Heme, cholorophyll, etc. atomically correct[1]

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16 January 2004
http://homepage.mac.com/whitby/

http://web.me.com/whitby/Octahedron/Welcome.html

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1. Excerpted from Octahedron1stEd.pdf—bookmark HEME—pages 385-388

HEME

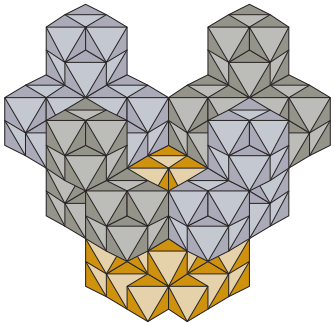
In order to model the heme group, the structure suggested by the chemical symbols of the chemistry texts must be interpreted into a structural association of octahedral atoms:

•there is a suggestion of fourfold symmetry in the arrangement of the N-atoms and the pyrrole rings which include them;

• the N-atoms are adjacent to the central Fe-atom.

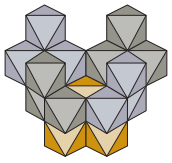
Pyrrole ring

The pyrrole ring is best realized as a C_6-ring with one of the vertical C-atoms removed and an N-atom substituted for the horizontal C-atom opposite the vacated vertical position.



Pyrrole ring with N-atom at bottom, epn-octa detail.

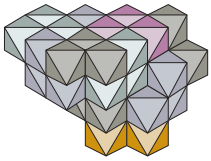
This will be represented in the following figures in He-octa detail.



Representation of pyrrole ring in He-octa detail

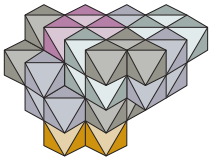
Pyrrole pair

A ring similar to the pyrrole ring could include a C-atom or an O-atom in place of the N-atom. This can join with the pyrrole ring to produce a stable assembly in which a horizontal C-atom of one ring fills the vertical C-atom vacancy of the other ring. This can happen in one of two ways. The next figure shows the pyrrole ring in the same orientation as the previous figure and a similar ring joined with it in the described manner. The added ring is



Pyrrole ring pair, left join

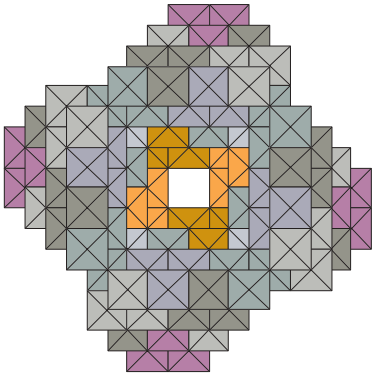
rotated 180° about an axis parallel to one of the vertexial diameters of the He-octa. It is slightly to the *left* of the pyrrole ring. In the next figure, the two rings have the same orientations but the added ring is slightly to the *right* of the pyrrole ring.



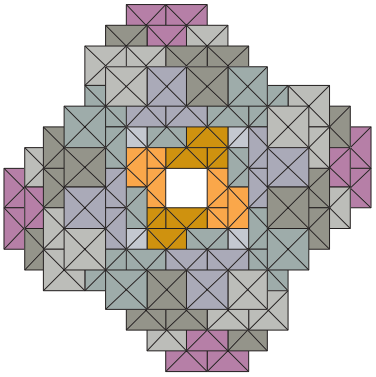
Pyrrole ring pair, right join

Tetrapyrrole

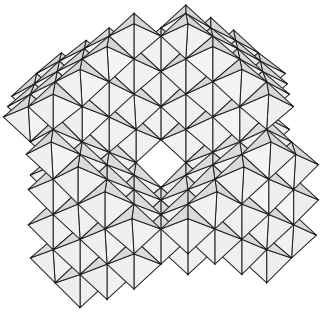
Four ring pairs of either hand can form a fourfold ring. The top left figure is the ring formed by leftly joined pairs. The view is parallel to the fourfold axis. The top right figure shows the ring formed by rightly joined pairs. The two ring assemblies have similar features. The bottom side is vertexially planar as can be seen in the lower right figure. There is a square aperture in the center of the assembly which will just accommodate an edgial equator of a He-octa. The lower left figure shows the other side of the ring which has a pyramidal concavity which is octahedral. This feature provides the utility of the assembly as a holder of atoms. The atom fits snugly in this concavity with its He-octa occupying the vertex of the pyramid.



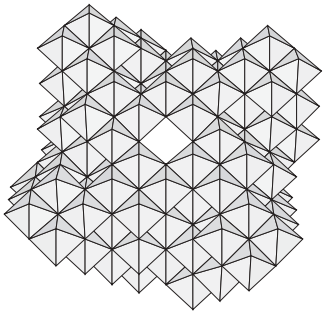
Ring formed by four pairs of leftly joined pyrrole rings.



Ring formed by four pairs of rightly joined pyrrole rings.

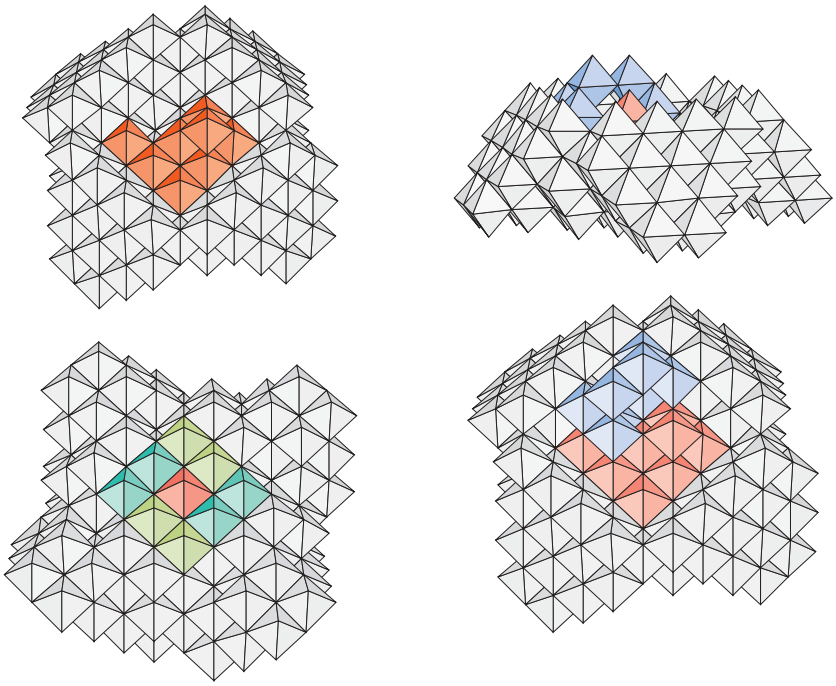


Pyrrole ring assembly, concave side.



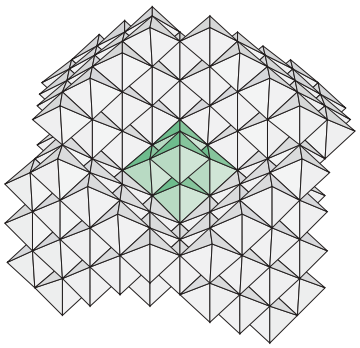
Pyrrole ring assembly, planar side

Heme and chlorophyll groups



Heme group

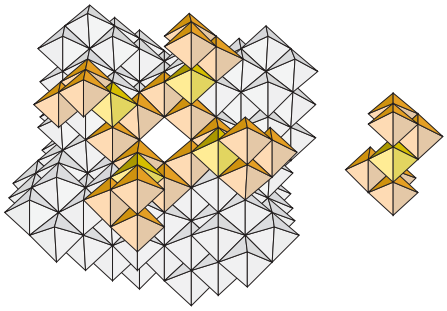
In the above figure, on the upper left there is a pyrrole ring assembly with an Fe-atom colored red occupying the concavity, as in the heme group. The obverse view just below it shows the He-octa of the Fe-atom at is center colored red. Two He-octas of each of the four N-atoms have been colored green. On the right, there are two views of the same group but with the addition of an O_2-group, as in oxy-hemoglobin. The top view shows the planar nature of the assembly. He-octas of the O_2 group protrude above the rim.



Chlorophyll group

The chlorophyll ring carries a Mg-atom which is colored green.

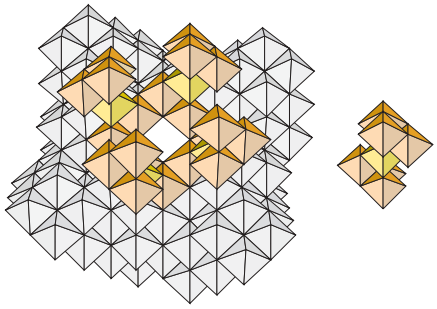
Connections to tetrapyrroles



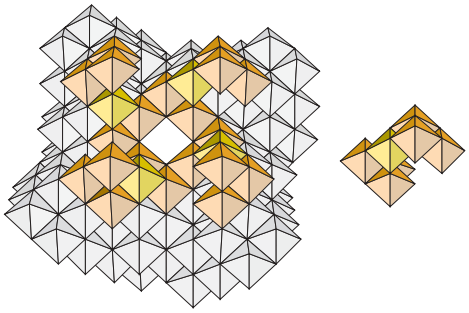
Pyrrole ring assembly: N-atom attachment at 120° clockwise

N to N connections

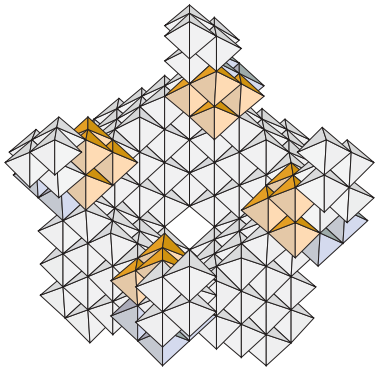
On the planar bottom, the four N-atoms are accessible for triplet-joins. This type of join can be one of three types which differ by the rotation between the pairing atoms. The next figure shows the assembly with four N-atoms joined to the N-atoms of the assembly and the inset shows the orientation between the joined pair. The next orientation between the joined N-atom pair is 120° counter-clockwise relative to the previous N-atom pair join. And the third type of N-atom pair join is 120° clockwise to the first pair join.



Pyrrole ring assembly: N-atom attachment, 0°

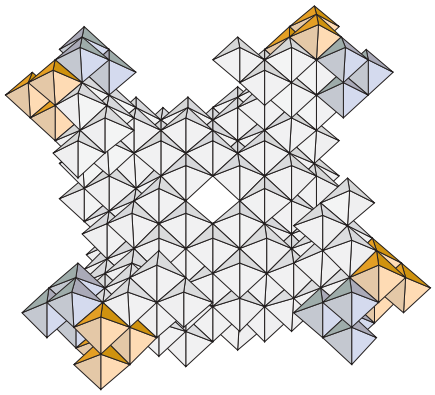


Pyrrole ring assembly: N-atom attachment at 120° counter-clockwise.



Pyrrole ring assembly: Gly attachment to C-atoms of rim

There are four places on the rim around the concavity where the NH_2-O group of a protein main chain unit can join to a C-atom of a pyrrole ring. This is shown in the next figure, with the protein units's beta chain axis normal to the plane of the ring assembly.



Pyrrole ring assembly: Gly attachments to C-atoms of planar surface.

Each of the four rings which are paired with the pyrrole rings might have a C-atom which could join cleftly with a C-atom of the protein unit. In the next figure, the C_α of the protein unit is cleftly joined to the C-atom of the ring.