Di-L-triplets

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http://homepage.mac.com/whitby/

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

Reference

1. Octahedron1stEd.pdf
2. COgroups.pdf
3. COassys.pdf

Introduction

The backbone of D-glucose is a di-L-triplet. This paper looks at each of the ways in which two identical L-triplets can join to form a di-L-triplet and assesses the ability of each to accommodate an H_2O-group on each of its six C-atoms.

The number of distinct orientations of the C-atom in the octahedral view chosen for the figures is four. Each orientation is coded with a color. There are six distinct orientations of a pair of L-joined C-atoms. Adjoining C-atoms are not in the same orientation and so they have different colors. The pairs are shown in the left column of the table in Figure 1 and, again, in the top row of the table. Each C-atom of a pair has two vacant clefts to which a third C-atom can join. The twenty-four triplets which are formed by the addition of an L-joined C-atom to each of those clefts are shown in the cells of the table. The three C-atoms of each triplet have different orientations and different colors.

The twenty-four triplets of the table consist of twelve distinctly oriented identical triplets each of which appears twice. The distinct triplets are shown in Figure 2. The triplet on the left of the top row which is labeled "ROB-1" was arbitrarily chosen to be the base triplet. The orange C-atom of this triplet was arbitrarily chosen as the place to join a second triplet[1]. Each of the eleven remaining distinct triplets that could join to one of the two clefts of the orange atom form the assemblies shown in Figure 3. Triplet OBG-3 could not be joined to the orange C-atom, each of the other triplets could. The assemblies are labeled according to the sequence of the colors of the C-atoms of the added triplet beginning with its free end. There are thirteen assemblies.

Each of the assemblies is represented in Figure 4 by a line of six octahedra. Each octahedron represents a C-atom of the triplet and is colored to match that C-atom. The leftmost octahedron represents the C-atom at the free end of the added triplet. Each of the assemblies is given a text code which consists of the first letter of the color of the octahedron. The letters are in the same order as the octahedra. The pattern of duplicate colors within each assembly is shown in the numbers to the left of the octahedra. These show that two of the assemblies are duplicates [Figure 5]. Three assemblies cannot accommodate an O-atom on each of their C-atoms [Figure 5].

The assemblies which can accommodate an O-atom on each of their C-atoms are shown in Figure 6. For two of these assemblies, an O-atom at one location prevents an adjacent O-atom from accommodating an H_2-group. The nature of this interference for the two assemblies is shown in Figure 7.

The seven di-L-triplets whose C-atoms can each accommodate an H_2O-group are shown in Figure 8.

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1. The two arbitrary choices affect only the orientations of the resulting di-triplet assemblies.

Fig. 1 L-triplets for the ROGB view.

There are six distinct pairs of left-joined C-atoms. These occupy the leftmost column and the topmost row. An L-triplet is formed by the addition of a C-atom to a cleft of one of the C-atoms of the L-pair. For the GO-pair, a red atom or a blue atom can join to either the orange atom or the green atom of the pair to form a triplet.

The C-atoms of an L-triplet are differently oriented and this means differently colored. The pair has two colors, so the addition is one of the other two colors. The pairs of the head row show how the third atom can be joined. Each C-atom has a color. The three possible L-joins requires a C-atom of one of the three remaining colors. Taking the green atom, there are three pairs in the top row which include a green atom. One has the orange atom of the index pair, so this cannot make a triplet. But the blue green and the red green work. The blue red pair does not work, because neither the red nor the blue is present in the index triplet.

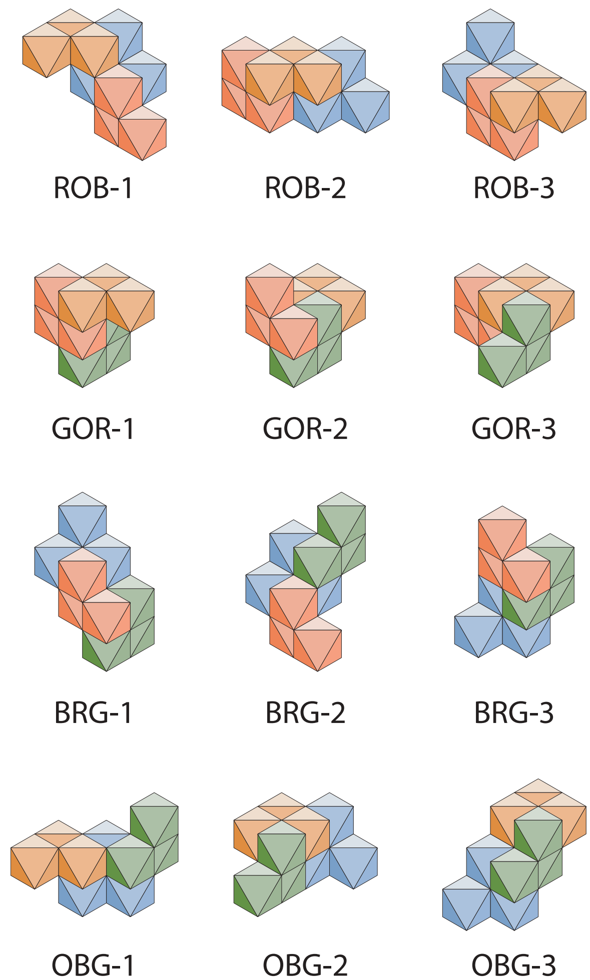
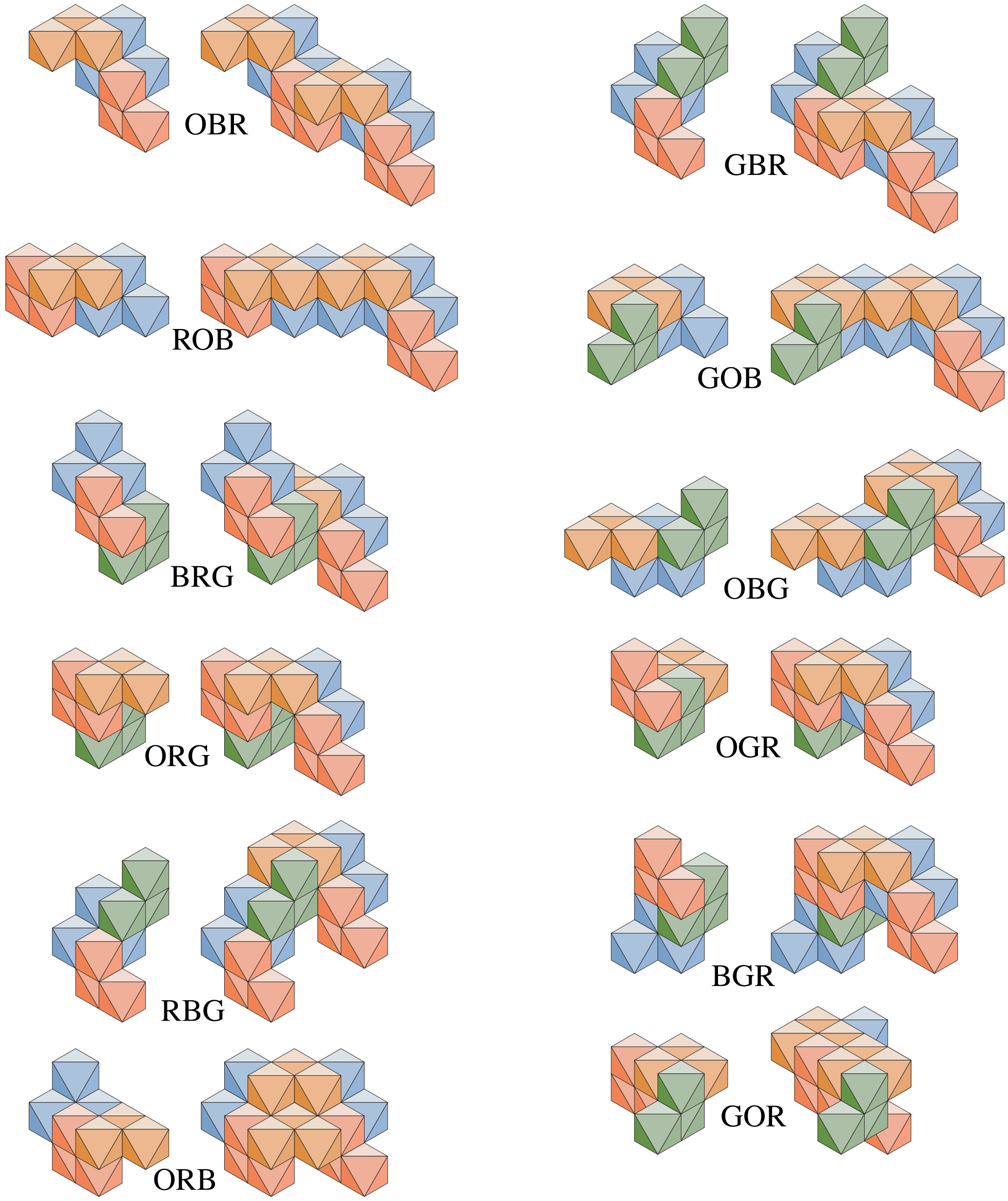


Fig. 2 The L-triplets

The table in the previous figure has twenty-four triplets. These are found to include twelve pairs of identical triplets. The twelve distinct triplets are shown in the figure. Each has been given a code. The code consists of a letter for each of the colors of the C-atoms followed by an integer. Each of the triplets in a row has the same three colors. The integer denotes the column in which it is placed. Each triplet is identical to each of the other eleven triplets. Each has a different orientation.



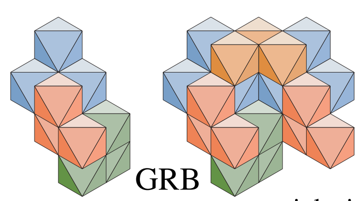


Fig. 3 di-L-triplets

The figure shows the thirteen ways in which a second L-triplet can be cleftly joined to one of the end atoms of the first triplet. The first triplet is in the ROB-1 orientation and is common to each of the thirteen assemblies, and each of the added triplets is joined to its orange atom. The second triplet is shown to the left of each of the assemblies which include it. Two of the resulting assemblies are not suitable as hexoses because O-atoms cannot be attached to one of its six C-atoms. These are shown at the bottom of the left column. The OBG-3 triplet cannot join with the orange atom of the ROB-1 triplet.

Fig. 4 di-L-triplet patterns

Each of the six atoms of each d-L-triplet is represented in the figure by a single octahedron. The color of the octahedron represents the orientation of the C-atom; its position represents the position of the C-atom relative to the adjoining C-atoms.

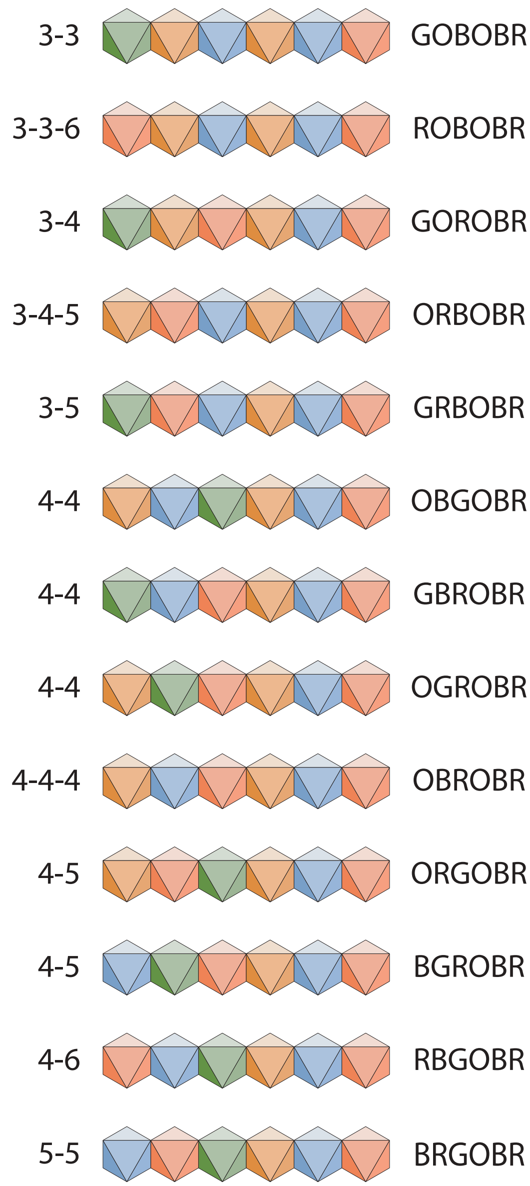
A code is shown to the right of the octahedral representation of the assembly. It is simply the first letter of the color used to differentiate the orientations of the C-atoms–Green Orange Blue Red.

The C-atom has four possible orientations. Adjoining C-atoms cannot have the same orientation. Each C-atom within an L-triplet must be differently oriented than either of the other C-atoms. It follows that two of the C-atoms of the second triplet must have the same orientation as two of the C-atoms of the first triplet. There are just three cases in which the three C-atoms of the second triplet have identically oriented counterparts in the first triplet.

The six octahedron arrangement reveals the patterns of like color within each di-triplet. The patterns are shown in the numbers to the left of the octahedral representation of the C-atoms of the triplet. The topmost di-triplet has two color duplications, orange and blue. The OBO-segment has three atoms and this is shown as a "3" on the left. The BOB-segment has three atoms, too, and this is shown on the left. Hence "3-3".

There are three di-triplets with the "4-4" arrangement. Each has a different positional pattern of duplication. OBGOBR has O--O-- and -B--B-. GBROBR has -B--B- and --R--R. OGROBR has O--O-- and --R--R. Each of the duplicates of OGROBR includes one of its end atoms. Only one of the duplicates of OBGOBR and GBROBR includes an end atom. OGROBR is clearly not the same as the other two triplets with the "4-4" arrangement. Examination of OBGOBR and GBROBR show that they are the same di-triplet in different orientations.

There are two "4-5" arrangements. ORGOBR has O--O-- and -R---R. BGROBR has B---B- and --R--R. These are not duplicates.



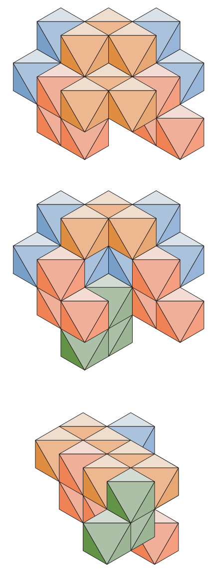


Fig. 5 Unsuitable di-triplets

Three of the di-triplets cannot accommodate an O-atom on each of its C-atoms.

The di-triplet labeled ORB cannot accommodate an O-atom on one orange C-atom because the second orange O-atom prevents it.

The di-triplet labeled GRB can accommodate an O-atom on either the orange C-atom or the leftmost red O-atom but not both.

The di-triplet GOR cannot accommodate an O-atom on its inner red atom because it is blocked by the outer red atom.

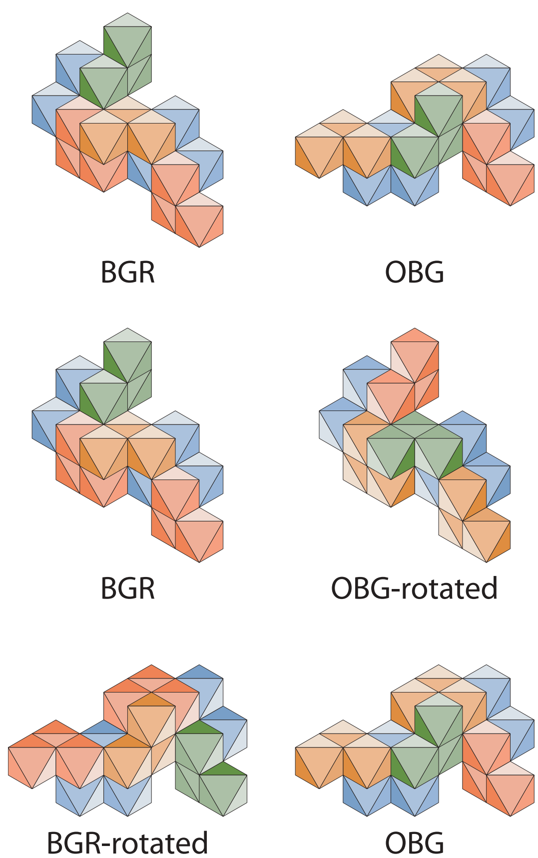


Fig. 5 Duplicate di-triplets

Two of the di-triplets have the same conformation but are differently oriented. They are shown at the top of the figure on the left. In the middle row, OBG has been rotated through one-third turn without change of coloration to show that it is the same assembly as BGR. In the bottom row, BGR has been rotated one-third turn and is shown to be identical to the unrotated OBG.

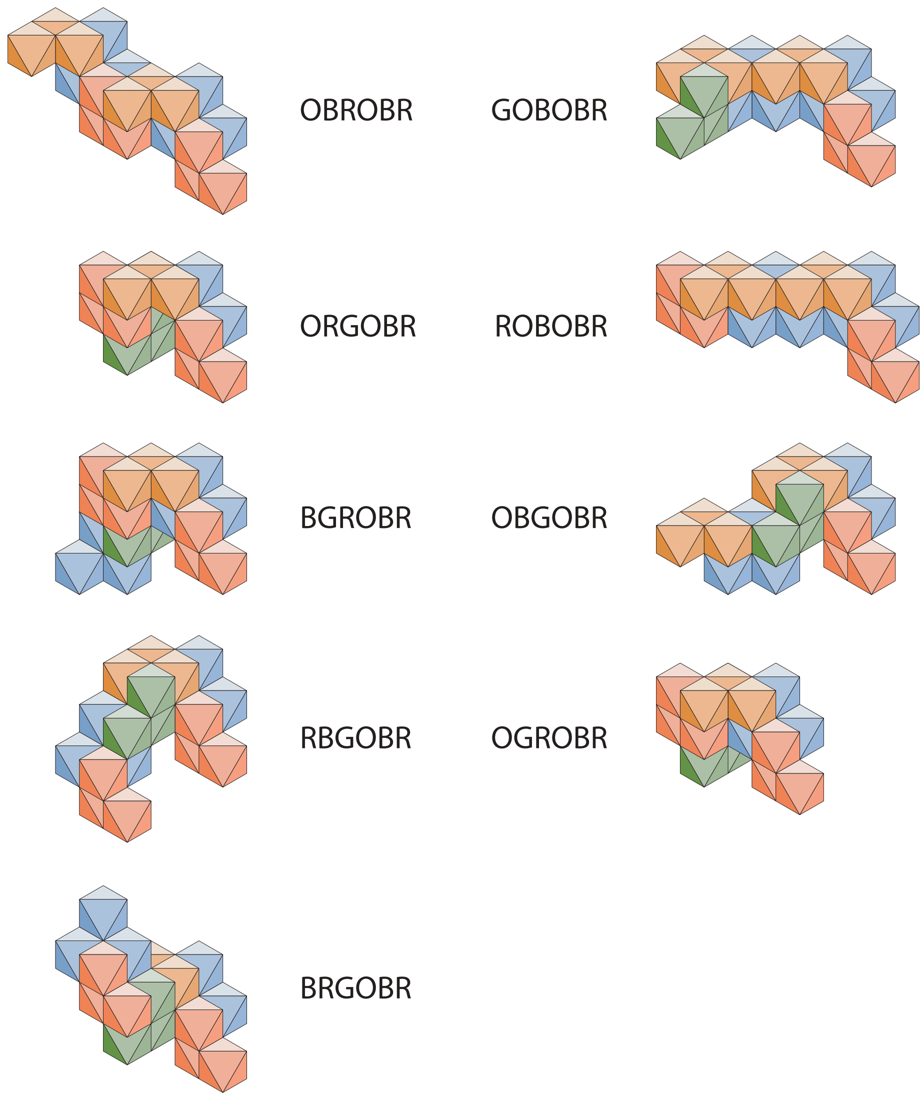


Fig. 6 di-L-triplets which can accommodate an O-atom on each C-atom

Each of the nine distinct di-L-triplets of the figure can accommodate an O-atom on each of its six C-atoms.

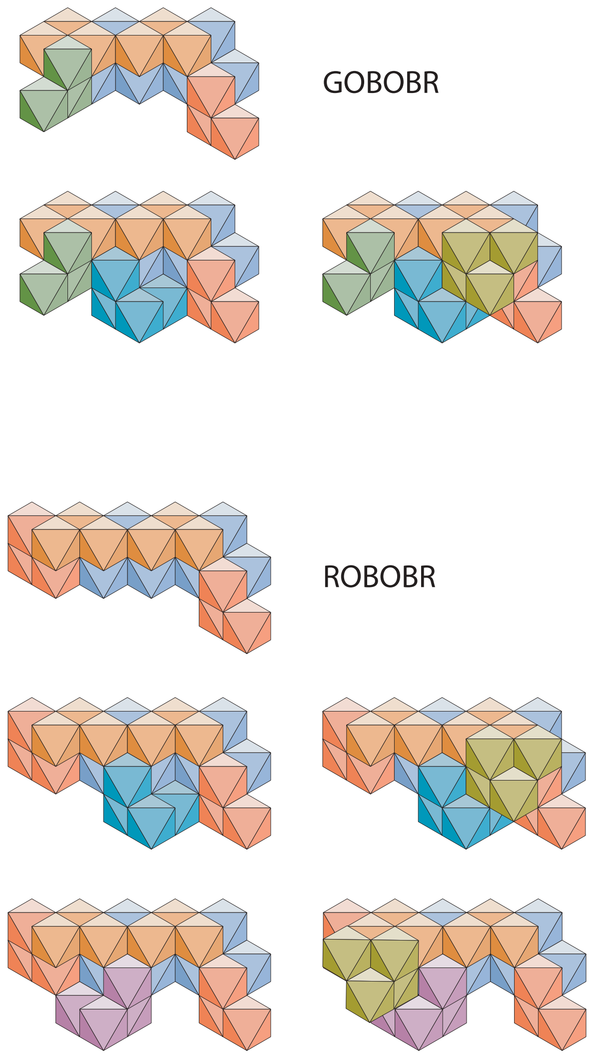


Fig. 7 di-triplets whose O-atoms interfere with H_2-groups

The figure shows two di-triplets which have an O-atom that cannot accommodate an H_2-group due to interference. GOBOBR is shown at the top of the figure. Just below it, an O-atom colored aqua has been added to the leftmost blue colored C-atom. To the right, a yellow O-atom has been added to the rightmost orange C-atom. A He-octa of the yellow O-atom fills the void of the aqua O-atom preventing it from accepting an H_2-group. No matter how these two O-atoms are oriented one will prevent the other from accommodating an H_2-group.

In the lower part of the figure, ROBOBR has the same type of conflict. If an aqua O-atom is joined to the leftmost blue atom, the yellow atom attached to the rightmost orange atom fills the space required for the H_2-group. If a violet O-atom is tried in place of the aqua O-atom, the yellow O-atom attached to the leftmost orange atom fills the space required for the H_2-group.

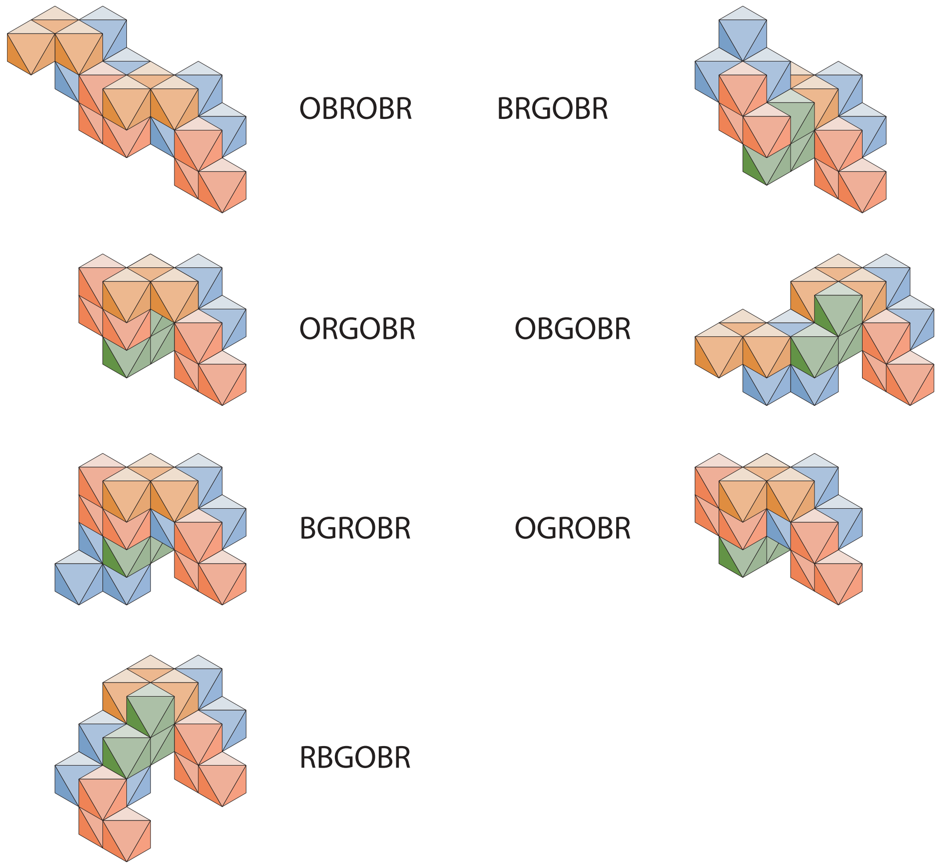


Fig. 8 L-di-triplets whose six C-atoms can each accommodate an H_2O-group

Each of the seven L-di-triplets shown in the figure can accommodate an O-atom with an H_2-group on each of its six C-atoms. In each of the seven assemblies, the triplet-to-triplet join is effected by an L-join between two C-atoms. None of the five assemblies in which the join between the triplets is an R-join can accommodate an H_2O-group on each of its C-atoms.