D-glucose candidates

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

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

Reference

1. Octahedron1stEd.pdf
2. LTriplets.pdf
3. SymLdiTriplets.pdf

Introduction

Unlike the symmetrical triplet, each of the three C-atoms of the L-triplet has a positional identity. Figure 1 shows each of the orientations of an L-triplet for an octahedral facial view. Each C-atoms is distinguishable by its coloration. Two coloring schemes are used to produce two sets of orientations. Each C-atom of one set is colored according to its orientation; each C-atom of the other set is colored according to its position within the triplet.

Additional di-L-triplets can be formed so that the red C-atom of one OBR triplet is joined to the red C-atom of an identical triplet in a different orientation (See Figure 2). These di-L-triplets were overlooked in Reference 2. Figure 6 shows each of the di-L-triplets arranged in columns according to the positional relationship of the joining C-atoms–orange to orange, orange to red, red to red. Figure 7 shows only the di-L-triplets which can accommodate an H_2O-group on each C-atom.

Figures 8, 9, and 10 show how O-atoms can join with each of the C-atoms of three different di-L-triplets. The ways were counted and used to produce the table below. The di-L-triplet has more ways to accommodate an H_2O-group than the di-triplet which consists of an L-triplet joined with a symmetrical triplet (See Reference 3). The di-L-triplet OBGOBR can accommodate an H_2O-group on each of its six C-atoms in 1600 ways; the highest number of combinations for a sym-L-di-triplets is 640.

Table 1: Combined ways of adding H_2O-groups to di-L-triplets

<table>
<tr><th rowspan="2">Di-triplet code</th><th colspan="6">H_2O-groups by position</th><th rowspan="2">Combinations</th></tr>
<tr><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th><th>6</th></tr>
<tr><td rowspan="2">OBROBR</td><td rowspan="2">6</td><td rowspan="2">2</td><td rowspan="2">2</td><td rowspan="2">2</td><td>2</td><td>4</td><td rowspan="2">960</td></tr>
<tr><td>2</td><td>6</td></tr>
<tr><td rowspan="2">OBGOBR</td><td>4</td><td>2</td><td rowspan="2">2</td><td rowspan="2">2</td><td>2</td><td>4</td><td rowspan="2">1600</td></tr>
<tr><td>6</td><td>2</td><td>2</td><td>6</td></tr>
<tr><td rowspan="2">BGROBR</td><td rowspan="2">6</td><td rowspan="2">2</td><td rowspan="2">2</td><td rowspan="2">2</td><td>2</td><td>4</td><td rowspan="2">960</td></tr>
<tr><td>2</td><td>6</td></tr>
</table>

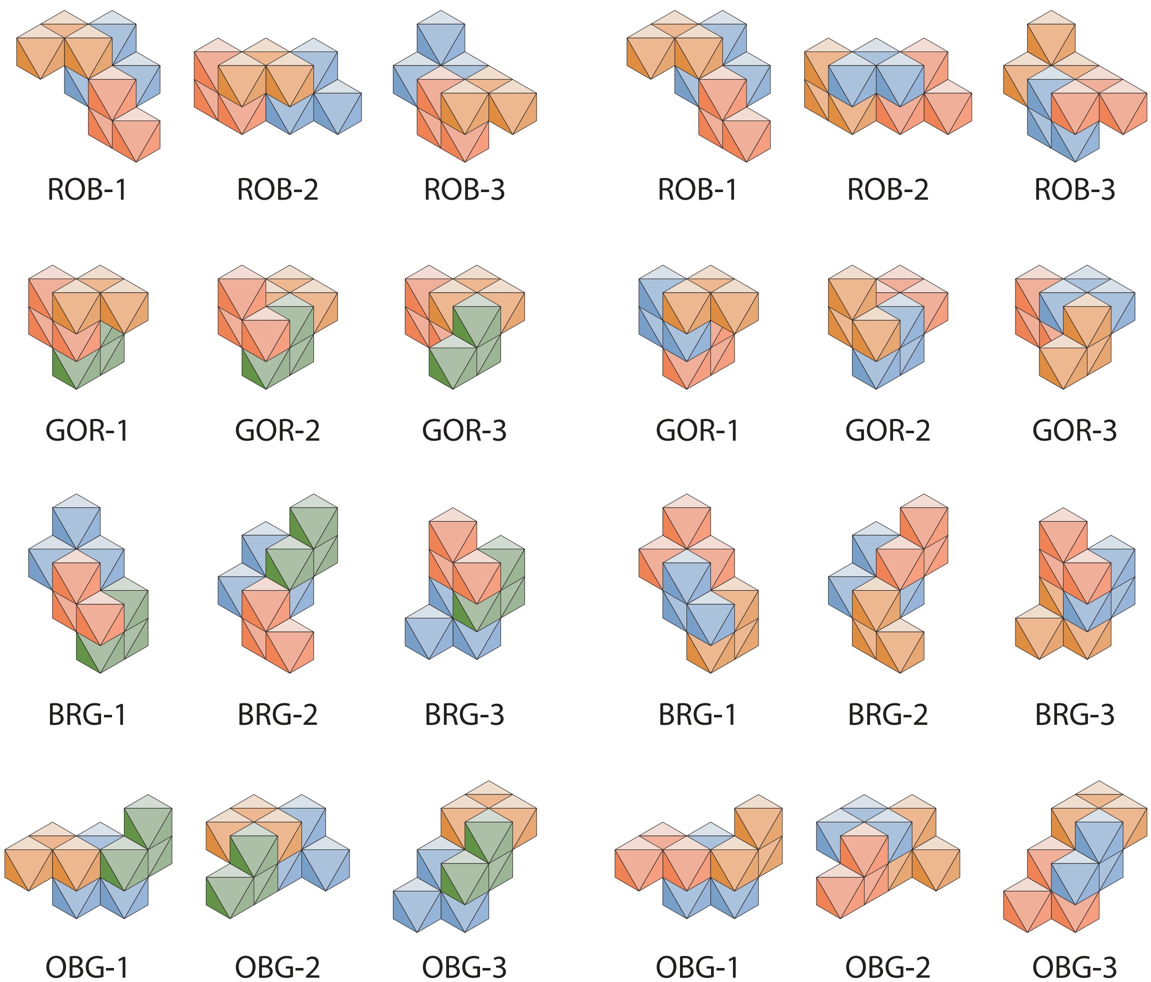

Fig. 1 Coloration of C-atoms–orientation vs. triplet position
Two identical sets of L-triplet orientations for the octahedral view are shown in the figure. The C-atoms of the set on the left have been colored according to their orientations; those on the right have been colored according to their positions within the triplet. The label is the same for the respective triplet orientation in each set, e.g. "ROB-1" in the left set refers to the same orientation as "ROB-1" in the right set. The orientation colors of the C-atoms of the ROB-1 triplet are used for the positional coloration–an orange C-atom in a triplet of the right hand set is the same positionally as the orange C-atom of the ROB-1 triplet of the left hand set.

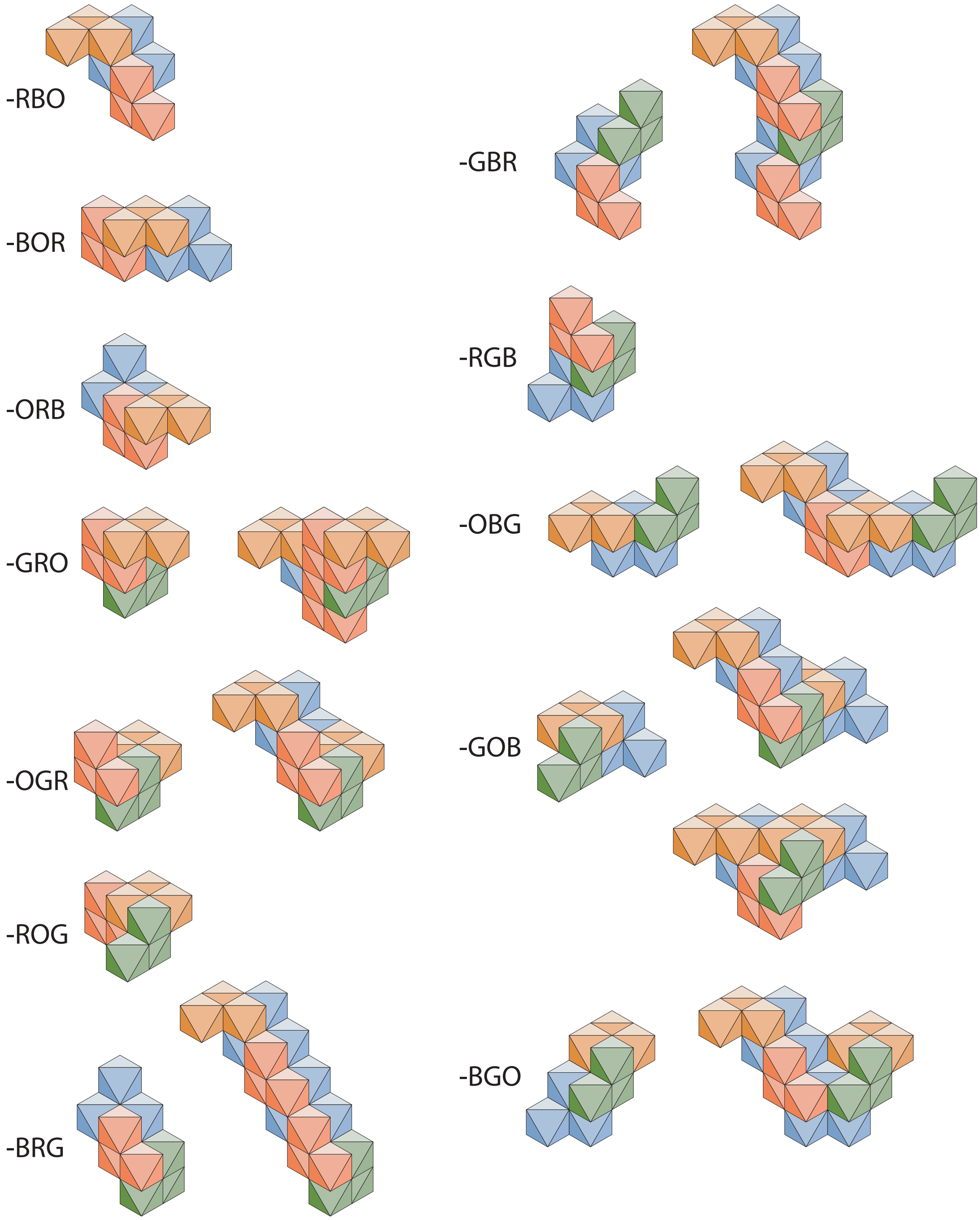

Fig. 2 Di-L-triplets formed by the joining of C-atoms in the red positions

Wherever possible, the C-atom in the red position of each of the L-triplet orientations is joined the red C-atom of the OBR triplet and the resulting di-triplet is shown in the figure. For the triplet “-GRO” there is the di-triplet OBR-OGR. The *positional* coloration would be OBR-RBO for each of the di-triplets.

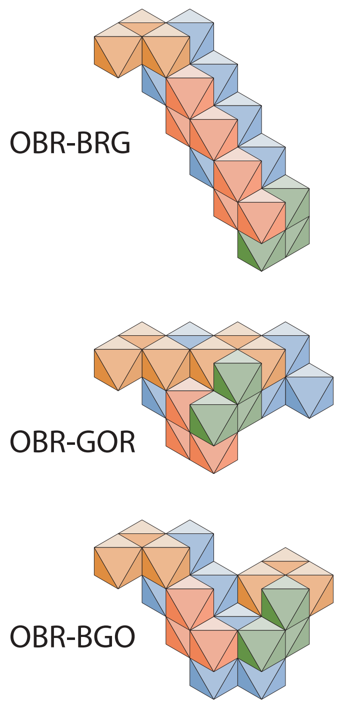

Fig. 3 OBR-(RBO) di-triplets which cannot accommodate an H_2O-group on each C-atom

The three di-triplets shown in the figure are unable to accommodate an H_2O-group on each of their C-atoms.

An O-atom joined to the blue C-atom between the two red atoms would prevent one of the C-atoms from accommodating an H_2O-group.

The orange atom on the right in the middle di-triplet is blocking the blue C-atom to its left.

Either the red C-atom or the green C-atom of the bottom di-triplet can accommodate the O-atom of an H_2O-group, but not both.

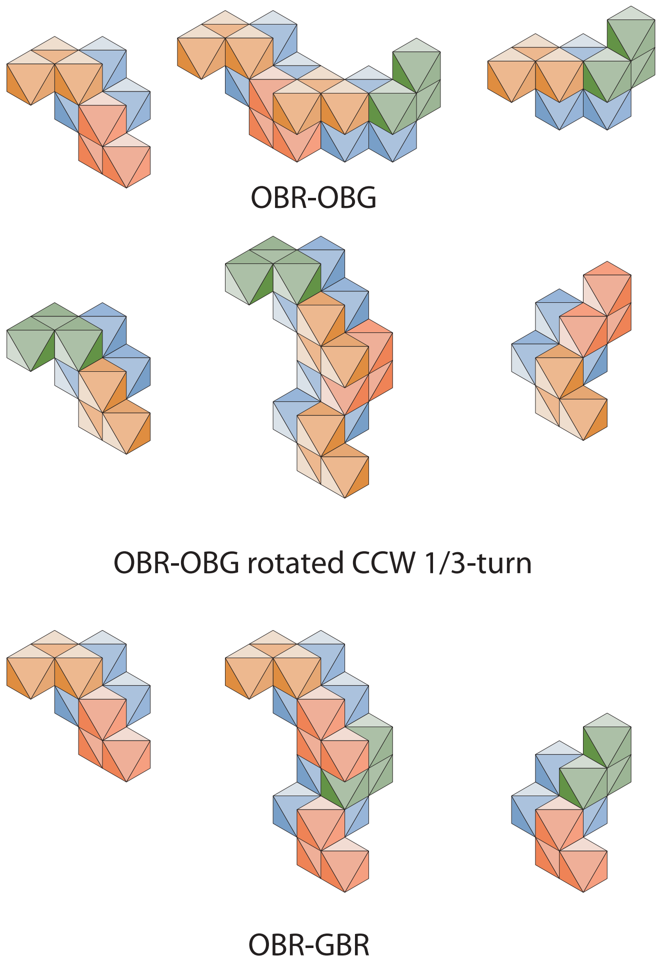

Fig. 4 OBR-GBR is a duplicate of OBR-OBG

The figure shows that di-triplet OBR-OBG is the same as di-triplet OBR-GBR. Di-triplet OBR-OBG is shown in the middle of the top row flanked by its two triplets. Di-triplet OBR-GBR is shown in the bottom row. The middle row shows OBR-OBG rotated 1/3-turn counter-clockwise. Comparison of middle and bottom rows shows the di-triplets and their flanking triplets to be the same.

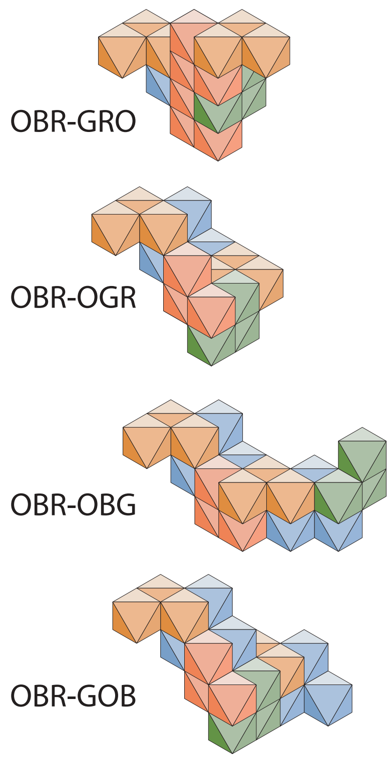

Fig. 5 OBR-(RBO) di-L-triplets suitable for hexose backbones

Each of the four di-L-triplets shown in the figure is a suitable backbone for a hexose. Each is of the type OBR-(RBO).

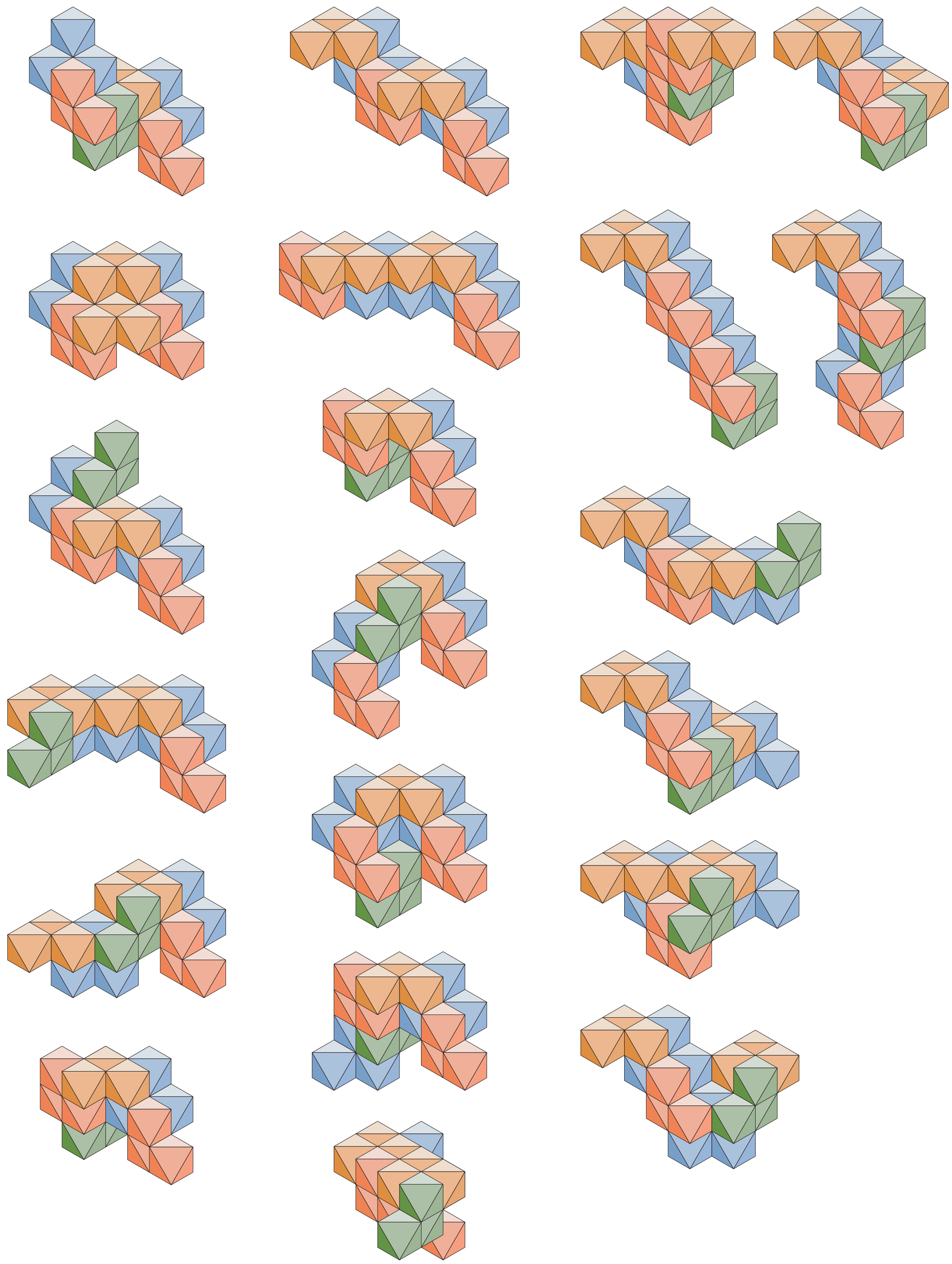

Fig. 6 Di-L-triplets arranged according to the triplet positions of the joining C-atoms

Each of the six di-triplets of the left hand column is formed by the join between C-atoms which are in the orange position of their respective triplets.

Each of the seven di-triplets of the center column is formed by the join between a C-atom in the red position of one triplet and a C-atom in the orange position of the other triplet.

Each of the eight di-triplets of the right hand column is formed by the join between C-atoms in the red position of their respective triplets.

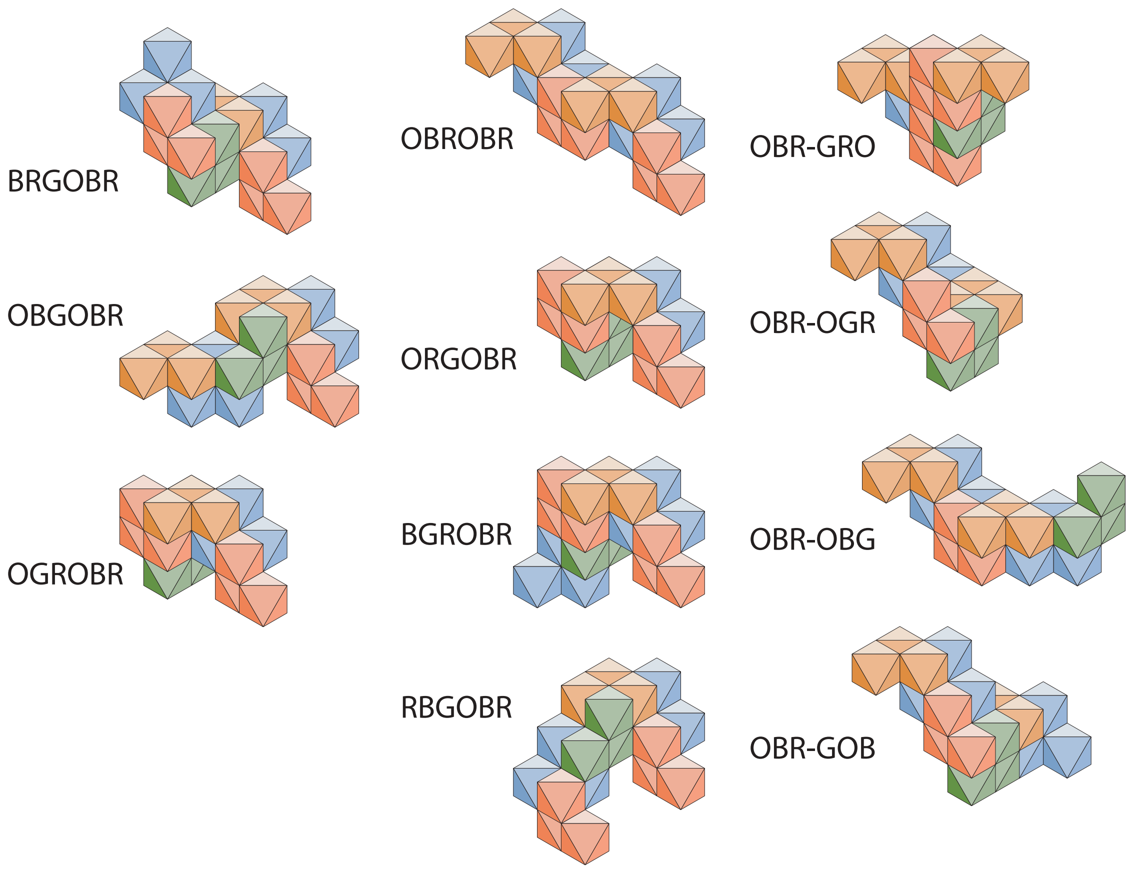

Fig. 7 Di-triplets capable of accommodating an H_2O-group on each C-atom

Each C-atom of each of the di-triplets in the figure can accommodate an H_2O-group.

The three di-triplets in the left hand column are formed by a cleft join between C-atoms in the red position of their respective triplets; the four in the middle column by a C-atom in the red position with a C-atom in the orange position; and the five in the right hand column by C-atoms in the red position.

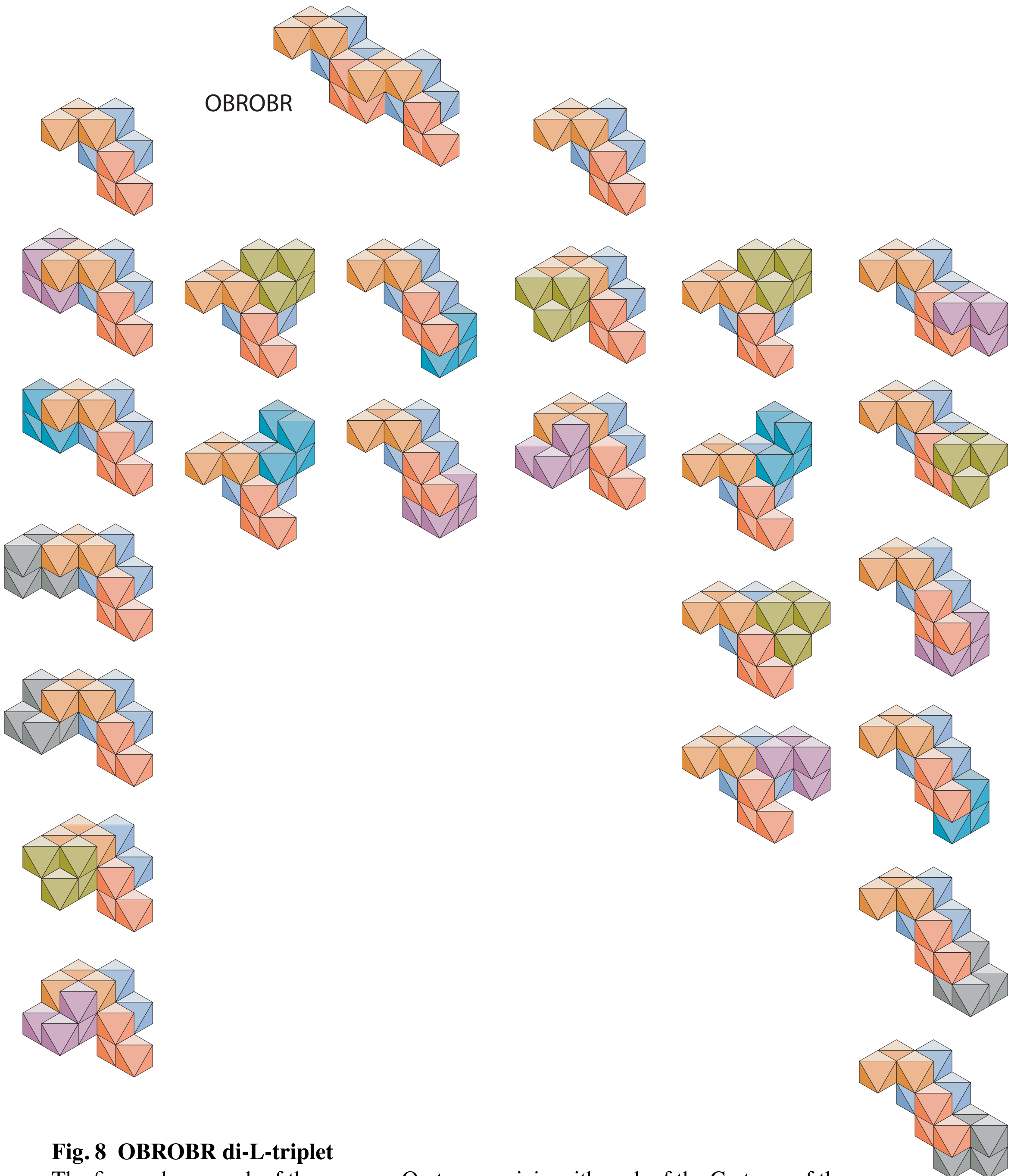

Fig. 8 OBROBR di-L-triplet

The figure shows each of the ways an O-atom can join with each of the C-atoms of the OBROBR di-triplet. The di-triplet has been separated into its two L-triplets to enable a clear view of the O-atom additions. Each of the columns represents one of the C-atoms of the di-triplet. Each of the assemblies in the column has an O-atom joined in a different way to the C-atom which the column represents. There are 960 ways in which the O-atoms can be combined.

The C-atoms of this di-triplet form two turns of a threefold helix whose axis is parallel to a facial diameter of the octahedron.

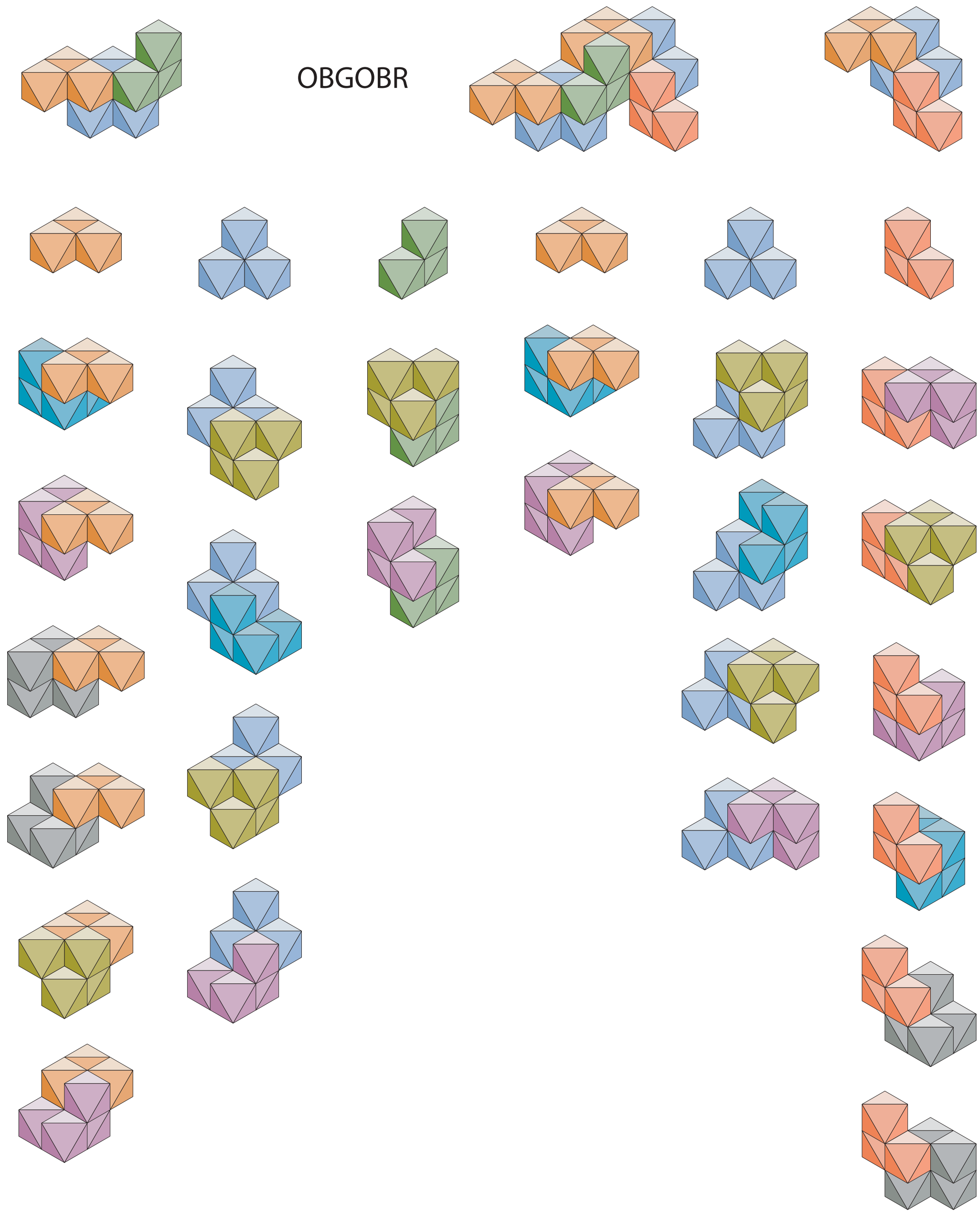

Fig. 9 OBGOBR di-L-triplet

The figure shows each of the ways in which an O-atom can join to each of the C-atoms of the OBGOBR di-L-triplet.

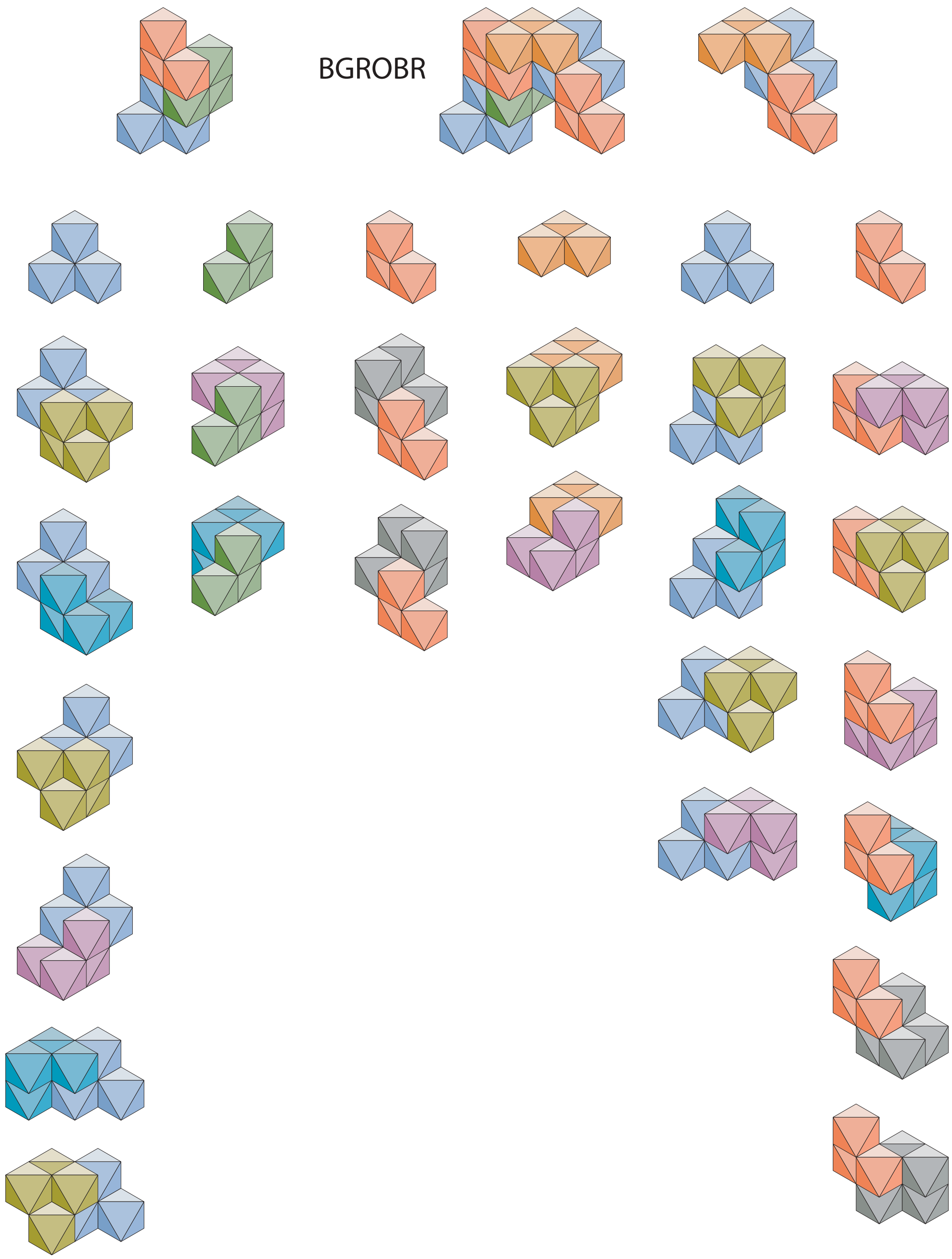

Fig. 10 BGROBR di-L-triplet
The figure shows each of the ways in which an O-atom can join to each of the C-atoms of the BGROBR di-L-triplet.

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