Polypyrrole monomer with aspartate

Robert William Whitby
19 May 2005
http://homepage.mac.com/whitby/

References

1. Octahedron1stEd.pdf by Robert William Whitby

The octahedral periodicity of the atomic elements and its implications, 500 pages
http://homepage.mac.com/whitby/FileSharing103.html
11Jun2002

2. Heme.pdf by Robert William Whitby

Heme, chlorophyll, etc., atomically correct. Excerpted from Octahedron1stEd.pdf.
http://homepage.mac.com/whitby/FileSharing114.html

3. Pthalo.pdf by Robert William Whitby

Porphyrin, phthalocyanine, and their relatives. Extends the material provided in the Heme chapter of Octahedron1stEd.pdf. Shows the formation of the rings which pair to provide the subunits for the atom-holding assemblies. Shows how the join between rings confers handedness to the assemblies. Shows how the atom-holding cavity is hemi-octahedral and that the cavity of one assembly is identical to that of each of the other assemblies. Shows how one porphyrin can join to another if they are of opposite hand and inverted relative to one another. Shows how the paired ring subunits can form chains if they are of the same hand.
http://homepage.mac.com/whitby/FileSharing115.html

4. ProteinFilesBook.pdf

Three excerpts from Octahedron1stEd.pdf--PROTEIN which shows the forms of the crystals of cytochrome and neuraminidase, AMINO which shows the amino acids, and PROTEIN CHAIN which shows how main chain units join to form the protein substructures.
http://homepage.mac.com/whitby/FileSharing128.html

5.ProteinFoldBook.pdf

Shows plausible conformations of the sidechains of the peptides, gives xyz-addresses of their He-octas, and describes testing the various folded conformations for interference.
http://homepage.mac.com/whitby/FileSharing127.html

6. Engineers Discover Way to Link Plastic to Biological Materials

News item describing the finding that an aspartate residue of the T59-peptide joins with polypyrrole.
http://www.physorg.com/news4111.html

7. Molecular Tissue Engineering, The Schmidt Lab, University of Texas at Austin

Link to the laboratory whose work is described in Reference 6.
http://www.bme.utexas.edu/faculty/schmidt/index.html

Introduction

This file shows two ways in which four pyrroles can join together to form the monomer of polypyrrole that is suggested by the literature. Each of the two monomers is the mirror of the other. The file also shows that the O_2-group of an aspartate residue can join with a C-atom of one of the internal pyrroles of the monomer.

Figure 1 shows a pyrolle group in each of the two orientations required to make a simple chain.

Figure 2 shows that there are two ways for pyrroles having the orientations of Figure 1 to join– each is a mirror of the other. When identical pairs join, the chains are also handed.

Figure 3 shows one of the chains in a vertexial view.

Figure 4 shows two ways in which an O_2-group can join with a C-atom of a pyrrole without interfering with its ability to participate in either of the chains of Figure 2. A chain is shown with an O_2-group joined to a C-atom of one of its four pyrroles.

Figure 5 shows how the O_2-group of an aspartate residue allows it to make the same join.

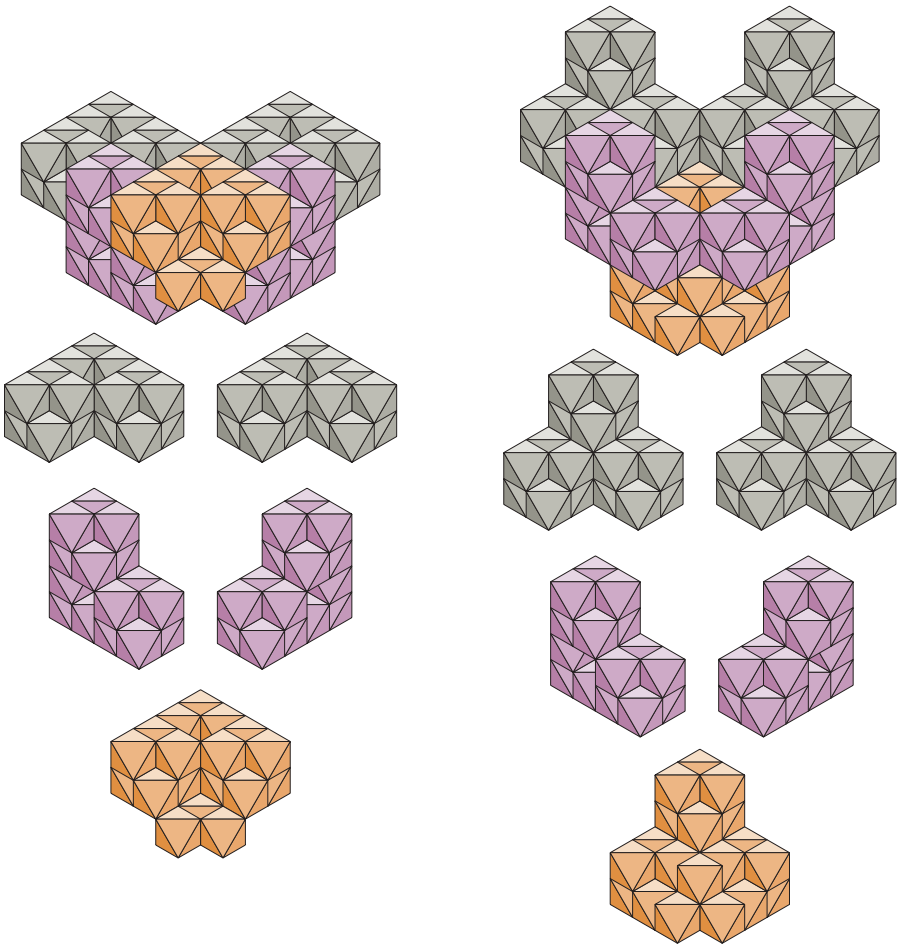

Fig. 1 Pyrrole group in two orientations

The figure shows a pyrrole group in two orientations. On the left, the plane of the pyrrole group makes an angle with the projection plane; on the right, the plane of the pyrrole group is parallel to the projection plane. Below each pyrolle group, each of the atoms which form it is shown separately in the orientation it has in the group. The gray and violet colored atoms are C-atoms; the orange colored atoms are N-atoms. Each octahedron is an epn.

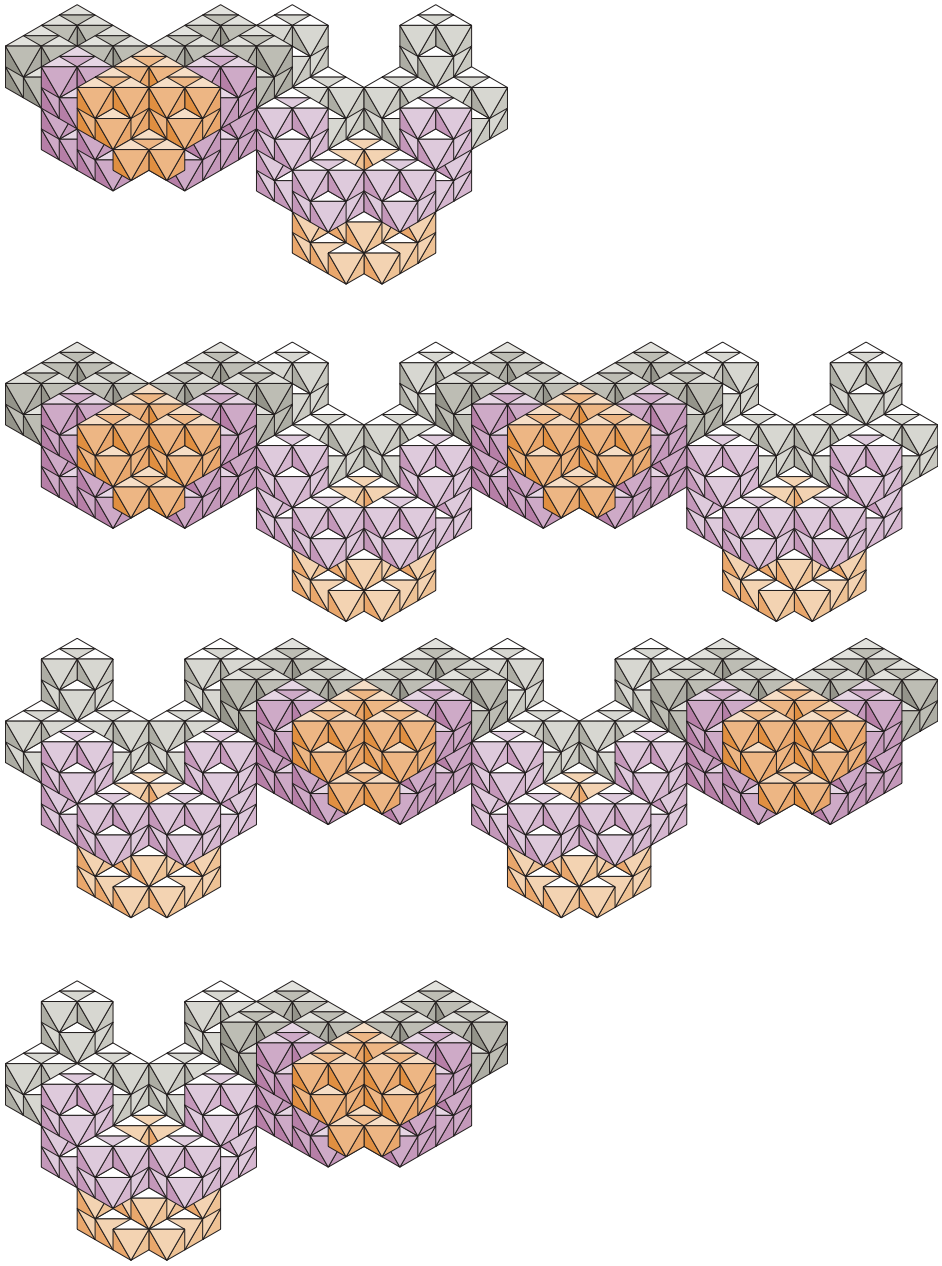

Fig. 2 Polypyrrole monomer

The figure shows how two pyrroles can form handed pairs–one at the top of the figure, one at the bottom of the figure. The chains formed by each of the two pairs are shown in the middle of the figure. Like the pairs, each chain is a mirror of the other.

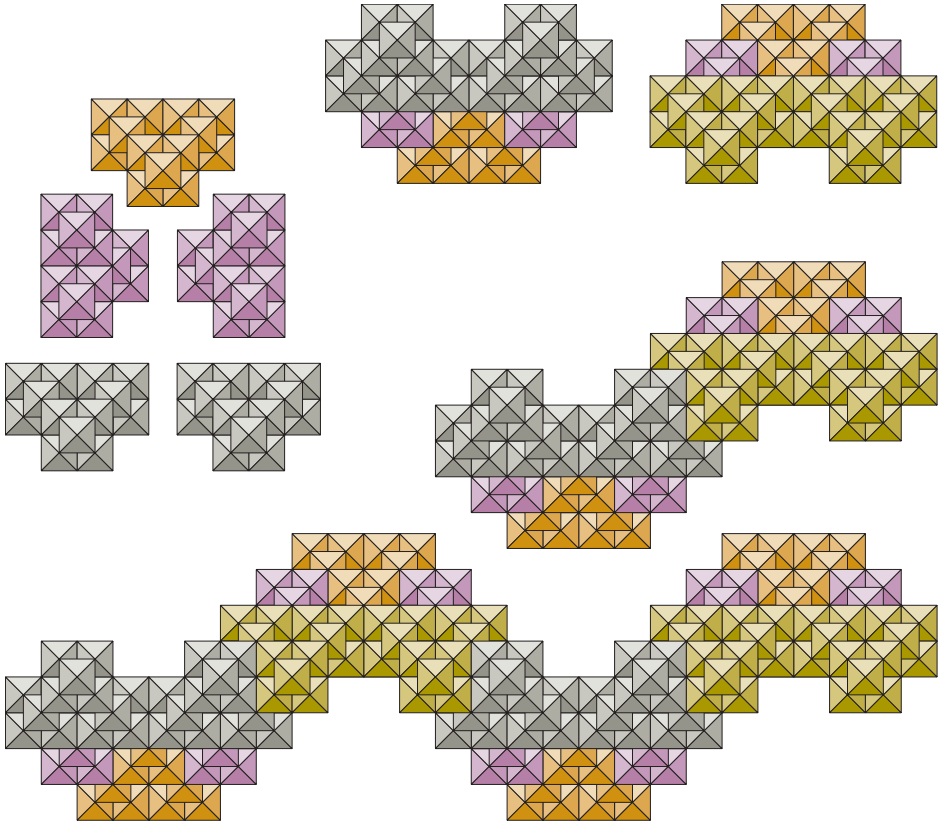

Fig. 3 Polypyrrole monomer–vertexial view

The figure shows how atoms form the pyrrole group, how identical pyrrole groups join as a pair, and how two pairs join as a polypyrrole monomer. In this figure, the C-atoms are colored gray, violet, or yellow; the N-atoms are colored orange.

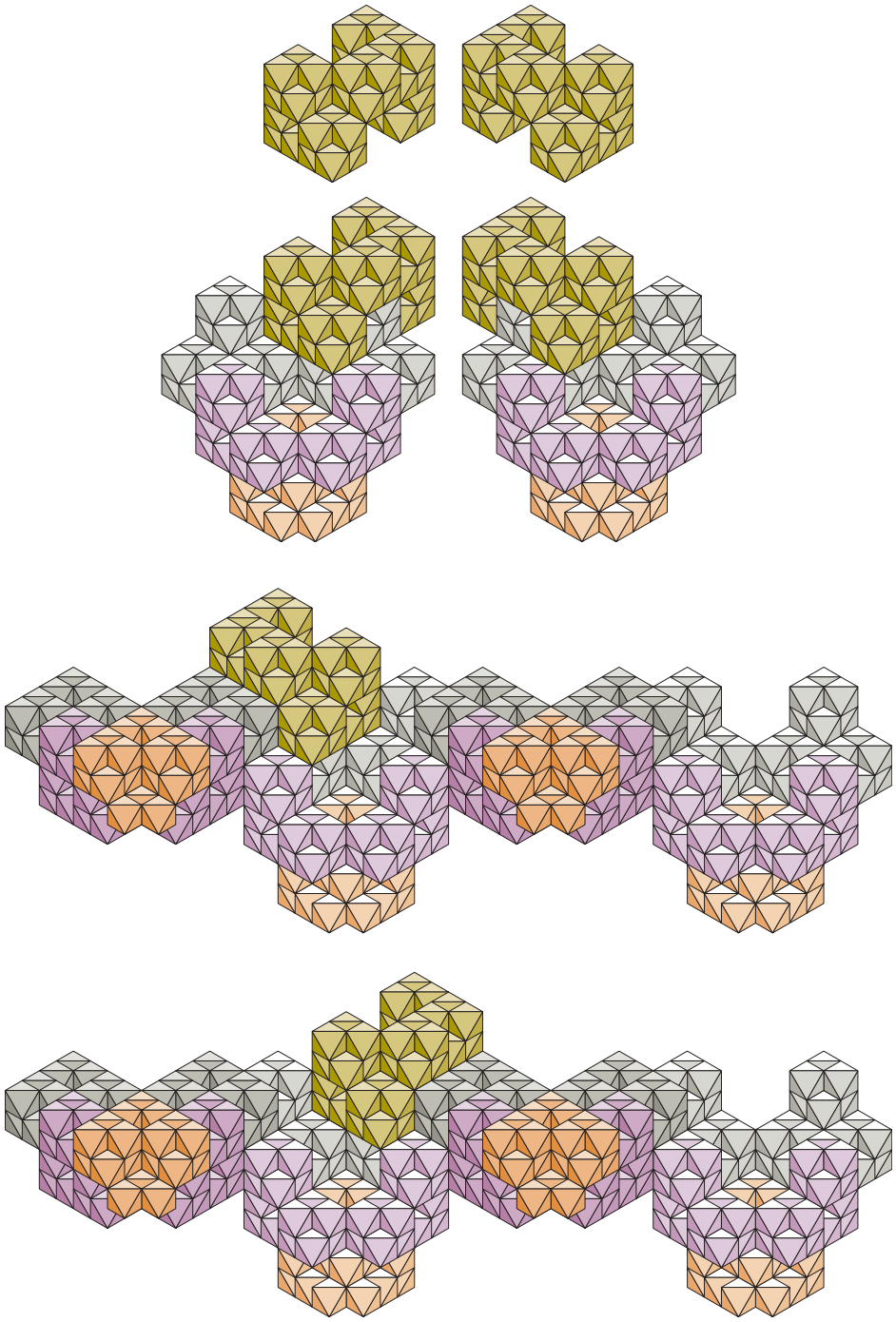

Fig. 4 Polypyrrole monomer with O_2-group

The figure shows two ways in which an O_2-group can join with a pyrrole unit without preventing its inclusion in a polypyrrole monomer. The pyrolle-O_2 groups are at top; the polypyrrole-O_2 monomers are at bottom.

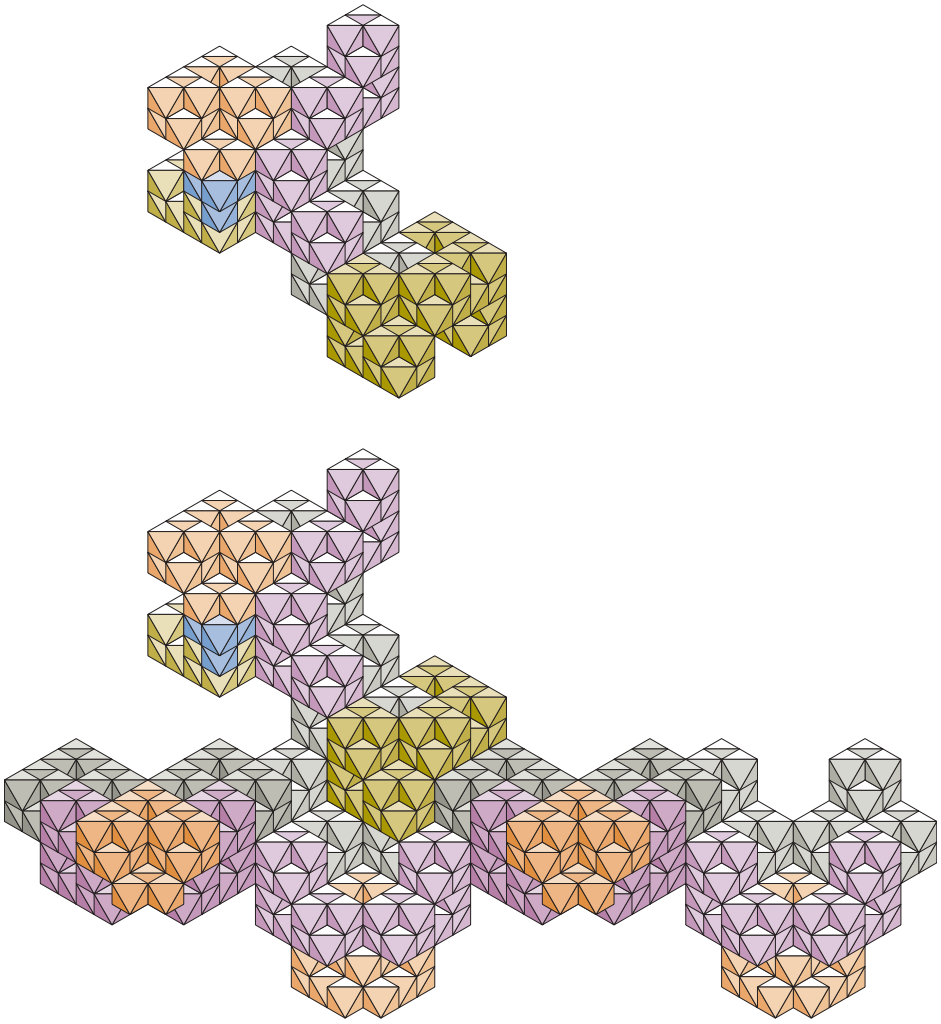

Fig. 5 Polypyrrole monomer with aspartate attached

The figure shows how an aspartate group can join with a polypyrrole monomer. The aspartate group is shown at the top; the monomer with aspartate group is at the bottom. The H_2-group of the aspartate is colored blue, C-atoms are either gray or violet, N-atoms are orange, and O-atoms are yellow.

8 Polypyrrole monomer with aspartate