48353400	4.13028300

1...C₇₀ (stagg.):

C	0.99542200	0.72321600	1.96375600
C	0.99542200	-0.72321600	1.96375600
C	1.95426600	-1.41985700	1.22296000
C	2.93914400	-0.69704800	0.44909100
C	2.93914400	0.69704800	0.44909100
C	1.95426600	1.41985700	1.22296000
C	-0.38021700	1.17018900	1.96375600
C	-1.23040900	0.00000000	1.96375600
C	-0.38021700	-1.17018900	1.96375600
C	-0.74646300	-2.29737700	1.22296000
C	1.57117800	-2.57989200	0.44909100
C	3.17138500	-1.41525900	-0.78404700
C	3.48895300	-0.73542000	-1.99271500
C	3.48895300	0.73542000	-1.99271500
C	3.17138500	1.41525900	-0.78404700
C	2.32600300	2.57882800	-0.78404700
C	1.57117800	2.57989200	0.44909100
C	0.24531300	3.01069200	0.44909100
C	-0.74646300	2.29737700	1.22296000
C	-2.41560500	0.00000000	1.22296000
C	-2.78753200	1.16366200	0.44909100
C	-1.96810300	2.29151000	0.44909100
C	-1.73383700	3.00906200	-0.78404700
C	-0.36597900	3.45350600	-0.78404700
C	0.37872000	3.54544900	-1.99271500
C	1.77757200	3.09093400	-1.99271500
C	2.32600300	-2.57882800	-0.78404700
C	0.37872000	-3.54544900	-1.99271500
C	-0.36597900	-3.45350600	-0.78404700
C	-1.73383700	-3.00906200	-0.78404700
C	-2.39035300	-2.64572300	-1.99271500
C	-3.25489200	-1.45578800	-1.99271500
C	-2.39035300	2.64572300	-1.99271500
C	-3.25489200	1.45578800	-1.99271500
C	-3.39757300	0.71912500	-0.78404700
C	-3.39757300	-0.71912500	-0.78404700

C	-2.78753200	-1.16366200	0.44909100	C	-3.48837900	0.73523900	2.11626700
C	-1.96810300	-2.29151000	0.44909100	C	-3.17058500	1.41490300	0.90757500
C	1.77757200	-3.09093400	-1.99271500	C	-2.32541700	2.57817600	0.90757500
C	0.24531300	-3.01069200	0.44909100	C	-1.57024100	2.57809000	-0.32469100
C	-3.39634700	0.71883900	-3.20145600	C	-0.24501200	3.00868300	-0.32469100
C	-3.39634700	-0.71883900	-3.20145600	C	0.74632500	2.29695300	-1.10082200
C	-1.73318500	3.00798500	-3.20145600	C	2.41515900	0.00000000	-1.10082200
C	-1.96803000	2.29091600	-4.43464400	C	2.78571500	1.16275400	-0.32469100
C	-2.78694600	1.16377600	-4.43464400	C	1.96667800	2.29006100	-0.32469100
C	-2.41771800	0.00000000	-5.21229500	C	1.73339800	3.00830300	0.90757500
C	-2.78694600	-1.16377600	-4.43464400	C	0.36588800	3.45263400	0.90757500
C	-1.96803000	-2.29091600	-4.43464400	C	-0.37871500	3.54484700	2.11626700
C	-1.73318500	-3.00798500	-3.20145600	C	-1.77722300	3.09044400	2.11626700
C	-0.36587300	-3.45225100	-3.20145600	C	-2.32541700	-2.57817600	0.90757500
C	0.24560300	-3.01016900	-4.43464400	C	-0.37871500	-3.54484700	2.11626700
C	-0.74711600	-2.29938600	-5.21229500	C	0.36588800	-3.45263400	0.90757500
C	-0.38141500	-1.17387600	-5.95996700	C	1.73339800	-3.00830300	0.90757500
C	-1.23428600	0.00000000	-5.95996700	C	2.38999500	-2.64523900	2.11626700
C	-0.38141500	1.17387600	-5.95996700	C	3.25432100	-1.45559700	2.11626700
C	-0.74711600	2.29938600	-5.21229500	C	2.38999500	2.64523900	2.11626700
C	2.32517900	2.57787600	-3.20145600	C	3.25432100	1.45559700	2.11626700
C	2.93873700	0.69661100	-4.43464400	C	3.39671600	0.71894200	0.90757500
C	1.95597500	1.42109900	-5.21229500	C	3.39671600	-0.71894200	0.90757500
C	1.57063600	2.57964000	-4.43464400	C	2.78571500	-1.16275400	-0.32469100
C	0.24560300	3.01016900	-4.43464400	C	1.96667800	-2.29006100	-0.32469100
C	-0.36587300	3.45225100	-3.20145600	C	-1.77722300	-3.09044400	2.11626700
C	3.17022500	-1.41477000	-3.20145600	C	-0.24501200	-3.00868300	-0.32469100
C	2.93873700	-0.69661100	-4.43464400	C	3.39597800	0.71880100	3.32502400
C	0.99855800	0.72549500	-5.95996700	C	3.39597800	-0.71880100	3.32502400
C	0.99855800	-0.72549500	-5.95996700	C	1.73303500	3.00764600	3.32502400
C	1.95597500	-1.42109900	-5.21229500	C	1.96806800	2.29093100	4.55840300
C	1.57063600	-2.57964000	-4.43464400	C	2.78697100	1.16380700	4.55840300
C	2.32517900	-2.57787600	-3.20145600	C	2.41789500	0.00000000	5.33614000
C	3.17022500	1.41477000	-3.20145600	C	2.78697100	-1.16380700	4.55840300
C	-0.97397000	0.70763100	5.50632900	C	1.96806800	-2.29093100	4.55840300
C	-0.97397000	-0.70763100	5.50632900	C	1.73303500	-3.00764600	3.32502400
C	0.37202300	-1.14497000	5.50632900	C	0.36579500	-3.45188900	3.32502400
C	1.20389300	0.00000000	5.50632900	C	-0.24562500	-3.01020400	4.55840300
C	0.37202300	1.14497000	5.50632900	C	0.74717100	-2.29955500	5.33614000
C	-2.01574100	1.46452200	4.98606300	C	0.38142700	-1.17391100	6.08360200
C	-2.01574100	-1.46452200	4.98606300	C	1.23432300	0.00000000	6.08360200
C	0.76994500	-2.36964600	4.98606300	C	0.38142700	1.17391100	6.08360200
C	2.49159300	0.00000000	4.98606300	C	0.74717100	2.29955500	5.33614000
C	0.76994500	2.36964600	4.98606300	C	-2.32490400	2.57762800	3.32502400
C	2.17344300	2.44054300	4.63595900	C	-2.93877600	0.69660100	4.55840300
C	2.99272500	1.31289800	4.63595900	C	-1.95611800	1.42120300	5.33614000
C	2.99272500	-1.31289800	4.63595900	C	-1.57063900	2.57968100	4.55840300
C	2.17344300	-2.44054300	4.63595900	C	-0.24562500	3.01020400	4.55840300
C	-1.64946300	-2.82123700	4.63595900	C	0.36579500	3.45188900	3.32502400
C	-0.32383800	-3.25195900	4.63595900	C	-3.16990400	-1.41458400	3.32502400
C	-3.19286800	-0.69692300	4.63595900	C	-2.93877600	-0.69660100	4.55840300
C	-3.19286800	0.69692300	4.63595900	C	-0.99858800	0.72551700	6.08360200
C	-1.64946300	2.82123700	4.63595900	C	-0.99858800	-0.72551700	6.08360200
C	-0.32383800	3.25195900	4.63595900	C	-1.95611800	-1.42120300	5.33614000
H	2.58421300	3.37685600	4.26061800	C	-1.57063900	-2.57968100	4.55840300
H	4.01014700	1.41422700	4.26061800	C	-2.32490400	-2.57762800	3.32502400
H	4.01014700	-1.41422700	4.26061800	C	-3.16990400	1.41458400	3.32502400
H	2.58421300	-3.37685600	4.26061800	C	1.21580900	0.00000000	-5.19787500
H	-2.41301500	-3.50123900	4.26061800	C	0.37570600	1.15630300	-5.19787500
H	-0.10580600	-4.25089600	4.26061800	C	0.78863000	2.42715500	-4.71326400
H	-4.07553900	-1.21297200	4.26061800	C	2.18799900	2.41936900	-4.43835900
H	-4.07553900	1.21297200	4.26061800	C	2.97708600	1.33328400	-4.43835900
H	-2.41301500	3.50123900	4.26061800	C	2.55206100	0.00000000	-4.71326400
H	-0.10580600	4.25089600	4.26061800	C	0.37570600	-1.15630300	-5.19787500

2...C₇₀ (eclip.):

C	-0.99636000	0.72389800	-1.84554300	C	-2.97708600	-1.33328400	-4.43835900
C	-0.99636000	-0.72389800	-1.84554300	C	2.18799900	-2.41936900	-4.43835900
C	-1.95390500	-1.41959500	-1.10082200	C	0.78863000	-2.42715500	-4.71326400
C	-2.93714000	-0.69671400	-0.32469100	C	-2.06466100	-1.50006400	-4.71326400
C	-2.93714000	0.69671400	-0.32469100	C	-1.62482800	-2.82853700	-4.43835900
C	-1.95390500	1.41959500	-1.10082200	C	-0.34805800	-3.24338400	-4.43835900
C	0.38057600	1.17129200	-1.84554300	C	-3.19219800	-0.67123800	-4.43835900
C	1.23156900	0.00000000	-1.84554300	C	-3.19219800	0.67123800	-4.43835900
C	0.38057600	-1.17129200	-1.84554300	C	-1.62482800	2.82853700	-4.43835900
C	0.74632500	-2.29695300	-1.10082200	C	-1.34451900	4.13800400	-3.74391700
C	-1.57024100	-2.57809000	-0.32469100	C	-4.35095400	0.00000000	-3.74391700
C	-3.17058500	-1.41490300	0.90757500	C	-1.34451900	-4.13800400	-3.74391700
C	-3.48837900	-0.73523900	2.11626700	C	3.51999600	-2.55742700	-3.74391700

C	3.51999600	2.55742700	-3.74391700	C	-1.95543200	-1.42070400	5.37966900
H	-1.36197700	4.19173300	-2.64834600	C	-1.57028300	-2.57899400	4.60188800
H	3.56570100	2.59063400	-2.64834600	C	-2.32509600	-2.57780000	3.36877400
H	4.31570800	3.13554600	-4.22805500	C	-3.17012800	1.41471400	3.36877400
H	-1.64845400	5.07341900	-4.22805500	C	0.98304300	-0.71422300	-5.18541000
H	3.56570100	-2.59063400	-2.64834600	C	0.98304300	0.71422300	-5.18541000
H	4.31570800	-3.13554600	-4.22805500	C	2.06690900	1.50169700	-4.70945200
H	-1.64845400	-5.07341900	-4.22805500	C	3.19496900	0.67154300	-4.44108100
H	-1.36197700	-4.19173300	-2.64834600	C	3.19496900	-0.67154300	-4.44108100
H	-5.33450900	0.00000000	-4.22805500	C	2.06690900	-1.50169700	-4.70945200
H	-4.40744900	0.00000000	-2.64834600	C	-0.37548900	-1.15563700	-5.18541000

2...C₇₀ (stagg.):

C	-0.99632500	0.72387300	-1.80115100	C	-0.37548900	1.15563700	-5.18541000
C	-0.99632500	-0.72387300	-1.80115100	C	-0.37548900	1.15563700	-5.18541000
C	-1.95231700	-1.41844100	-1.05496800	C	-0.78948900	2.42979800	-4.70945200
C	-2.93788300	-0.69646200	-0.28088400	C	1.62597500	2.83107800	-4.44108100
C	-2.93788300	0.69646200	-0.28088400	C	1.62597500	-2.83107800	-4.44108100
C	-1.95231700	1.41844100	-1.05496800	C	0.34862400	-3.24611500	-4.44108100
C	0.38056200	1.17125000	-1.80115100	C	-0.78948900	-2.42979800	-4.70945200
C	1.23152600	0.00000000	-1.80115100	C	-2.55484000	0.00000000	-4.70945200
C	0.38056200	-1.17125000	-1.80115100	C	-2.97950800	-1.33466600	-4.44108100
C	0.74571900	-2.29508600	-1.05496800	C	-2.19006100	-2.42124600	-4.44108100
C	-1.57023000	-2.57887500	-0.28088400	C	-2.97950800	1.33466600	-4.44108100
C	-3.17084700	-1.41502300	0.95145000	C	-2.19006100	2.42124600	-4.44108100
C	-3.48907000	-0.73532300	2.16019800	C	0.34862400	3.24611500	-4.44108100
C	-3.48907000	0.73532300	2.16019800	C	1.35201500	4.16107400	-3.78690400
C	-3.17084700	1.41502300	0.95145000	C	-3.53962100	2.57168500	-3.78690400
C	-2.32561300	2.57838900	0.95145000	C	-3.53962100	-2.57168500	-3.78690400
C	-1.57023000	2.57887500	-0.28088400	C	1.35201500	-4.16107400	-3.78690400
C	-0.24548100	3.00931200	-0.28088400	C	4.37521200	0.00000000	-3.78690400
C	0.74571900	2.29508600	-1.05496800	H	1.37996600	4.24709800	-2.69254500
C	2.41319600	0.00000000	-1.05496800	H	4.46566300	0.00000000	-2.69254500
C	2.78616800	1.16339500	-0.28088400	H	5.34307800	0.00000000	-4.30191600
C	1.96742800	2.29029400	-0.28088400	H	1.65110200	5.08156900	-4.30191600
C	1.73354000	3.00855500	0.95145000	H	1.37996600	-4.24709800	-2.69254500
C	0.36592200	3.45292100	0.95145000	H	1.65110200	-5.08156900	-4.30191600
C	-0.37884900	3.54553000	2.16019800	H	-4.32264100	-3.14058200	-4.30191600
C	-1.77751500	3.09107500	2.16019800	H	-3.61279800	-2.62485100	-2.69254500
C	-2.32561300	-2.57838900	0.95145000	H	-4.32264100	3.14058200	-4.30191600
C	-0.37884900	-3.54553000	2.16019800	H	-3.61279800	2.62485100	-2.69254500
C	0.36592200	-3.45292100	0.95145000				
C	1.73354000	-3.00855500	0.95145000				
C	2.39050500	-2.64571200	2.16019800				
C	3.25492900	-1.45593500	2.16019800				
C	2.39050500	2.64571200	2.16019800				
C	3.25492900	1.45593500	2.16019800				
C	3.39699900	0.71899900	0.95145000				
C	3.39699900	-0.71899900	0.95145000				
C	2.78616800	-1.16339500	-0.28088400				
C	1.96742800	-2.29029400	-0.28088400				
C	-1.77751500	-3.09107500	2.16019800				
C	-0.24548100	-3.00931200	-0.28088400				
C	3.39623500	0.71882700	3.36877400				
C	3.39623500	-0.71882700	3.36877400				
C	1.73313900	3.00788200	3.36877400				
C	1.96752500	2.29038100	4.60188800				
C	2.78628000	1.16346100	4.60188800				
C	2.41704600	0.00000000	5.37966900				
C	2.78628000	-1.16346100	4.60188800				
C	1.96752500	-2.29038100	4.60188800				
C	1.73313900	-3.00788200	3.36877400				
C	0.36585000	-3.45214100	3.36877400				
C	-0.24550900	-3.00943900	4.60188800				
C	0.74690800	-2.29874800	5.37966900				
C	0.38142300	-1.17389800	6.12857500				
C	1.23430900	0.00000000	6.12857500				
C	0.38142300	1.17389800	6.12857500				
C	0.74690800	2.29874800	5.37966900				
C	-2.32509600	2.57780000	3.36877400				
C	-2.93801300	0.69647500	4.60188800				
C	-1.95543200	1.42070400	5.37966900				
C	-1.57028300	2.57899400	4.60188800				
C	-0.24550900	3.00943900	4.60188800				
C	0.36585000	3.45214100	3.36877400				
C	-3.17012800	-1.41471400	3.36877400				
C	-2.93801300	-0.69647500	4.60188800				
C	-0.99857700	0.72550900	6.12857500				
C	-0.99857700	-0.72550900	6.12857500				

3...C₇₀ (eclip.):

C	-0.99509000	0.72297500	-1.40618300	C	-0.99509000	-0.72297500	-1.40618300
C	-0.99509000	-0.72297500	-1.40618300	C	-1.95402700	-1.41968400	-0.66739600
C	-1.95402700	-1.41968400	-0.66739600	C	-2.93927800	-0.69715600	0.10557300
C	-2.93927800	-0.69715600	0.10557300	C	-2.93927800	0.69715600	0.10557300
C	-1.95402700	1.41968400	-0.66739600	C	-1.95402700	1.41968400	-0.66739600
C	0.38009100	1.16979800	-1.40618300	C	0.38009100	1.16979800	-1.40618300
C	1.22999900	0.00000000	-1.40618300	C	1.22999900	0.00000000	-1.40618300
C	0.38009100	-1.16979800	-1.40618300	C	0.38009100	-1.16979800	-1.40618300
C	0.74637200	-2.29709600	-0.66739600	C	0.74637200	-2.29709600	-0.66739600
C	-1.57132100	-2.57998700	0.10557300	C	-1.57132100	-2.57998700	0.10557300
C	-3.17161700	-1.41518000	1.33806000	C	-3.17161700	-1.41518000	1.33806000
C	-3.48915700	-0.73535100	2.54687900	C	-3.48915700	-0.73535100	2.54687900
C	-3.48915700	0.73535100	2.54687900	C	-3.17161700	1.41518000	1.33806000
C	-3.17161700	1.41518000	1.33806000	C	-2.32600000	2.57907200	1.33806000
C	-2.32600000	2.57907200	1.33806000	C	-1.57132100	2.57998700	0.10557300
C	-1.57132100	2.57998700	0.10557300	C	-0.24525300	3.01085300	0.10557300
C	-0.24525300	3.01085300	0.10557300	C	0.74637200	2.29709600	-0.66739600
C	0.74637200	2.29709600	-0.66739600	C	2.41531000	0.00000000	-0.66739600
C	2.41531000	0.00000000	-0.66739600	C	2.78770400	1.16365400	0.10557300
C	2.78770400	1.16365400	0.10557300	C	1.96814800	2.29167500	0.10557300
C	1.96814800	2.29167500	0.10557300	C	1.73407000	3.00913500	1.33806000
C	1.73407000	3.00913500	1.33806000	C	0.36583300	3.45370200	1.33806000
C	0.36583300	3.45370200	1.33806000	C	-0.37884800	3.54562100	2.54687900
C	-0.37884800	3.54562100	2.54687900	C	-1.77756900	3.09114900	2.54687900
C	-1.77756900	3.09114900	2.54687900	C	-2.32600000	-2.57907200	1.33806000
C	-2.32600000	-2.57907200	1.33806000	C	-0.37884800	-3.54562100	2.54687900
C	-0.37884800	-3.54562100	2.54687900	C	0.36583300	-3.45370200	1.33806000
C	0.36583300	-3.45370200	1.33806000	C	1.73407000	-3.00913500	1.33806000
C	1.73407000	-3.00913500	1.33806000	C	2.39055900	-2.64578700	2.54687900
C	2.39055900	-2.64578700	2.54687900	C	3.25501600	-1.45596300	2.54687900
C	3.25501600	-1.45596300	2.54687900	C	2.39055900	2.64578700	2.54687900
C	2.39055900	2.64578700	2.54687900	C	3.25501600	1.45596300	2.54687900
C	3.25501600	1.45596300	2.54687900	C	3.39771400	0.71932500	1.33806000
C	3.39771400	0.71932500	1.33806000	C	3.39771400	-0.71932500	1.33806000
C	3.39771400	-0.71932500	1.33806000	C	2.78770400	-1.16365400	0.10557300
C	2.78770400	-1.16365400	0.10557300	C	1.96814800	-2.29167500	0.10557300
C	1.96814800	-2.29167500	0.10557300				

C	0.98043700	0.71232900	-4.64548300	C	3.25496300	1.45600900	-2.39381900
C	0.98043700	-0.71232900	-4.64548300	C	3.39686800	0.71905000	-3.60250000
C	-0.37449400	-1.15257200	-4.64548300	C	3.39686800	-0.71905000	-3.60250000
C	-0.78605900	-2.41924000	-4.18719900	C	2.78742500	-1.16384400	-4.83561000
C	-3.00267500	-1.32034900	-3.86912400	C	1.96824300	-2.29135100	-4.83561000
C	-4.17125700	2.05188700	-3.22947100	C	-1.77750000	-3.09115500	-2.39381900
C	-3.24045000	3.33303300	-3.22947100	C	-0.24551900	-3.01064600	-4.83561000
C	0.32784900	3.26372400	-3.86912400	C	3.39643700	0.71936400	-1.18479900
C	1.65313300	2.83311300	-3.86912400	C	3.39643700	-0.71936400	-1.18479900
C	2.05792800	1.49517200	-4.18719900	C	1.73371200	3.00790700	-1.18479900
C	2.05792800	-1.49517200	-4.18719900	C	1.96700600	2.28996900	0.04687700
C	3.20529700	-0.69674300	-3.86912400	C	2.78572800	1.16309500	0.04687700
C	3.20529700	0.69674300	-3.86912400	C	2.41559400	0.00000000	0.82292000
C	2.16854900	4.11181500	-3.22947100	C	2.78572800	-1.16309500	0.04687700
C	0.66247100	4.60116900	-3.22947100	C	1.96700600	-2.28996900	0.04687700
C	-3.24045000	-3.33303300	-3.22947100	C	1.73371200	-3.00790700	-1.18479900
C	0.66247100	-4.60116900	-3.22947100	C	0.36540100	-3.45249900	-1.18479900
C	2.16854900	-4.11181500	-3.22947100	C	-0.24533100	-3.00880100	0.04687700
C	4.58068700	0.79179200	-3.22947100	C	0.74646000	-2.29736700	0.82292000
C	4.58068700	-0.79179200	-3.22947100	C	0.38061400	-1.17140800	1.56700400
C	1.65313300	-2.83311300	-3.86912400	C	1.23169100	0.00000000	1.56700400
C	0.32784900	-3.26372400	-3.86912400	C	0.38061400	1.17140800	1.56700400
C	-4.17125700	-2.05188700	-3.22947100	C	0.74646000	2.29736700	0.82292000
C	-2.18360500	-2.44770400	-3.86912400	C	-2.32494300	2.57835300	-1.18479900
H	2.59923000	3.98655400	-2.22696500	C	-2.93735100	0.69644700	0.04687700
H	0.24041700	4.75297900	-2.22696500	C	-1.95425700	1.41985100	0.82292000
H	2.85172100	4.71699000	-3.84054600	C	-1.57005200	2.57837300	0.04687700
H	0.46548600	5.49232400	-3.84054600	C	-0.24533100	3.00880100	0.04687700
H	5.36735400	1.25451800	-3.84054600	C	0.36540100	3.45249900	-1.18479900
H	4.59464500	1.24010100	-2.22696500	C	-3.17060600	-1.41439800	-1.18479900
H	5.36735400	-1.25451800	-3.84054600	C	-2.93735100	-0.69644700	0.04687700
H	4.59464500	-1.24010100	-2.22696500	C	-0.99645900	0.72397000	1.56700400
H	2.85172100	-4.71699000	-3.84054600	C	-0.99645900	-0.72397000	1.56700400
H	2.59923000	-3.98655400	-2.22696500	C	-1.95425700	-1.41985100	0.82292000
H	0.46548600	-5.49232400	-3.84054600	C	-1.57005200	-2.57837300	0.04687700
H	0.24041700	-4.75297900	-2.22696500	C	-2.32494300	-2.57835300	-1.18479900
H	-2.98823200	-3.70392700	-2.22696500	C	-3.17060600	1.41439800	-1.18479900
H	-3.60489300	-4.16977800	-3.84054600	C	-0.97491400	-0.70831600	4.98594100
H	-4.44605900	-1.69740100	-2.22696500	C	-0.97491400	0.70831600	4.98594100
H	-5.07966800	-2.13992500	-3.84054600	C	-2.05433700	1.49256300	4.45969300
H	-4.44605900	1.69740100	-2.22696500	C	-3.17891700	0.70229700	4.11985800
H	-5.07966800	2.13992500	-3.84054600	C	-3.17891700	-0.70229700	4.11985800
H	-2.98823200	3.70392700	-2.22696500	C	-2.05433700	-1.49256300	4.45969300
H	-3.60489300	4.16977800	-3.84054600	C	0.37238400	-1.14608000	4.98594100

4...C₇₀ (eclip.):

C	-0.99846600	0.72542800	-6.36069400	C	0.78468700	2.41501800	4.45969300
C	-0.99846600	-0.72542800	-6.36069400	C	-1.65026400	2.80630800	4.11985800
C	-1.95632900	-1.42135600	-5.61310200	C	-4.51874500	0.67467400	3.35151900
C	-2.93916400	-0.69683800	-4.83561000	C	-4.51874500	-0.67467400	3.35151900
C	-2.93916400	0.69683800	-4.83561000	C	-1.65026400	-2.80630800	4.11985800
C	-1.95632900	1.42135600	-5.61310200	C	-0.31441500	-3.24035200	4.11985800
C	0.38138000	1.17376700	-6.36069400	C	0.78468700	-2.41501800	4.45969300
C	1.23417200	0.00000000	-6.36069400	C	2.53930000	0.00000000	4.45969300
C	0.38138000	-1.17376700	-6.36069400	C	2.98459800	-1.30035000	4.11985800
C	0.74725100	-2.29980200	-5.61310200	C	2.15899800	-2.43669100	4.11985800
C	-1.57098400	-2.57997600	-4.83561000	C	-0.75471600	-4.50606700	3.35151900
C	-3.17077100	-1.41490500	-3.60250000	C	-2.03802200	-4.08909600	3.35151900
C	-3.48914100	-0.73528400	-2.39381900	C	-0.75471600	4.50606700	3.35151900
C	-3.48914100	0.73528400	-2.39381900	C	3.25917800	3.20187400	3.35151900
C	-3.17077100	1.41490500	-3.60250000	C	4.05230500	2.11022900	3.35151900
C	-2.32547700	2.57835300	-3.60250000	C	3.25917800	-3.20187400	3.35151900
C	-1.57098400	2.57997600	-4.83561000	C	4.05230500	-2.11022900	3.35151900
C	-0.24551900	3.01064600	-4.83561000	C	2.98459800	1.30035000	4.11985800
C	0.74725100	2.29980200	-5.61310200	C	2.15899800	2.43669100	4.11985800
C	2.41815500	0.00000000	-5.61310200	C	-2.03802200	4.08909600	3.35151900
C	2.78742500	1.16384400	-4.83561000	C	-0.31441500	3.24035200	4.11985800
C	1.96824300	2.29135100	-4.83561000	H	-0.23495100	5.36950700	2.94889200
C	1.73354700	3.00841500	-3.60250000	H	-2.96603800	4.48212300	2.94889200
C	0.36583300	3.45281200	-3.60250000	H	-5.17930900	1.43581700	2.94889200
C	-0.37890800	3.54558500	-2.39381900	H	-5.17930900	-1.43581700	2.94889200
C	-1.77750000	3.09115500	-2.39381900	H	-2.96603800	-4.48212300	2.94889200
C	-2.32547700	-2.57835300	-3.60250000	H	-0.23495100	-5.36950700	2.94889200
C	-0.37890800	-3.54558500	-2.39381900	H	3.34619700	-4.20592200	2.94889200
C	0.36583300	-3.45281200	-3.60250000	H	5.03410100	-1.88272100	2.94889200
C	1.73354700	-3.00841500	-3.60250000	H	5.03410100	1.88272100	2.94889200
C	2.39058500	-2.64572200	-2.39381900	H	3.34619700	4.20592200	2.94889200
C	3.25496300	-1.45600900	-2.39381900				
C	2.39058500	2.64572200	-2.39381900				

4...C₇₀ (stagg.):

C	1.73337600	-3.00824600	4.09975000	H	-4.28703200	1.60508200	-1.89048100
C	0.36587300	-3.45257500	4.09975000	H	-2.85128900	3.58121200	-1.89048100
C	-0.24553200	-3.01021000	5.33283700	H	2.52483800	3.81839300	-1.89048100
C	0.74711700	-2.29939000	6.11042200	H	4.41172500	-1.22131500	-1.89048100
C	0.38140500	-1.17384300	6.85820300	H	0.20175800	-4.57320700	-1.89048100
C	1.23425100	0.00000000	6.85820300	H	-4.28703200	-1.60508200	-1.89048100
C	0.38140500	1.17384300	6.85820300				
C	0.74711700	2.29939000	6.11042200				
C	-2.32537000	2.57813700	4.09975000				
C	-2.93875300	0.69669100	5.33283700	5...C ₇₀ (stagg.):			
C	-1.95597800	1.42110100	6.11042200	C	-0.99563800	0.72337400	-0.99463700
C	-1.57071700	2.57963100	5.33283700	C	-0.99563800	-0.72337400	-0.99463700
C	-0.24553200	3.01021000	5.33283700	C	-1.95207500	-1.41826500	-0.25130000
C	0.36587300	3.45257500	4.09975000	C	-2.93832800	-0.69710700	0.52093400
C	-3.17053300	-1.41487000	4.09975000	C	-2.93832800	0.69710700	0.52093400
C	-2.93875300	-0.69669100	5.33283700	C	-1.95207500	1.41826500	-0.25130000
C	-0.99853000	0.72547500	6.85820300	C	0.38030000	1.17044300	-0.99463700
C	-0.99853000	-0.72547500	6.85820300	C	1.23067600	0.00000000	-0.99463700
C	-1.95597800	-1.42110100	6.11042200	C	0.38030000	-1.17044300	-0.99463700
C	-1.57071700	-2.57963100	5.33283700	C	0.74562600	-2.29480100	-0.25130000
C	-2.32537000	-2.57813700	4.09975000	C	-1.57098100	-2.57909900	0.52093400
C	-3.17053300	1.41487000	4.09975000	C	-3.17159800	-1.41526300	1.75307000
C	0.37284000	1.14748400	-4.38161500	C	-3.48931600	-0.73537200	2.96183000
C	-0.97610800	0.70918400	-4.38161500	C	-3.48931600	0.73537200	2.96183000
C	-2.02179100	1.46891700	-3.85699400	C	-3.17159800	1.41526300	1.75307000
C	-1.65199900	2.82031800	-3.50589100	C	-2.32607300	2.57902800	1.75307000
C	-0.32124600	3.25270600	-3.50589100	C	-1.57098100	2.57909900	0.52093400
C	0.77225600	2.37675800	-3.85699400	C	-0.24500600	3.00993400	0.52093400
C	1.20653600	0.00000000	-4.38161500	C	0.74562600	2.29480100	-0.25130000
C	0.37284000	-1.14748400	-4.38161500	C	2.41289700	0.00000000	-0.25130000
C	-0.97610800	-0.70918400	-4.38161500	C	2.78690700	1.16313500	0.52093400
C	-2.02179100	-1.46891700	-3.85699400	C	1.96740900	2.29107700	0.52093400
C	-3.19277800	0.69961800	-3.50589100	C	1.73400600	3.00919000	1.75307000
C	-2.55568900	3.87730000	-2.90855100	C	0.36591800	3.45370900	1.75307000
C	-0.21142400	4.63899800	-2.90855100	C	-0.37887800	3.54577900	2.96183000
C	2.89778000	3.62875600	-2.90855100	C	-1.77763800	3.09129400	2.96183000
C	2.17178600	2.44267100	-3.50589100	C	-2.32607300	-2.57902800	1.75307000
C	2.99423700	1.31066500	-3.50589100	C	-0.37887800	-3.54577900	2.96183000
C	2.49907100	0.00000000	-3.85699400	C	0.36591800	-3.45370900	1.75307000
C	0.77225600	-2.37675800	-3.85699400	C	1.73400600	-3.00919000	1.75307000
C	2.17178600	-2.44267100	-3.50589100	C	2.39067500	-2.64589600	2.96183000
C	2.99423700	-1.31066500	-3.50589100	C	3.25515600	-1.45604000	2.96183000
C	4.34661600	-1.63460500	-2.90855100	C	2.39067500	2.64589600	2.96183000
C	4.34661600	1.63460500	-2.90855100	C	3.25515600	1.45604000	2.96183000
C	-4.47728300	1.23245300	-2.90855100	C	3.39774700	0.71924700	1.75307000
C	-4.47728300	-1.23245300	-2.90855100	C	3.39774700	-0.71924700	1.75307000
C	-2.55568900	-3.87730000	-2.90855100	C	2.78690700	-1.16313500	0.52093400
C	2.89778000	-3.62875600	-2.90855100	C	1.96740900	-2.29107700	0.52093400
C	-0.21142400	-4.63899800	-2.90855100	C	-1.77763800	-3.09129400	2.96183000
C	-0.32124600	-3.25270600	-3.50589100	C	-0.24500600	-3.00993400	0.52093400
C	-1.65199900	-2.82031800	-3.50589100	C	3.39641900	0.71887100	4.17048900
C	-3.19277800	-0.69961800	-3.50589100	C	3.39641900	-0.71887100	4.17048900
C	-5.41716400	0.00000000	-2.89153800	C	1.73323800	3.00804300	4.17048900
C	-1.67399600	-5.15202900	-2.89153800	C	1.96789500	2.29085000	5.40370600
C	4.38257800	-3.18412900	-2.89153800	C	2.78684000	1.16366800	5.40370600
C	4.38257800	3.18412900	-2.89153800	C	2.41761100	0.00000000	6.18145900
C	-1.67399600	5.15202900	-2.89153800	C	2.78684000	-1.16366800	5.40370600
H	-4.89470800	2.07114800	-3.47918900	C	1.96789500	-2.29085000	5.40370600
H	-4.89470800	-2.07114800	-3.47918900	C	1.73323800	-3.00804300	4.17048900
H	-3.48232700	-4.01512400	-3.47918900	C	0.36586400	-3.45233000	4.17048900
H	0.45723100	-5.29516400	-3.47918900	C	-0.24553300	-3.01003600	5.40370600
H	2.74251100	-4.55263100	-3.47918900	C	0.74708300	-2.29928500	6.18145900
H	5.17729200	-1.20144300	-3.47918900	C	0.38142800	-1.17391300	6.92973300
H	5.17729200	1.20144300	-3.47918900	C	1.23432500	0.00000000	6.92973300
H	2.74251100	4.55263100	-3.47918900	C	0.38142800	1.17391300	6.92973300
H	0.45723100	5.29516400	-3.47918900	C	0.74708300	2.29928500	6.18145900
H	-3.48232700	4.01512400	-3.47918900	C	-2.32521900	2.57794400	4.17048900
H	-6.09515000	0.00000000	-2.03042000	C	-2.93858800	0.69663700	5.40370600
H	-6.02927300	0.00000000	-3.80210300	C	-1.95588900	1.42103600	6.18145900
H	-1.86314800	-5.73417900	-3.80210300	C	-1.57061500	2.57949000	5.40370600
H	-1.88350500	-5.79683200	-2.03042000	C	-0.24553300	3.01003600	5.40370600
H	4.87778400	-3.54391800	-3.80210300	C	0.36586400	3.45233000	4.17048900
H	4.93108000	-3.58263900	-2.03042000	C	-3.17030300	-1.41478600	4.17048900
H	4.93108000	3.58263900	-2.03042000	C	-2.93858800	-0.69663700	5.40370600
H	4.87778400	3.54391800	-3.80210300	C	-0.99859000	0.72551800	6.92973300
H	-1.88350500	5.79683200	-2.03042000	C	-0.99859000	-0.72551800	6.92973300
H	-1.86314800	5.73417900	-3.80210300	C	-1.95588900	-1.42103600	6.18145900
H	-2.85128900	-3.58121200	-1.89048100	C	-1.57061500	-2.57949000	5.40370600
H	2.52483800	-3.81839300	-1.89048100	C	-2.32521900	-2.57794400	4.17048900
H	4.41172500	1.22131500	-1.89048100	C	-3.17030300	1.41478600	4.17048900
H	0.20175800	4.57320700	-1.89048100	C	0.97647200	0.70944900	-4.39139100

C	-0.37297900	1.14791200	-4.39139100	C	-3.17209100	-1.41518900	1.51013400
C	-0.77211800	2.37633600	-3.86298400	C	-3.48921200	-0.73545700	2.71931400
C	0.31944700	3.24873100	-3.50301300	C	-3.48921200	0.73545700	2.71931400
C	1.65111800	2.81604400	-3.50301300	C	-3.17209100	1.41518900	1.51013400
C	2.02143200	1.46865600	-3.86298400	C	-2.32615400	2.57952000	1.51013400
C	0.97647200	-0.70944900	-4.39139100	C	-1.57236100	2.58183400	0.27659700
C	-0.37297900	-1.14791200	-4.39139100	C	-0.24549700	3.01295900	0.27659700
C	-1.20698600	0.00000000	-4.39139100	C	0.74723900	2.29976400	-0.49497700
C	-2.49862700	0.00000000	-3.86298400	C	2.41811500	0.00000000	-0.49497700
C	-2.16799400	2.44051200	-3.50301300	C	2.78963100	1.16453700	0.27659700
C	0.20962600	4.62312400	-2.87939400	C	1.96958400	2.29323500	0.27659700
C	2.54781400	3.86340100	-2.87939400	C	1.73444800	3.00942000	1.51013400
C	4.46163100	1.22925800	-2.87939400	C	0.36569500	3.45415500	1.51013400
C	3.18844100	0.70010100	-3.50301300	C	-0.37876500	3.54570700	2.71931400
C	3.18844100	-0.70010100	-3.50301300	C	-1.77768700	3.09117000	2.71931400
C	2.02143200	-1.46865600	-3.86298400	C	-2.32615400	-2.57952000	1.51013400
C	-0.77211800	-2.37633600	-3.86298400	C	-0.37876500	-3.54570700	2.71931400
C	0.31944700	-3.24873100	-3.50301300	C	0.36569500	-3.45415500	1.51013400
C	1.65111800	-2.81604400	-3.50301300	C	1.73444800	-3.00942000	1.51013400
C	2.54781400	-3.86340100	-2.87939400	C	2.39054200	-2.64590400	2.71931400
C	4.46163100	-1.22925800	-2.87939400	C	3.25512300	-1.45591100	2.71931400
C	-2.88699500	3.61697100	-2.87939400	C	2.39054200	2.64590400	2.71931400
C	-4.33207500	1.62799000	-2.87939400	C	3.25512300	1.45591100	2.71931400
C	-4.33207500	-1.62799000	-2.87939400	C	3.39810200	0.71959600	1.51013400
C	0.20962600	-4.62312400	-2.87939400	C	3.39810200	-0.71959600	1.51013400
C	-2.88699500	-3.61697100	-2.87939400	C	2.78963100	-1.16453700	0.27659700
C	-2.16799400	-2.44051200	-3.50301300	C	1.96958400	-2.29323500	0.27659700
C	-2.99101200	-1.30772500	-3.50301300	C	-1.77768700	-3.09117000	2.71931400
C	-2.99101200	1.30772500	-3.50301300	C	-0.24549700	-3.01295900	0.27659700
C	-4.37164600	3.17618700	-2.86512000	C	3.39678200	0.71891800	3.92818300
C	-4.37164600	-3.17618700	-2.86512000	C	3.39678200	-0.71891800	3.92818300
C	1.66982000	-5.13917800	-2.86512000	C	1.73339600	3.00837400	3.92818300
C	5.40365200	0.00000000	-2.86512000	C	1.96805200	2.29104400	5.16136300
C	1.66982000	5.13917800	-2.86512000	C	2.78707300	1.16375700	5.16136300
H	-2.72949400	4.55333500	-3.42823400	C	2.41773600	0.00000000	5.93908200
H	-5.17393900	1.18884500	-3.42823400	C	2.78707300	-1.16375700	5.16136300
H	-5.17393900	-1.18884500	-3.42823400	C	1.96805200	-2.29104400	5.16136300
H	-2.72949400	-4.55333500	-3.42823400	C	1.73339600	-3.00837400	3.92818300
H	-0.46817700	-5.28808100	-3.42823400	C	0.36593100	-3.45269000	3.92818300
H	3.48701900	-4.00296100	-3.42823400	C	-0.24554600	-3.01028500	5.16136300
H	4.88459000	-2.07936900	-3.42823400	C	0.74712200	-2.29940400	5.93908200
H	4.88459000	2.07936900	-3.42823400	C	0.38141500	-1.17387400	6.68722200
H	3.48701900	4.00296100	-3.42823400	C	1.23428500	0.00000000	6.68722200
H	-0.46817700	5.28808100	-3.42823400	C	0.38141500	1.17387400	6.68722200
H	-4.92231100	3.57626900	-2.00595800	C	0.74712200	2.29940400	5.93908200
H	-4.86384400	3.53379000	-3.77831400	C	-2.32548500	2.57819600	3.92818300
H	-4.86384400	-3.53379000	-3.77831400	C	-2.93882900	0.69670100	5.16136300
H	-4.92231100	-3.57626900	-2.00595800	C	-1.95599000	1.42111000	5.93908200
H	1.85782300	-5.71779200	-3.77831400	C	-1.57075100	2.57970000	5.16136300
H	1.88015600	-5.78652400	-2.00595800	C	-0.24554600	3.01028500	5.16136300
H	6.08431200	0.00000000	-2.00595800	C	0.36593100	3.45269000	3.92818300
H	6.01204200	0.00000000	-3.77831400	C	-3.17062400	-1.41496100	3.92818300
H	1.88015600	5.78652400	-2.00595800	C	-2.93882900	-0.69670100	5.16136300
H	1.85782300	5.71779200	-3.77831400	C	-0.99855700	0.72549400	6.68722200
H	-4.37168700	-1.22128700	-1.85662100	C	-0.99855700	-0.72549400	6.68722200
H	-0.18941300	-4.53511900	-1.85662100	C	-1.95599000	-1.42111000	5.93908200
H	4.25462300	-1.58157100	-1.85662100	C	-1.57075100	-2.57970000	5.16136300
H	2.81891400	3.55765500	-1.85662100	C	-2.32548500	-2.57819600	3.92818300
H	-2.51243800	3.78032300	-1.85662100	C	-3.17062400	1.41496100	3.92818300
H	-0.18941300	4.53511900	-1.85662100	C	-0.99107500	0.72005800	-4.34185500
H	4.25462300	1.58157100	-1.85662100	C	-0.99107500	-0.72005800	-4.34185500
H	2.81891400	-3.55765500	-1.85662100	C	-2.05950700	-1.49631900	-3.95470200
H	-2.51243800	-3.78032300	-1.85662100	C	-3.28061900	-0.75733300	-3.66745500
H	-4.37168700	1.22128700	-1.85662100	C	-3.28061900	0.75733300	-3.66745500
				C	-2.05950700	1.49631900	-3.95470200
				C	0.37855700	1.16507800	-4.34185500
				C	1.22503600	0.00000000	-4.34185500
				C	0.37855700	-1.16507800	-4.34185500
				C	0.78666200	-2.42109500	-3.95470200
				C	-1.73403400	-2.88602600	-3.66745500
				C	-4.51349500	-1.18441800	-3.27440100
				C	-4.51349500	1.18441800	-3.27440100
				C	-2.52119500	3.92658400	-3.27440100
				C	-1.73403400	2.88602600	-3.66745500
				C	-0.29350100	3.35408300	-3.66745500
				C	0.78666200	2.42109500	-3.95470200
				C	2.54569000	0.00000000	-3.95470200
				C	3.09922600	1.31560400	-3.66745500
				C	2.20892800	2.54099500	-3.66745500
				C	2.95531100	3.61118000	-3.27440100
				C	-0.26829900	4.65859400	-3.27440100
6...C ₇₀ (eclip.):							
C	-0.99587300	0.72354400	-1.22942000				
C	-0.99587300	-0.72354400	-1.22942000				
C	-1.95629600	-1.42133200	-0.49497700				
C	-2.94135700	-0.69757400	0.27659700				
C	-2.94135700	0.69757400	0.27659700				
C	-1.95629600	1.42133200	-0.49497700				
C	0.38039000	1.17071900	-1.22942000				
C	1.23096700	0.00000000	-1.22942000				
C	0.38039000	-1.17071900	-1.22942000				
C	0.74723900	-2.29976400	-0.49497700				
C	-1.57236100	-2.58183400	0.27659700				

C	-2.52119500	-3.92658400	-3.27440100	C	2.78698800	1.16373300	5.21165700
C	-0.26829900	-4.65859400	-3.27440100	C	2.41786200	0.00000000	5.98949100
C	2.95531100	-3.61118000	-3.27440100	C	2.78698800	-1.16373300	5.21165700
C	4.34767800	1.69475200	-3.27440100	C	1.96800200	-2.29097000	5.21165700
C	4.34767800	-1.69475200	-3.27440100	C	1.73309400	-3.00773100	3.97832100
C	3.09922600	-1.31560400	-3.66745500	C	0.36579700	-3.45199200	3.97832100
C	2.20892800	-2.54099500	-3.66745500	C	-0.24554900	-3.01019700	5.21165700
C	-0.29350100	-3.35408300	-3.66745500	C	0.74716100	-2.29952400	5.98949100
C	-1.66488700	-5.12399600	-2.99106900	C	0.38142800	-1.17391500	6.73746000
C	4.35873100	-3.16680400	-2.99106900	C	1.23432800	0.00000000	6.73746000
C	4.35873100	3.16680400	-2.99106900	C	0.38142800	1.17391500	6.73746000
C	-1.66488700	5.12399600	-2.99106900	C	0.74716100	2.29952400	5.98949100
C	-5.38768800	0.00000000	-2.99106900	C	-2.32496600	2.57771000	3.97832100
H	-3.59817700	-3.92213300	-3.16515800	C	-2.93874600	0.69667100	5.21165700
H	0.60561500	-5.28802800	-3.16515800	C	-1.95609200	1.42118400	5.98949100
H	2.61827200	-4.63407600	-3.16515800	C	-1.57069600	2.57963000	5.21165700
H	5.21635800	-1.05811700	-3.16515800	C	-0.24554900	3.01019700	5.21165700
H	5.21635800	1.05811700	-3.16515800	C	0.36579700	3.45199200	3.97832100
H	2.61827200	4.63407600	-3.16515800	C	-3.17000200	-1.41461800	3.97832100
H	0.60561500	5.28802800	-3.16515800	C	-2.93874600	-0.69667100	5.21165700
H	-3.59817700	3.92213300	-3.16515800	C	-0.99859200	0.72552000	6.73746000
H	-4.84206800	2.21006400	-3.16515800	C	-0.99859200	-0.72552000	6.73746000
H	-4.84206800	-2.21006400	-3.16515800	C	-1.95609200	-1.42118400	5.98949100
H	-1.77124400	-5.45132900	-1.94139300	C	-1.57069600	-2.57963000	5.21165700
H	-1.94847900	-5.99680000	-3.60448700	C	-2.32496600	-2.57771000	3.97832100
H	5.10118300	-3.70622600	-3.60448700	C	-3.17000200	1.41461800	3.97832100
H	4.63717800	-3.36910700	-1.94139300	C	-0.37839600	1.16458400	-4.34449800
H	5.10118300	3.70622600	-3.60448700	C	-1.22451600	0.00000000	-4.34449800
H	4.63717800	3.36910700	-1.94139300	C	-2.54875400	0.00000000	-3.97671600
H	-1.77124400	5.45132900	-1.94139300	C	-3.10480200	1.31850100	-3.70528000
H	-1.94847900	5.99680000	-3.60448700	C	-2.21340600	2.54540300	-3.70528000
H	-5.73186700	0.00000000	-1.94139300	C	-0.78760800	2.42400900	-3.97671600
H	-6.30540900	0.00000000	-3.60448700	C	0.99065500	0.71975300	-4.34449800

6...C₇₀ (stagg.):

C	-0.99458200	0.72260600	-1.17410900	C	-0.37839600	-1.16458400	-4.34449800
C	-0.99458200	-0.72260600	-1.17410900	C	-0.78760800	-2.42400900	-3.97671600
C	-1.95764800	-1.42231400	-0.44565500	C	-3.10480200	-1.31850100	-3.70528000
C	-2.94192500	-0.69736600	0.32731900	C	-4.35839900	1.70209300	-3.33403000
C	-2.94192500	0.69736600	0.32731900	C	-2.96560600	3.61910800	-3.33403000
C	-1.95764800	1.42231400	-0.44565500	C	0.27196700	4.67106000	-3.33403000
C	0.37989700	1.16920100	-1.17410900	C	0.29453300	3.36028100	-3.70528000
C	1.22937100	0.00000000	-1.17410900	C	1.73684200	2.89164700	-3.70528000
C	0.37989700	-1.16920100	-1.17410900	C	2.06198500	1.49812000	-3.97671600
C	0.74775500	-2.30135300	-0.44565500	C	2.06198500	-1.49812000	-3.97671600
C	-1.57233900	-2.58243900	0.32731900	C	3.28683300	-0.75826700	-3.70528000
C	-3.17216700	-1.41509100	1.56031700	C	3.28683300	0.75826700	-3.70528000
C	-3.48877700	-0.73530500	2.76952200	C	4.52648400	1.18478100	-3.33403000
C	-3.48877700	0.73530500	2.76952200	C	2.52555400	3.93882500	-3.33403000
C	-3.17216700	1.41509100	1.56031700	C	-4.35839900	-1.70209300	-3.33403000
C	-2.32608500	2.57962300	1.56031700	C	-2.96560600	-3.61910800	-3.33403000
C	-1.57233900	2.58243900	0.32731900	C	0.27196700	-4.67106000	-3.33403000
C	-0.24587000	3.01343500	0.32731900	C	4.52648400	-1.18478100	-3.33403000
C	0.74775500	2.30135300	-0.44565500	C	2.52555400	-3.93882500	-3.33403000
C	2.41978600	0.00000000	-0.44565500	C	1.73684200	-2.89164700	-3.70528000
C	2.78996900	1.16503900	0.32731900	C	0.29453300	-3.36028100	-3.70528000
C	1.97016600	2.29340100	0.32731900	C	-2.21340600	-2.54540300	-3.70528000
C	1.73456800	3.00938600	1.56031700	C	-4.37273400	-3.17697700	-3.06409200
C	0.36557800	3.45419700	1.56031700	C	1.67023600	-5.14045700	-3.06409200
C	-0.37877400	3.54524600	2.76952200	C	5.40499600	0.00000000	-3.06409200
C	-1.77740800	3.09080200	2.76952200	C	1.67023600	5.14045700	-3.06409200
C	-2.32608500	-2.57962300	1.56031700	C	-4.37273400	3.17697700	-3.06409200
C	-0.37877400	-3.54524600	2.76952200	H	-5.22809500	-1.06551400	-3.23039100
C	0.36557800	-3.45419700	1.56031700	H	-2.62893500	-4.64295100	-3.23039100
C	1.73456800	-3.00938600	1.56031700	H	-0.60220600	-5.30147600	-3.23039100
C	2.39027800	-2.64552600	2.76952200	H	3.60332400	-3.93501600	-3.23039100
C	3.25468100	-1.45577700	2.76952200	H	4.85591100	-2.21097800	-3.23039100
C	2.39027800	2.64552600	2.76952200	H	4.85591100	2.21097800	-3.23039100
C	3.25468100	1.45577700	2.76952200	H	3.60332400	3.93501600	-3.23039100
C	3.39810700	0.71972000	1.56031700	H	-0.60220600	5.30147600	-3.23039100
C	3.39810700	-0.71972000	1.56031700	H	-2.62893500	4.64295100	-3.23039100
C	2.78996900	-1.16503900	0.32731900	H	-5.22809500	1.06551400	-3.23039100
C	1.97016600	-2.29340100	0.32731900	H	-4.66429700	-3.38881000	-2.01943300
C	-1.77740800	-3.09080200	2.76952200	H	-5.10819800	-3.71132300	-3.69035200
C	-0.24587000	-3.01343500	0.32731900	H	1.95115800	-6.00504700	-3.69035200
C	3.39607700	0.71883100	3.97832100	H	1.78160300	-5.48321000	-2.01943300
C	3.39607700	-0.71883100	3.97832100	H	6.31408000	0.00000000	-3.69035200
C	1.73309400	3.00773100	3.97832100	H	5.76538800	0.00000000	-2.01943300
C	1.96800200	2.29097000	5.21165700	H	1.78160300	5.48321000	-2.01943300
				H	1.95115800	6.00504700	-3.69035200
				H	-4.66429700	3.38881000	-2.01943300
				H	-5.10819800	3.71132300	-3.69035200

7...C₇₀ (eclip.):

C	-0.99566300	0.72339200	-1.28116000
C	-0.99566300	-0.72339200	-1.28116000
C	-1.95435700	-1.41992300	-0.53996000
C	-2.93815000	-0.69647800	0.23513500
C	-2.93815000	0.69647800	0.23513500
C	-1.95435700	1.41992300	-0.53996000
C	0.38030900	1.17047200	-1.28116000
C	1.23070700	0.00000000	-1.28116000
C	0.38030900	-1.17047200	-1.28116000
C	0.74649800	-2.29748400	-0.53996000
C	-1.57032800	-2.57912300	0.23513500
C	-3.17118800	-1.41509200	1.46652500
C	-3.48909500	-0.73524800	2.67522300
C	-3.48909500	0.73524800	2.67522300
C	-3.17118800	1.41509200	1.46652500
C	-2.32578400	2.57869100	1.46652500
C	-1.57032800	2.57912300	0.23513500
C	-0.24554900	3.00957000	0.23513500
C	0.74649800	2.29748400	-0.53996000
C	2.41571700	0.00000000	-0.53996000
C	2.78639200	1.16353900	0.23513500
C	1.96763400	2.29046300	0.23513500
C	1.73377400	3.00881100	1.46652500
C	0.36588200	3.45326600	1.46652500
C	-0.37892800	3.54553000	2.67522300
C	-1.77745200	3.09112200	2.67522300
C	-2.32578400	-2.57869100	1.46652500
C	-0.37892800	-3.54553000	2.67522300
C	0.36588200	-3.45326600	1.46652500
C	1.73377400	-3.00881100	1.46652500
C	2.39056900	-2.64566600	2.67522300
C	3.25490500	-1.45601100	2.67522300
C	2.39056900	2.64566600	2.67522300
C	3.25490500	1.45601100	2.67522300
C	3.39731500	0.71914400	1.46652500
C	3.39731500	-0.71914400	1.46652500
C	2.78639200	-1.16353900	0.23513500
C	1.96763400	-2.29046300	0.23513500
C	-1.77745200	-3.09112200	2.67522300
C	-0.24554900	-3.00957000	0.23513500
C	3.39622400	0.71887700	3.88367500
C	3.39622400	-0.71887700	3.88367500
C	1.73318400	3.00785500	3.88367500
C	1.96779900	2.29066300	5.11679300
C	2.78663300	1.16363400	5.11679300
C	2.41744600	0.00000000	5.89441800
C	2.78663300	-1.16363400	5.11679300
C	1.96779900	-2.29066300	5.11679300
C	1.73318400	-3.00785500	3.88367500
C	0.36579800	-3.45214600	3.88367500
C	-0.24556500	-3.00982800	5.11679300
C	0.74703200	-2.29912800	5.89441800
C	0.38139700	-1.17382000	6.64229400
C	1.23422800	0.00000000	6.64229400
C	0.38139700	1.17382000	6.64229400
C	0.74703200	2.29912800	5.89441800
C	-2.32505700	2.57783400	3.88367500
C	-2.93840000	0.69654200	5.11679300
C	-1.95575500	1.42093900	5.89441800
C	-1.57046700	2.57934100	5.11679300
C	-0.24556500	3.00982800	5.11679300
C	0.36579800	3.45214600	3.88367500
C	-3.17014800	-1.41466600	3.88367500
C	-2.93840000	-0.69654200	5.11679300
C	-0.99851100	0.72546100	6.64229400
C	-0.99851100	-0.72546100	6.64229400
C	-1.95575500	-1.42093900	5.89441800
C	-1.57046700	-2.57934100	5.11679300
C	-2.32505700	-2.57783400	3.88367500
C	-3.17014800	1.41466600	3.88367500
C	0.37315100	1.14844100	-4.63446800
C	-0.97692200	0.70977600	-4.63446800
C	-2.01996900	1.46759300	-4.09875600
C	-1.64339900	2.80921600	-3.73583500
C	-0.32167800	3.23866900	-3.73583500
C	0.77155900	2.37461500	-4.09875600
C	1.20754200	0.00000000	-4.63446800

C	0.37315100	-1.14844100	-4.63446800
C	-0.97692200	-0.70977600	-4.63446800
C	-2.01996900	-1.46759300	-4.09875600
C	-3.17956200	0.69487000	-3.73583500
C	-2.49782100	3.87860700	-3.10941600
C	-0.25900900	4.60604100	-3.10941600
C	2.91690600	3.57412400	-3.10941600
C	2.16388500	2.43106100	-3.73583500
C	2.98075400	1.30673800	-3.73583500
C	2.49681800	0.00000000	-4.09875600
C	0.77155900	-2.37461500	-4.09875600
C	2.16388500	-2.43106100	-3.73583500
C	2.98075400	-1.30673800	-3.73583500
C	4.30056800	-1.66967700	-3.10941600
C	4.30056800	1.66967700	-3.10941600
C	-4.46064400	1.17701300	-3.10941600
C	-4.46064400	-1.17701300	-3.10941600
C	-2.49782100	-3.87860700	-3.10941600
C	2.91690600	-3.57412400	-3.10941600
C	-0.25900900	-4.60604100	-3.10941600
C	-0.32167800	-3.23866900	-3.73583500
C	-1.64339900	-2.80921600	-3.73583500
C	-3.17956200	-0.69487000	-3.73583500
H	-5.02063800	1.87566500	-3.74957600
H	-5.02063800	-1.87566500	-3.74957600
H	-3.33532600	-4.19529800	-3.74957600
H	0.23240100	-5.35452300	-3.74957600
H	2.95929300	-4.46850200	-3.74957600
H	5.16427000	-1.43361200	-3.74957600
H	5.16427000	1.43361200	-3.74957600
H	2.95929300	4.46850200	-3.74957600
H	0.23240100	5.35452300	-3.74957600
H	-3.33532600	4.19529800	-3.74957600
H	-2.91308500	-3.53424500	-2.14528200
H	2.46107400	-3.86265000	-2.14528200
H	4.43411200	1.14699600	-2.14528200
H	0.27935900	4.57153300	-2.14528200
H	-4.26145900	1.67836700	-2.14528200
H	-2.91308500	3.53424500	-2.14528200
H	2.46107400	3.86265000	-2.14528200
H	4.43411200	-1.14699600	-2.14528200
H	0.27935900	-4.57153300	-2.14528200
H	-4.26145900	-1.67836700	-2.14528200
O	-1.62601600	-5.00436100	-2.90372100
O	-5.26189700	0.00000000	-2.90372100
O	-1.62601600	5.00436100	-2.90372100
O	4.25696400	3.09286500	-2.90372100
O	4.25696400	-3.09286500	-2.90372100

7...C₇₀ (stagg.):

C	-0.99542400	0.72321800	-1.28054100
C	-0.99542400	-0.72321800	-1.28054100
C	-1.95261500	-1.41865800	-0.53839800
C	-2.93942700	-0.69715100	0.23358200
C	-2.93942700	0.69715100	0.23358200
C	-1.95261500	1.41865800	-0.53839800
C	0.38021800	1.17019100	-1.28054100
C	1.23041200	0.00000000	-1.28054100
C	0.38021800	-1.17019100	-1.28054100
C	0.74583300	-2.29543700	-0.53839800
C	-1.57136300	-2.58013000	0.23358200
C	-3.17234400	-1.41590400	1.46529000
C	-3.48938100	-0.73536300	2.67371200
C	-3.48938100	0.73536300	2.67371200
C	-3.17234400	1.41590400	1.46529000
C	-2.32691300	2.57954000	1.46529000
C	-1.57136300	2.58013000	0.23358200
C	-0.24530300	3.01099300	0.23358200
C	0.74583300	2.29543700	-0.53839800
C	2.41356500	0.00000000	-0.53839800
C	2.78782200	1.16374400	0.23358200
C	1.96827100	2.29175900	0.23358200
C	1.73423200	3.01014700	1.46529000
C	0.36629700	3.45461600	1.46529000
C	-0.37890600	3.54583900	2.67371200
C	-1.77765000	3.09135900	2.67371200
C	-2.32691300	-2.57954000	1.46529000
C	-0.37890600	-3.54583900	2.67371200
C	0.36629700	-3.45461600	1.46529000

C	-3.17005500	-1.41465800	3.89131200	C	0.74574800	-2.29517600	-0.44386000
C	-2.93852600	-0.69660800	5.12469300	C	-1.57141900	-2.57985600	0.32795300
C	-0.99854100	0.72548300	6.65049000	C	-3.17195100	-1.41536000	1.56005000
C	-0.99854100	-0.72548300	6.65049000	C	-3.48913300	-0.73527100	2.76896300
C	-1.95593500	-1.42107000	5.90246600	C	-3.48913300	0.73527100	2.76896300
C	-1.57056800	-2.57944000	5.12469300	C	-3.17195100	1.41536000	1.56005000
C	-2.32502100	-2.57774800	3.89131200	C	-2.32627400	2.57933400	1.56005000
C	-3.17005500	1.41465800	3.89131200	C	-1.57141900	2.57985600	0.32795300
C	0.37329000	1.14886800	-4.63602800	C	-0.24509700	3.01080400	0.32795300
C	-0.97728500	0.71003900	-4.63602800	C	0.74574800	2.29517600	-0.44386000
C	-2.01833000	1.46640300	-4.09381600	C	2.41329100	0.00000000	-0.44386000
C	-1.64363600	2.80614400	-3.71992300	C	2.78770600	1.16349000	0.32795300
C	-0.31968100	3.23632300	-3.71992300	C	1.96799300	2.29172800	0.32795300
C	0.77093400	2.37269000	-4.09381600	C	1.73423500	3.00947600	1.56005000
C	1.20799100	0.00000000	-4.63602800	C	0.36590000	3.45407500	1.56005000
C	0.37329000	-1.14886800	-4.63602800	C	-0.37891800	3.54557400	2.76896300
C	-0.97728500	-0.71003900	-4.63602800	C	-1.77748500	3.09115200	2.76896300
C	-2.01833000	-1.46640300	-4.09381600	C	-2.32627400	-2.57933400	1.56005000
C	-3.17671300	0.69604400	-3.71992300	C	-0.37891800	-3.54557400	2.76896300
C	-2.51917100	3.85276100	-3.08176100	C	0.36590000	-3.45407500	1.56005000
C	-0.22654400	4.59768100	-3.08176100	C	1.73423500	-3.00947600	1.56005000
C	2.88572700	3.58644300	-3.08176100	C	2.39058700	-2.64570700	2.76896300
C	2.16089000	2.43033600	-3.71992300	C	3.25494900	-1.45601400	2.76896300
C	2.97913900	1.30411300	-3.71992300	C	2.39058700	2.64570700	2.76896300
C	2.49479400	0.00000000	-4.09381600	C	3.25494900	1.45601400	2.76896300
C	0.77093400	-2.37269000	-4.09381600	C	3.39809000	0.71937600	1.56005000
C	2.16089000	-2.43033600	-3.71992300	C	3.39809000	-0.71937600	1.56005000
C	2.97913900	-1.30411300	-3.71992300	C	2.78770600	-1.16349000	0.32795300
C	4.30264900	-1.63621700	-3.08176100	C	1.96799300	-2.29172800	0.32795300
C	4.30264900	1.63621700	-3.08176100	C	-1.77748500	-3.09115200	2.76896300
C	-4.44266000	1.20530600	-3.08176100	C	-0.24509700	-3.01080400	0.32795300
C	-4.44266000	-1.20530600	-3.08176100	C	3.39590200	0.71885000	3.97760400
C	-2.51917100	-3.85276100	-3.08176100	C	3.39590200	-0.71885000	3.97760400
C	2.88572700	-3.58644300	-3.08176100	C	1.73305900	3.00755700	3.97760400
C	-0.22654400	-4.59768100	-3.08176100	C	1.96790700	2.29085000	5.21097300
C	-0.31968100	-3.23632300	-3.71992300	C	2.78684400	1.16367900	5.21097300
C	-1.64363600	-2.80614400	-3.71992300	C	2.41784900	0.00000000	5.98868400
C	-3.17671300	-0.69604400	-3.71992300	C	2.78684400	-1.16367900	5.21097300
H	-4.93681400	1.97783200	-3.69067700	C	1.96790700	-2.29085000	5.21097300
H	-4.93681400	-1.97783200	-3.69067700	C	1.73305900	-3.00755700	3.97760400
H	-3.40659000	-4.08400600	-3.69067700	C	0.36572400	-3.45183100	3.97760400
H	0.35547100	-5.30637300	-3.69067700	C	-0.24554300	-3.01004300	5.21097300
H	2.83142600	-4.50188700	-3.69067700	C	0.74715700	-2.29951100	5.98868400
H	5.15650700	-1.30168700	-3.69067700	C	0.38139800	-1.17382300	6.73624100
H	5.15650700	1.30168700	-3.69067700	C	1.23423000	0.00000000	6.73624100
H	2.83142600	4.50188700	-3.69067700	C	0.38139800	1.17382300	6.73624100
H	0.35547100	5.30637300	-3.69067700	C	0.74715700	2.29951100	5.98868400
H	-3.40659000	4.08400600	-3.69067700	C	-2.32481300	2.57762300	3.97760400
H	-2.88187500	-3.48566200	-2.10306600	C	-2.93859800	0.69663000	5.21097300
H	2.42451300	-3.81795500	-2.10306600	C	-1.95608100	1.42117600	5.98868400
H	4.38030700	1.12603600	-2.10306600	C	-1.57061100	2.57950200	5.21097300
H	0.28266600	4.51388400	-2.10306600	C	-0.24554300	3.01004300	5.21097300
H	-4.20561000	1.66369800	-2.10306600	C	0.36572400	3.45183100	3.97760400
H	-2.88187500	3.48566200	-2.10306600	C	-3.16987200	-1.41449900	3.97760400
H	2.42451300	3.81795500	-2.10306600	C	-2.93859800	-0.69663000	5.21097300
H	4.38030700	-1.12603600	-2.10306600	C	-0.99851300	0.72546300	6.73624100
H	0.28266600	-4.51388400	-2.10306600	C	-0.99851300	-0.72546300	6.73624100
H	-4.20561000	-1.66369800	-2.10306600	C	-1.95608100	-1.42117600	5.98868400
N	-5.29031700	0.00000000	-2.96802300	C	-1.57061100	-2.57950200	5.21097300
N	-1.63479800	-5.03139100	-2.96802300	C	-2.32481300	-2.57762300	3.97760400
N	4.27995600	-3.10957000	-2.96802300	C	-3.16987200	1.41449900	3.97760400
N	4.27995600	3.10957000	-2.96802300	C	0.97701900	0.70984600	-4.59517000
N	-1.63479800	5.03139100	-2.96802300	C	-0.37318800	1.14855500	-4.59517000
H	-5.82414600	0.00000000	-2.10665300	C	-0.77189100	2.37563500	-4.06146100
H	-1.79976000	-5.53909200	-2.10665300	C	0.31943800	3.23855000	-3.68994600
H	4.71183300	-3.42334700	-2.10665300	C	1.64514200	2.80780300	-3.68994600
H	4.71183300	3.42334700	-2.10665300	C	2.02083600	1.46822300	-4.06146100
H	-1.79976000	5.53909200	-2.10665300	C	0.97701900	-0.70984600	-4.59517000
				C	-0.37318800	-1.14855500	-4.59517000
				C	-1.20766200	0.00000000	-4.59517000
				C	-2.49789000	0.00000000	-4.06146100
				C	-2.16200200	2.43228100	-3.68994600
				C	0.23032400	4.59864000	-3.04782600
				C	2.51667700	3.85575900	-3.04782600
				C	4.44474100	1.20200700	-3.04782600
				C	3.17875600	0.69696400	-3.68994600
				C	3.17875600	-0.69696400	-3.68994600
				C	2.02083600	-1.46822300	-4.06146100
				C	-0.77189100	-2.37563500	-4.06146100
				C	0.31943800	-3.23855000	-3.68994600
				C	1.64514200	-2.80780300	-3.68994600

8...C₇₀ (stagg.):

C	-0.99561600	0.72335700	-1.18665400
C	-0.99561600	-0.72335700	-1.18665400
C	-1.95239300	-1.41849700	-0.44386000
C	-2.93918400	-0.69728900	0.32795300
C	-2.93918400	0.69728900	0.32795300
C	-1.95239300	1.41849700	-0.44386000
C	0.38029100	1.17041600	-1.18665400
C	1.23064900	0.00000000	-1.18665400
C	0.38029100	-1.17041600	-1.18665400

C	2.51667700	-3.85575900	-3.04782600	C	1.96941100	-2.29238900	0.19030200
C	4.44474100	-1.20200700	-3.04782600	C	-1.77773600	-3.09164400	2.63058100
C	-2.88934900	3.58499700	-3.04782600	C	-0.24585400	-3.01217200	0.19030200
C	-4.30239300	1.64010900	-3.04782600	C	3.39620400	0.71888000	3.83895900
C	-4.30239300	-1.64010900	-3.04782600	C	3.39620400	-0.71888000	3.83895900
C	0.23032400	-4.59864000	-3.04782600	C	1.73318100	3.00783600	3.83895900
C	-2.88934900	-3.58499700	-3.04782600	C	1.96790500	2.29077700	5.07210800
C	-2.16200200	-2.43228100	-3.68994600	C	2.78677400	1.16369900	5.07210800
C	-2.98133300	-1.30457000	-3.68994600	C	2.41765400	0.00000000	5.84976300
C	-2.98133300	1.30457000	-3.68994600	C	2.78677400	-1.16369900	5.07210800
H	-2.81405100	4.51150200	-3.63657500	C	1.96790500	-2.29077700	5.07210800
H	-5.16028300	1.28219100	-3.63657500	C	1.73318100	-3.00783600	3.83895900
H	-5.16028300	-1.28219100	-3.63657500	C	0.36578900	-3.45212900	3.83895900
H	-2.81405100	-4.51150200	-3.63657500	C	-0.24558300	-3.00998300	5.07210800
H	-0.37517900	-5.30394000	-3.63657500	C	0.74709600	-2.29932600	5.84976300
H	3.42110400	-4.07045300	-3.63657500	C	0.38141700	-1.17387900	6.59745500
H	4.92841000	-1.99582400	-3.63657500	C	1.23429000	0.00000000	6.59745500
H	4.92841000	1.99582400	-3.63657500	C	0.38141700	1.17387900	6.59745500
H	3.42110400	4.07045300	-3.63657500	C	0.74709600	2.29932600	5.84976300
H	-0.37517900	5.30394000	-3.63657500	C	-2.32504000	2.57782500	3.83895900
H	-4.36326200	-1.15652500	-2.05266900	C	-2.93855300	0.69657200	5.07210800
H	-0.24840200	-4.50709400	-2.05266900	C	-1.95592400	1.42106200	5.84976300
H	4.20974100	-1.62901300	-2.05266900	C	-1.57054300	2.57947700	5.07210800
H	2.85016500	3.50030900	-2.05266900	C	-0.24558300	3.00998300	5.07210800
H	-2.44824200	3.79232300	-2.05266900	C	0.36578900	3.45212900	3.83895900
H	-0.24840200	4.50709400	-2.05266900	C	-3.17013400	-1.41465300	3.83895900
H	4.20974100	1.62901300	-2.05266900	C	-2.93855300	-0.69657200	5.07210800
H	2.85016500	-3.50030900	-2.05266900	C	-0.99856100	0.72549700	6.59745500
H	-2.44824200	-3.79232300	-2.05266900	C	-0.99856100	-0.72549700	6.59745500
H	-4.36326200	1.15652500	-2.05266900	C	-1.95592400	-1.42106200	5.84976300
N	-4.28858200	3.11583700	-2.97869800	C	-1.57054300	-2.57947700	5.07210800
N	-4.28858200	-3.11583700	-2.97869800	C	-2.32504000	-2.57782500	3.83895900
N	1.63809300	-5.04153000	-2.97869800	C	-3.17013400	1.41465300	3.83895900
N	5.30097900	0.00000000	-2.97869800	C	0.37236100	1.14601000	-4.59325700
N	1.63809300	5.04153000	-2.97869800	C	-0.97485400	0.70827300	-4.59325700
H	-4.75529200	3.45492200	-2.14525700	C	-2.02015800	1.46773100	-4.08103100
H	-4.75529200	-3.45492200	-2.14525700	C	-1.65448700	2.83067500	-3.74396700
H	1.81636000	-5.59018100	-2.14525700	C	-0.32532100	3.26254700	-3.74396700
H	5.87786400	0.00000000	-2.14525700	C	0.77163200	2.37483900	-4.08103100
H	1.81636000	5.59018100	-2.14525700	C	1.20498600	0.00000000	-4.59325700

9...C₇₀ (eclip.):

C	-0.99501300	0.72291900	-1.31939100	C	-0.97485400	-0.70827300	-4.59325700
C	-0.99501300	-0.72291900	-1.31939100	C	-2.02015800	-1.46773100	-4.08103100
C	-1.95562800	-1.42084700	-0.58298500	C	-3.20339700	0.69878400	-3.74396700
C	-2.94071900	-0.69699100	0.19030200	C	-2.65226400	3.83348200	-3.21484000
C	-2.94071900	0.69699100	0.19030200	C	-0.10753700	4.66031400	-3.21484000
C	-1.95562800	1.42084700	-0.58298500	C	2.82626300	3.70706500	-3.21484000
C	0.38006100	1.16970800	-1.31939100	C	2.18086700	2.44823700	-3.74396700
C	1.22990400	0.00000000	-1.31939100	C	3.00233700	1.31758100	-3.74396700
C	0.38006100	-1.16970800	-1.31939100	C	2.49705300	0.00000000	-4.08103100
C	0.74698300	-2.29897900	-0.58298500	C	0.77163200	-2.37483900	-4.08103100
C	-1.57161000	-2.58140800	0.19030200	C	2.18086700	-2.44823700	-3.74396700
C	-3.17254200	-1.41571400	1.42197900	C	3.00233700	-1.31758100	-3.74396700
C	-3.48967800	-0.73535700	2.63058100	C	4.39899100	-1.54239000	-3.21484000
C	-3.48967800	0.73535700	2.63058100	C	4.39899100	1.54239000	-3.21484000
C	-3.17254200	1.41571400	1.42197900	C	-4.46545300	1.33784200	-3.21484000
C	-2.32679300	2.57978700	1.42197900	C	-4.46545300	-1.33784200	-3.21484000
C	-1.57161000	2.58140800	0.19030200	C	-2.65226400	-3.83348200	-3.21484000
C	-0.24585400	3.01217200	0.19030200	C	2.82626300	-3.70706500	-3.21484000
C	0.74698300	2.29897900	-0.58298500	C	-0.10753700	-4.66031400	-3.21484000
C	2.41728900	0.00000000	-0.58298500	C	-0.32532100	-3.26254700	-3.74396700
C	2.78877300	1.16463400	0.19030200	C	-1.65448700	-2.83067500	-3.74396700
C	1.96941100	2.29238900	0.19030200	C	-3.20339700	-0.69878400	-3.74396700
C	1.73450500	3.01010900	1.42197900	H	-4.84561200	2.11727400	-3.88392300
C	0.36605400	3.45474600	1.42197900	H	-4.84561200	-2.11727400	-3.88392300
C	-0.37900400	3.54611900	2.63058100	H	-3.51102400	-3.95417700	-3.88392300
C	-1.77773600	3.09164400	2.63058100	H	0.51627100	-5.26272400	-3.88392300
C	-2.32679300	-2.57978700	1.42197900	H	2.67567900	-4.56109000	-3.88392300
C	-0.37900400	-3.54611900	2.63058100	H	5.16468500	-1.13526800	-3.88392300
C	0.36605400	-3.45474600	1.42197900	H	5.16468500	1.13526800	-3.88392300
C	1.73450500	-3.01010900	1.42197900	H	2.67567900	4.56109000	-3.88392300
C	2.39097700	-2.64609800	2.63058100	H	0.51627100	5.26272400	-3.88392300
C	3.25544100	-1.45626500	2.63058100	H	-3.51102400	3.95417700	-3.88392300
C	2.39097700	2.64609800	2.63058100	H	-3.02379800	-3.52227100	-2.22972700
C	3.25544100	1.45626500	2.63058100	H	2.41547400	-3.96424400	-2.22972700
C	3.39877600	0.71943700	1.42197900	H	4.51664200	1.07223300	-2.22972700
C	3.39877600	-0.71943700	1.42197900	H	0.37596500	4.62692000	-2.22972700
C	2.78877300	-1.16463400	0.19030200	H	-4.28428300	1.78736100	-2.22972700
				H	-3.02379800	3.52227100	-2.22972700
				H	2.41547400	3.96424400	-2.22972700
				H	4.51664200	-1.07223300	-2.22972700

H	0.37596500	-4.62692000	-2.22972700	C	-2.32499800	-2.57770000	3.90514100
H	-4.28428300	-1.78736100	-2.22972700	C	-3.17000200	1.41465100	3.90514100
S	-1.77163400	-5.45252900	-3.07763600	C	0.97435400	0.70790900	-4.57658100
S	-5.73312800	0.00000000	-3.07763600	C	-0.37217000	1.14542200	-4.57658100
S	-1.77163400	5.45252900	-3.07763600	C	-0.77285200	2.37859300	-4.07680500
S	4.63819800	3.36984800	-3.07763600	C	0.32545700	3.26588400	-3.74447800
S	4.63819800	-3.36984800	-3.07763600	C	1.65633800	2.83345400	-3.74447800

9...C₇₀ (stagg.):

C	-0.99418300	0.72231700	-1.24896800	C	0.10858200	4.66079100	-3.20725200
C	-0.99418300	-0.72231700	-1.24896800	C	2.65169900	3.83448200	-3.20725200
C	-1.95498800	-1.42038200	-0.51524200	C	4.46622900	1.33699600	-3.20725200
C	-2.94188700	-0.69763600	0.25614100	C	3.20661100	0.69968600	-3.74447800
C	-2.94188700	0.69763600	0.25614100	C	3.20661100	-0.69968600	-3.74447800
C	-1.95498800	1.42038200	-0.51524200	C	2.02335200	-1.47005100	-4.07680500
C	0.37974400	1.16873300	-1.24896800	C	-0.77285200	-2.37859300	-4.07680500
C	1.22887800	0.00000000	-1.24896800	C	0.32545700	-3.26588400	-3.74447800
C	0.37974400	-1.16873300	-1.24896800	C	1.65633800	-2.83345400	-3.74447800
C	0.74673900	-2.29822700	-0.51524200	C	2.65169900	-3.83448200	-3.20725200
C	-1.57258400	-2.58232000	0.25614100	C	4.46622900	-1.33699600	-3.20725200
C	-3.17361100	-1.41661700	1.48818500	C	-2.82738900	3.70683600	-3.20725200
C	-3.48978900	-0.73554500	2.69664400	C	-4.39912200	1.54353100	-3.20725200
C	-3.48978900	0.73554500	2.69664400	C	-4.39912200	-1.54353100	-3.20725200
C	-3.17361100	1.41661700	1.48818500	C	0.10858200	-4.66079100	-3.20725200
C	-2.32798200	2.58052500	1.48818500	C	-2.82738900	-3.70683600	-3.20725200
C	-1.57258400	2.58232000	0.25614100	C	-2.18293800	-2.45085700	-3.74447800
C	-0.24560200	3.01348200	0.25614100	C	-3.00546800	-1.31874100	-3.74447800
C	0.74673900	2.29822700	-0.51524200	C	-3.00546800	1.31874100	-3.74447800
C	2.41649800	0.00000000	-0.51524200	H	-2.67600300	4.56581200	-3.86983500
C	2.79009700	1.16479900	0.25614100	H	-5.16927500	1.13411700	-3.86983500
C	1.96997700	2.29359700	0.25614100	H	-5.16927500	-1.13411700	-3.86983500
C	1.73483900	3.01146900	1.48818500	H	-2.67600300	-4.56581200	-3.86983500
C	0.36658300	3.45604200	1.48818500	H	-0.51878500	-5.26673400	-3.86983500
C	-0.37885900	3.54628200	2.69664400	H	3.51541500	-3.95594400	-3.86983500
C	-1.77794900	3.09169000	2.69664400	H	4.84864900	-2.12090400	-3.86983500
C	-2.32798200	-2.58052500	1.48818500	H	4.84864900	2.12090400	-3.86983500
C	-0.37885900	-3.54628200	2.69664400	H	3.51541500	3.95594400	-3.86983500
C	0.36658300	-3.45604200	1.48818500	H	-0.51878500	5.26673400	-3.86983500
C	1.73483900	-3.01146900	1.48818500	H	-4.51103200	-1.07581900	-2.22006600
C	2.39095600	-2.64631500	2.69664400	H	-0.37082000	-4.62269200	-2.22006600
C	3.25564100	-1.45617800	2.69664400	H	4.28185200	-1.78116200	-2.22006600
C	2.39095600	2.64631500	2.69664400	H	3.01715100	3.52187400	-2.22006600
C	3.25564100	1.45617800	2.69664400	H	-2.41715000	3.95780000	-2.22006600
C	3.40017200	0.71933500	1.48818500	H	-0.37082000	4.62269200	-2.22006600
C	3.40017200	-0.71933500	1.48818500	H	4.28185200	1.78116200	-2.22006600
C	2.79009700	-1.16479900	0.25614100	H	3.01715100	-3.52187400	-2.22006600
C	1.96997700	-2.29359700	0.25614100	H	-2.41715000	-3.95780000	-2.22006600
C	-1.77794900	-3.09169000	2.69664400	H	-4.51103200	1.07581900	-2.22006600
C	-0.24560200	-3.01348200	0.25614100	S	-4.63955100	-3.37083100	-3.07246600
C	3.39609700	0.71880400	3.90514100	S	-4.63955100	3.37083100	-3.07246600
C	3.39609700	-0.71880400	3.90514100	S	1.77215100	5.45411900	-3.07246600
C	1.73307500	3.00775700	3.90514100	S	5.73480000	0.00000000	-3.07246600
C	1.96780600	2.29065900	5.13829100	S	1.77215100	-5.45411900	-3.07246600
C	2.78663100	1.16364200	5.13829100				
C	2.41754400	0.00000000	5.91600600				
C	2.78663100	-1.16364200	5.13829100				
C	1.96780600	-2.29065900	5.13829100				
C	1.73307500	-3.00775700	3.90514100	H	-4.11728000	-1.70483400	-2.27617000
C	0.36582800	-3.45200300	3.90514100	H	-5.60418600	0.00000000	-1.89087800
C	-0.24557300	-3.00982900	5.13829100	H	-1.73178900	-5.32989700	-1.89087800
C	0.74706200	-2.29922100	5.91600600	H	4.53388100	-3.29405800	-1.89087800
C	0.38142000	-1.17389000	6.66380700	H	4.53388100	3.29405800	-1.89087800
C	1.23430100	0.00000000	6.66380700	H	-1.73178900	5.32989700	-1.89087800
C	0.38142000	1.17389000	6.66380700	C	-1.59900800	4.92124000	-2.89816900
C	0.74706200	2.29922100	5.91600600	C	-5.17449800	0.00000000	-2.89816900
C	-2.32499800	2.57770000	3.90514100	C	-1.59900800	-4.92124000	-2.89816900
C	-2.93840400	0.69653500	5.13829100	C	4.18625600	-3.04149300	-2.89816900
C	-1.95583400	1.42099700	5.91600600	C	4.18625600	3.04149300	-2.89816900
C	-1.57046100	2.57934700	5.13829100	H	4.84087500	-3.51710100	-3.64134300
C	-0.24557300	3.00982900	5.13829100	H	-1.84905000	-5.69078900	-3.64134300
C	0.36582800	3.45200300	3.90514100	H	-5.98365000	0.00000000	-3.64134300
C	-3.17000200	-1.41465100	3.90514100	H	-1.84905000	5.69078900	-3.64134300
C	-2.93840400	-0.69653500	5.13829100	H	4.84087500	3.51710100	-3.64134300
C	-0.99857000	0.72550400	6.66380700	N	-0.20420500	4.48101500	-3.12991400
C	-0.99857000	-0.72550400	6.66380700	N	-2.46867000	3.74524600	-3.12991400
C	-1.95583400	-1.42099700	5.91600600	N	-4.32480100	-1.19050000	-3.12991400
C	-1.57046100	-2.57934700	5.13829100	N	-4.32480100	1.19050000	-3.12991400

N	-2.46867000	-3.74524600	-3.12991400
N	-0.20420500	-4.48101500	-3.12991400
N	2.79908000	-3.50518900	-3.12991400
N	4.19859600	-1.57892000	-3.12991400
N	4.19859600	1.57892000	-3.12991400
N	2.79908000	3.50518900	-3.12991400