AN INVESTIGATION OF SYMMETRY OPERATIONS WITH CLIFFORD ALGEBRA

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After presenting Clifford algebra and quaternions, the symmetry operations with Clifford algebra and quaternions are defined. This symmetry operations are applied to a Platonic solid, which is called as dodecahedron. Also, the vertices of a dodecahedron presented in the Cartesian coordinates are calculated.

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1 Introduction

The geometric algebra produces the new fields of view in the modern mathematical physics, definition of bodies and rearranging for equations of mathematics and physics. The new mathematical approaches play an important role in the progress of physics.

Wessel, Argand and Gauss used the complex numbers in the solutions of two-dimensional problems. The exponential form of complex numbers is useful in the theory of rotational motions. The quaternion algebra, which was defined by Sir W. R. Hamilton, was generalized for the three dimensional complex numbers [1]. The quaternion algebra is the Clifford algebra of the two-dimensional anti-Eucliedean space. Quaternions in the three-dimensional spaces have more useful appearances for the subalgebras of Clifford algebra. We know that Grassmann was affected from Hamilton. This can be easily understood from Grassmann's studies. In the n-dimensional spaces, Grassmann carried on the studies for the multi-dimensional bodies and defined the central product, which includes the both interior and exterior products. The Grassmann's central product is the Clifford product of vectors. This result was found by Grassmann independently from Clifford. Later, Clifford tried to combine the Grassmann's algebra and quaternions in a mathematical system. Then this study, which was entitled "Application of Grassmann's Extensive Algebra", was published [2].

Today, Clifford algebra has an important role in the investigations of the symmetry properties of systems, crystallography, molecular and solid state physics.

The method of point groups in the multi-dimensional spaces is derived by transforming in to the parameters of the reflections and possible rotational operations. In the three-dimensional spaces, Altmann showed that the Euler's angles are not useful for the rotational operations but the Euler-Rodriques' parameters are more advantageous [3]. To know the rotational pole and

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angle for each rotational operations is necessary and enough. So, there is a similarity between the proper and improper operations in \mathbb{R}^3 .

The rest of paper is organized within 4 sections. Section 2 reveals the quaternions and symmetry operations in \mathbb{R}^3 . In section 3, the Clifford algebra and symmetry operations are showed. An application of the symmetry operations with Clifford algebra is given in section 4. Conclusions are drawn in the last section.

2 Quaternions and Symmetry Operations in \mathbb{R}^3

A quaternion is a quantity represented symbolically by \mathbf{A} and it is defined through the following equations

$$\mathbf{A} = \mathbf{a}\mathbf{1} + A_x \mathbf{i} + A_y \mathbf{j} + A_z \mathbf{k},\tag{1}$$

or

$$\mathbf{A} = [\mathbf{a}, \vec{\mathbf{A}}], \ \vec{\mathbf{A}} = (A_x, A_y, A_z), \tag{2}$$

where all a, A_x , A_y , A_z coefficients are the real numbers. The unitary quaternions **i**, **j**, **k** satisfy the multiplication rules as follows:

$$\mathbf{i} \mathbf{j} = \mathbf{k}, \ \mathbf{j} \mathbf{i} = -\mathbf{k}, \ \mathbf{j} \mathbf{k} = \mathbf{i}, \ \mathbf{k} \mathbf{j} = -\mathbf{i}, \ \mathbf{i} \mathbf{k} = -\mathbf{j}, \ \mathbf{k} \mathbf{i} = \mathbf{j}.$$
 (3)

Also i, j and k can be written as \mathbf{e}_1 , \mathbf{e}_2 and \mathbf{e}_3 , reciprocally. The vector quaternion **A** with components $[0, A_x, A_y, A_z]$ and a vector $\overrightarrow{\mathbf{A}}$ of the Euclidean tridimensional space with components (A_x, A_y, A_z) are reciprocally associated [4].

If A and B quaternions are

$$\mathbf{A} = \mathbf{a}\mathbf{1} + A_x \mathbf{e}_1 + A_y \mathbf{e}_2 + A_z \mathbf{e}_3 = [\mathbf{a}, \mathbf{A}],\tag{4}$$

and

$$\mathbf{B} = \mathbf{b}\mathbf{1} + B_x \mathbf{e}_1 + B_y \mathbf{e}_2 + B_z \mathbf{e}_3 = [\mathbf{b}, \mathbf{B}'],\tag{5}$$

the product of two quaternions, namely A and B, is given by

$$\mathbf{AB} = [\mathbf{ab} - \overrightarrow{\mathbf{A}} \cdot \overrightarrow{\mathbf{B}}, \mathbf{a}\overrightarrow{\mathbf{B}} + \mathbf{b}\overrightarrow{\mathbf{A}} + \overrightarrow{\mathbf{A}} \times \overrightarrow{\mathbf{B}}],\tag{6}$$

$$\mathbf{AB} = (\mathbf{ab} - A_x B_x - A_y B_y - A_z B_z) + \mathbf{e}_1 (A_x \mathbf{b} + \mathbf{a} B_x + A_y B_z - A_z B_y) + \mathbf{e}_2 (\mathbf{a} B_y + A_y \mathbf{b} - A_x B_z + A_z B_x) + \mathbf{e}_3 (\mathbf{a} B_z + A_z \mathbf{b} + A_x B_y - A_y B_x),$$
(7)

where the result is a quaternion. It must be noted that the product of quaternions is not commutative, but associative. The product of A and B quaternions in the matrix form can be written as

$$\mathbf{AB} = (1, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) \begin{bmatrix} a & -A_x & -A_y & -A_z \\ A_x & a & -A_z & A_y \\ A_y & A_z & a & -A_x \\ A_z & -A_y & A_x & a \end{bmatrix} \begin{bmatrix} b \\ B_x \\ B_y \\ B_z \end{bmatrix}$$
$$= (1, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) \begin{bmatrix} 1 \\ C_x \\ C_y \\ C_z \end{bmatrix}.$$
(8)

We can calculate the quaternion product of A, B and C quaternions,

ABC =

$$(1, \mathbf{e}_{1}, \mathbf{e}_{2}, \mathbf{e}_{3}) \begin{bmatrix} \mathbf{a} & -A_{x} & -A_{y} & -A_{z} \\ A_{x} & \mathbf{a} & -A_{z} & A_{y} \\ A_{y} & A_{z} & \mathbf{a} & -A_{x} \\ A_{z} & -A_{y} & A_{x} & \mathbf{a} \end{bmatrix} \begin{bmatrix} \mathbf{b} & -B_{x} & -B_{y} & -B_{z} \\ B_{y} & B_{z} & \mathbf{b} & -B_{z} \\ B_{z} & -B_{y} & B_{x} & \mathbf{b} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ C_{x} \\ C_{y} \\ C_{z} \end{bmatrix}$$
(9)
$$= (1, \mathbf{e}_{1}, \mathbf{e}_{2}, \mathbf{e}_{3}) \begin{bmatrix} 1 \\ D_{x} \\ D_{y} \\ D_{z} \end{bmatrix},$$

where **D** is equivalent to a quaternion. Also, each quaternion matrix is determined by the first column (or row) alone, which simplifies the construction of the corresponding (4×4) -matrix algebra considerably.

For each quaternion A, its conjugate is [5]

$$\mathbf{A}^* = \mathbf{a}\mathbf{1} - A_x \mathbf{e}_1 - A_y \mathbf{e}_2 - A_z \mathbf{e}_3. \tag{10}$$

The rotation of arbitrary points on an unit sphere ($\mathbf{R}(\gamma \mathbf{k})$) can be defined by γ angle around of the definite k-axis ($0 \le \gamma \le \pi$). The poles of rotational operations are defined on the every half-sphere. In general, the rotations (counterclokwise) are accepted to be positive direction. If $\mathbf{R}(\beta \mathbf{l})$ and $\mathbf{R}(\alpha \mathbf{m})$ are the rotations with β and α angles around of \mathbf{l} and \mathbf{m} axes, respectively, then the result of two rotational operations has to be equal to a new rotation with γ -angle around of k- axis, *i.e.*

$$\mathbf{R}(\beta \mathbf{l}) \ \mathbf{R}(\alpha \mathbf{m}) = \mathbf{R}(\gamma \mathbf{k}), \tag{11}$$

where k, l, m are the axial vectors that correspond to the k, l, m rotation axes, respectively. Rodriques [6] defined the geometrical structure and algebra for the angles γ , β , α and the axes k, l, m in the following forms

$$\cos\frac{\gamma}{2} = \cos\frac{\alpha}{2}\cos\frac{\beta}{2} - \sin\frac{\alpha}{2}\sin\frac{\beta}{2}\mathbf{m}\cdot\mathbf{l},\tag{12}$$

$$\sin\frac{\gamma}{2}\mathbf{k} = \sin\frac{\alpha}{2}\cos\frac{\beta}{2}\mathbf{m} - \cos\frac{\alpha}{2}\sin\frac{\beta}{2}\mathbf{l} + \sin\frac{\alpha}{2}\sin\frac{\beta}{2}\mathbf{m} \times \mathbf{l}.$$
(13)

The rotational operations with the normalized quaternions can be written as

$$\mathbf{R}(\alpha \mathbf{m}) = \left[\cos\frac{\alpha}{2}, \sin\frac{\alpha}{2}\mathbf{m}\right],\tag{14}$$

$$\mathbf{R}(\beta \mathbf{l}) = \left[\cos\frac{\beta}{2}, \sin\frac{\beta}{2}\mathbf{l}\right].$$
(15)

In the similar way, from eqs. (11, 14, 15), $\mathbf{R}(\gamma \mathbf{k})$ can be defined by the following equations

$$\mathbf{R}(\gamma \mathbf{k}) = \left[\cos\frac{\alpha}{2}, \sin\frac{\alpha}{2}\mathbf{m}\right] \left[\cos\frac{\beta}{2}, \sin\frac{\beta}{2}\mathbf{l}\right],\tag{16}$$

$$\mathbf{R}(\gamma \mathbf{k}) = \left[\cos\frac{\gamma}{2}, \sin\frac{\gamma}{2}\mathbf{k}\right].$$
(17)

Any point represented by \mathbf{R} quaternion transforms to the a new quaternionic point at the end of a rotation defined by \mathbf{A} unit quaternion. This new quaternion is

$$\mathbf{R}' = \mathbf{A} \mathbf{R} \mathbf{A}^*, \tag{18}$$

where \mathbf{A}^* is complex conjugate of \mathbf{A} .

3 Clifford Algebra and Symmetry Operations

Clifford algebra in physics is used for the studies of symmetry. There are three basic units e_i (*i*=1, 2, 3) in Clifford algebra such that

$$\mathbf{e}_i \mathbf{e}_j + \mathbf{e}_j \mathbf{e}_i = 2\delta_{ij},\tag{19}$$

which are equivalent to

$$\mathbf{e}_i \mathbf{e}_j = 1, \tag{20}$$

$$\mathbf{e}_i \mathbf{e}_j = -\mathbf{e}_j \mathbf{e}_i. \tag{21}$$

Using \mathbf{e}_1 , \mathbf{e}_2 and \mathbf{e}_3 , which are the terms of second and third rank, $\mathbf{e}_i \mathbf{e}_j$ and $\mathbf{e}_i \mathbf{e}_j \mathbf{e}_k$, can be defined as follows [7]:

$$\mathbf{e}_1 \mathbf{e}_1 = 1, \tag{22}$$

$$(\mathbf{e}_2\mathbf{e}_1)(\mathbf{e}_2\mathbf{e}_1) = \mathbf{e}_2\mathbf{e}_1\mathbf{e}_2\mathbf{e}_1 = -\mathbf{e}_2\mathbf{e}_1\mathbf{e}_1\mathbf{e}_2 = -1,$$
(23)

$$(\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3)(\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3) = -1.$$
 (24)



Fig. 1. Directional area with e_1 and e_1

The result of e_1e_2 product is neither scalar nor vector. This product is called bivector. The e_1e_2 product is represented by e_{12} that shows the oriented plane area of the square with sides e_1 and e_2 .

1, \mathbf{e}_1 , \mathbf{e}_2 , \mathbf{e}_{12} form the basis of the Clifford algebra Cl_2 of the vector plane \mathbb{R}^2 . An arbitrary element of Cl_2 is

$$\mathbf{u} = u_0 + u_1 \mathbf{e}_1 + u_2 \mathbf{e}_2 + u_{12} \mathbf{e}_{12},\tag{25}$$

where $u, u_1, u_2, u_{12} \in \mathbb{R}$. The Clifford algebra Cl_2 is the four-dimensional linear space and its basis elements have the multiplication Table 1 as follows:

Table 1. The basis of Clifford Algebra

The basis of Clifford Algebra	\mathbf{e}_1	\mathbf{e}_2	\mathbf{e}_{12}
\mathbf{e}_1	1	\mathbf{e}_{12}	\mathbf{e}_2
\mathbf{e}_2	$-{f e}_{12}$	1	$-\mathbf{e}_1$
\mathbf{e}_{12}	$-\mathbf{e}_2$	\mathbf{e}_1	-1

The Clifford product of two vectors, namely $\overrightarrow{\mathbf{a}}$ and $\overrightarrow{\mathbf{b}}$, with components

$$\vec{\mathbf{a}} = a_1 \mathbf{e}_1 + a_2 \mathbf{e}_2,\tag{26}$$

and

$$\overrightarrow{\mathbf{b}} = b_1 \mathbf{e}_1 + b_2 \mathbf{e}_2,\tag{27}$$

is given by



Fig. 2. The geometrical meaning of $\overrightarrow{\mathbf{a}} \wedge \overrightarrow{\mathbf{b}}$.

$$\overrightarrow{\mathbf{a}} \quad \overrightarrow{\mathbf{b}} = \overrightarrow{\mathbf{a}} \cdot \overrightarrow{\mathbf{b}} + \overrightarrow{\mathbf{a}} \wedge \overrightarrow{\mathbf{b}} = a_1 b_1 + a_2 b_2 + (a_1 b_2 - a_2 b_1) \mathbf{e}_{12}, \tag{28}$$

where " \wedge " is called as the wedge product [7].

The bivector $\vec{a} \wedge \vec{b}$ represents the oriented plane segment of the parallelogram with sides \vec{a} and \vec{b} . The magnitude of the bivector $\vec{a} \wedge \vec{b}$ is the area of this parallelogram, *i.e.*

$$\left|\overrightarrow{\mathbf{a}} \wedge \overrightarrow{\mathbf{b}}\right| = \left|a_1 b_2 - b_1 a_2\right|. \tag{29}$$

The bivectors $\vec{a} \wedge \vec{b}$ and $\vec{b} \wedge \vec{a}$ have the same magnitude but opposite senses of rotation. This can be expressed as

$$\vec{\mathbf{a}} \wedge \vec{\mathbf{b}} = -\vec{\mathbf{b}} \wedge \vec{\mathbf{a}}.$$
 (30)

The reflection of $\overrightarrow{\mathbf{r}}$ across the line $\overrightarrow{\mathbf{a}}$, namely the mirror image $\overrightarrow{\mathbf{r}}$ of $\overrightarrow{\mathbf{r}}$ with respect to $\overrightarrow{\mathbf{a}}$, is given by

$$\overrightarrow{\mathbf{r}}' = \overrightarrow{\mathbf{a}} \ \overrightarrow{\mathbf{r}} \ \overrightarrow{\mathbf{a}}^{-1}. \tag{31}$$

Equation (31) can be directly obtained from using the commutation properties of Clifford algebra [7]. The composition of two reflections, first across \vec{a} and then across \vec{b} , is given by

$$\widetilde{\mathbf{r}}' = \overrightarrow{\mathbf{b}} \ \overrightarrow{\mathbf{r}}' \ \overrightarrow{\mathbf{b}}^{-1} = \overrightarrow{\mathbf{b}} (\overrightarrow{\mathbf{a}} \ \overrightarrow{\mathbf{r}} \ \overrightarrow{\mathbf{a}}^{-1}) \ \overrightarrow{\mathbf{b}}^{-1} = (\overrightarrow{\mathbf{b}} \ \overrightarrow{\mathbf{a}}) \ \overrightarrow{\mathbf{r}} \ (\overrightarrow{\mathbf{b}} \ \overrightarrow{\mathbf{a}})^{-1}.$$
(32)

The composite of these two reflections is a rotation by twice the angle between \overrightarrow{a} and \overrightarrow{b} .



Fig. 3. The rotation and reflection operations of $\overrightarrow{\mathbf{a}}$ and $\overrightarrow{\mathbf{b}}$ vectors.

Now, the symmetry operations in the three-dimensional space must be mapped on the elements of the Clifford algebra, Cl_3 [8]. The Clifford algebra Cl_3 of \mathbb{R}^3 is the real associative algebra generated by the set of \mathbf{e}_1 , \mathbf{e}_2 , \mathbf{e}_3 , which are the eight-dimensional with the following basis

An arbitrary element in Cl_3 is a sum of a scalar, a vector, a bivector and a volume element, and can be written as

$$\mathbf{u} = u_0 + u_1 \mathbf{e}_1 + u_2 \mathbf{e}_2 + u_3 \mathbf{e}_3 + u_{12} \mathbf{e}_{12} + u_{13} \mathbf{e}_{13} + u_{23} \mathbf{e}_{23} + u_{123} \mathbf{e}_{123}.$$
 (34)

The Clifford units, \mathbf{e}_i 's, are identified with orthogonal reflections (mirrors)

$$\mathbf{e}_1 \leftrightarrow \sigma_{yz}, \, \mathbf{e}_2 \leftrightarrow \sigma_{xz}, \, \mathbf{e}_3 \leftrightarrow \sigma_{xy}. \tag{35}$$

The mappings between the Clifford bivectors $\mathbf{e}_i \mathbf{e}_j$ and the corresponding quaternion units are defined

$$\mathbf{e}_{3}\mathbf{e}_{2} \leftrightarrow \sigma_{xy}\sigma_{xz} = C_{2x} \leftrightarrow [0, (1, 0, 0)], \tag{36}$$

$$\mathbf{e}_1 \mathbf{e}_3 \leftrightarrow \sigma_{yz} \sigma_{xy} = C_{2y} \leftrightarrow [0, (0, 1, 0)], \tag{37}$$

$$\mathbf{e}_2 \mathbf{e}_1 \leftrightarrow \sigma_{xz} \sigma_{yz} = C_{2z} \leftrightarrow [0, (0, 0, 1)]. \tag{38}$$



Fig. 4. A dodecahedron, whose vertices are indexed as Cartesian coordinates in Table 3

The inversion, which is a product of three reflections, is obtained by a trivector as follows:

$$\mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3 \leftrightarrow \sigma_{yz} \sigma_{xz} \sigma_{xy} = i, \tag{39}$$

where $\mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3 \in Cl_3$ is performed.

4 An Application of The Symmetry Operations with Clifford Algebra

The reflection and rotation operations in the solid state physics and molecular physics play an important role. The symmetry operations can be easily applied on the regular polyhedra, which are called *Platonic Solids*. The Platonic solids are tetrahedron, cube, octahedron, icosahedron and dodecahedron. Some important numbers for the Platonic solids are shown in Table 2.

Table 2. Numbers for the five Platonic solids

	Number of faces	Number of edges	Number of vertices	Edges per face
Tatushaduau	1	6	о 4	2
Cuba	4	0	4	5
Cube	0	12	8	4
Uctanedron	8 20	12	0	2
Dodecabedron	12	30	20	5
Douccalleuron	12	30	20	5

A dodecahedron has twenty-vertices. The vertices of a dodecahedron, whose origin was chosen at the centre of body, are indexed as cartesian coordinates in Table 3.

Assuming the distances of midpoints of all the edges to the origin of the dodecahedron are normalized, we provide the cartesian coordinates of the 20 numbered vertices in Table 3.

Table 3. The vertices of a dodecahedron for the model shown in Fig. 4.

no	х	У	z
1	0.618	0.618	-0.618
2	-0.618	0.618	-0.618
3	-0.618	-0.618	-0.618
4	0.618	-0.618	-0.618
5	0.618	0.618	0.618
6	-0.618	0.618	0.618
7	-0.618	-0.618	0.618
8	0.618	-0.618	0.618
9	0	1	-0.382
10	0	1	0.382
11	1	0.382	0
12	1	-0.382	0
13	0	-1	0.382
14	0	-1	-0.382
15	0.382	0	-1
16	-0.382	0	-1
17	-1	0.382	0
18	-1	-0.382	0
19	-0.382	0	1
20	0.382	0	1

Now, for example, from eqs.(9), (10) and (18), the C_2 rotation of 19th vertex around the z-axis is

$\mathbf{R}' =$	$\mathbf{A}_{\mathbf{z}}\mathbf{R}$	$_{19}\mathbf{a}_{\mathrm{z}}^{*}$								
=	$\left[\begin{array}{c} 0\\ 0\\ 0\\ 1\end{array}\right]$	${0 \\ 0 \\ 1 \\ 0 }$	$\begin{array}{c} 0 \\ -1 \\ 0 \\ 0 \end{array}$	$\begin{bmatrix} -1\\0\\0\\0 \end{bmatrix}$	$\begin{array}{c} 0\\ -0.382\\ 0\\ 1\end{array}$	$\begin{array}{c} 0.382 \\ 0 \\ 1 \\ 0 \end{array}$	$\begin{array}{c} 0 \\ -1 \\ 0 \\ -0.382 \end{array}$	$\begin{array}{c} -1 \\ 0 \\ 0.382 \\ 0 \end{array}$	$\left[\begin{array}{c}0\\0\\-1\end{array}\right]$	
=) 882) L	,							(40)

where A_z , R_{19} and a_z^* are the (4×4)-matrix representations of rotation z-axis and 19th vertex,

 (4×1) -column matrix representation of the (4×4) matrix of \mathbf{A}_{z}^{*} respectively. This result of the matrix operation defines the 20th vertex of the dodecahedron.

This method is the conventional geometrical method of the rotation operation for dodecahedron. Using quaternions, the same calculation can be obtained as follows:

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$$\mathbf{R}' = \mathbf{a}_{z} \ \mathbf{R}_{19} \ \mathbf{a}_{z}^{*},$$

$$= (a_{z_{0}} \mathbf{e}_{0} + a_{z_{1}} \mathbf{e}_{1} + a_{z_{2}} \mathbf{e}_{2} + a_{z_{3}} \mathbf{e}_{3})$$

$$\times (\mathbf{R}_{19_{0}} \mathbf{e}_{0} + \mathbf{R}_{19x} \mathbf{e}_{1} + \mathbf{R}_{19y} \mathbf{e}_{2} + \mathbf{R}_{19z} \mathbf{e}_{3}) (a_{z_{0}} \mathbf{e}_{0} + a_{z_{1}} \mathbf{e}_{1} + a_{z_{2}} \mathbf{e}_{2} + a_{z_{3}} \mathbf{e}_{3})$$

$$= (1\mathbf{e}_{3})(-0, 382\mathbf{e}_{1} + 1\mathbf{e}_{3})(-1\mathbf{e}_{3}) = (0.382\mathbf{e}_{1} + 1\mathbf{e}_{3}).$$

$$(41)$$

This result is equal to the quaternionic definition of 20th vertex, as well.

Now we investigate another rotation operation of 20th vertex around the straight line, which connects the 5th vertex to origin. The rotation 120° of 20th vertex around this straight line named \mathbf{a}_5 must give the 11th vertex. From the eq. (18), **R**' is

$$\mathbf{R}' = \mathbf{a}_5 \ \mathbf{R}_{20} \ \mathbf{a}_5^*, \tag{42}$$

where $\mathbf{a_5}$ and \mathbf{R}_{20} are the quaternions representing the rotation axis and 20th vertex. \mathbf{a}_5^* is the quaternion, which is the complex conjugate of $\mathbf{a_5}$. The quaternion $\mathbf{a_5}$ can be written as

$$\mathbf{a}_5 = \mathbf{e}_0 \cos\left(\frac{120^\circ}{2}\right) + \vec{\mathbf{a}}_5 \sin\left(\frac{120^\circ}{2}\right). \tag{43}$$

 $\vec{\mathbf{a}}_5$ denotes a pure unit quaternion that describes the direction of the rotation axis. $\vec{\mathbf{a}}_5$ can be written in terms of the direction cosines with the cartesian axes as follows [9]:

$$\vec{\mathbf{a}}_{5} = \frac{a_{5x}}{\sqrt{a_{5x}^{2} + a_{5y}^{2} + a_{5z}^{2}}} \mathbf{e}_{1} + \frac{a_{5y}}{\sqrt{a_{5x}^{2} + a_{5y}^{2} + a_{5z}^{2}}} \mathbf{e}_{2} + \frac{a_{5z}}{\sqrt{a_{5x}^{2} + a_{5y}^{2} + a_{5z}^{2}}} \mathbf{e}_{3} = \frac{0.618}{\sqrt{0.618^{2} + 0.618^{2} + 0.618^{2}}} \mathbf{e}_{1} + \frac{0.618}{\sqrt{0.618^{2} + 0.618^{2} + 0.618^{2}}} \mathbf{e}_{2} + \frac{0.618}{\sqrt{0.618^{2} + 0.618^{2} + 0.618^{2}}} \mathbf{e}_{3}.$$
(44)

Then equation (43) becomes

$$\mathbf{a}_5 = 0.5\mathbf{e}_0 + 0.5\mathbf{e}_1 + 0.5\mathbf{e}_2 + 0.5\mathbf{e}_3. \tag{45}$$

The quaternion \mathbf{R}' , which gives 11th vertex, is found as follows:

$$\mathbf{R}' = (0.5\mathbf{e}_0 + 0.5\mathbf{e}_1 + 0.5\mathbf{e}_2 + 0.5\mathbf{e}_3)(0.382\mathbf{e}_1 + 1\mathbf{e}_3)(0.5\mathbf{e}_0 - 0.5\mathbf{e}_1 - 0.5\mathbf{e}_2 - 0.5\mathbf{e}_3)$$

= 1\mathbf{e}_1 + 0.382\mathbf{e}_2. (46)

Let us apply to the two consecutive operations for 20th vertex. After the 20th vertex is rotated of 120° around the straight line, which connects the 5th vertex to origin, we obtain the 11th vertex.

This 11th vertex will be rotated around the z-axis with 180° , as well. At the end of this operation, the quaternionic definition of vertex \mathbf{R}'' is found as

$$\mathbf{R}'' = \mathbf{a}_{z} \mathbf{R}' \mathbf{a}_{z}^{*}$$
(47)
= $\mathbf{a}_{z} (\mathbf{a}_{5} \mathbf{R}_{20} \mathbf{a}_{5}^{*}) \mathbf{a}_{z}^{*}$
= $(\mathbf{a}_{z} \mathbf{a}_{5}) \mathbf{R}_{20} (\mathbf{a}_{z} \mathbf{a}_{5})^{*}$
= $((1\mathbf{e}_{3}) (0.5\mathbf{e}_{0} + 0.5\mathbf{e}_{1} + 0.5\mathbf{e}_{2} + 0.5\mathbf{e}_{3})) (0.382\mathbf{e}_{1} + 1\mathbf{e}_{3})$
× $((1\mathbf{e}_{3}) (0.5\mathbf{e}_{0} + 0.5\mathbf{e}_{1} + 0.5\mathbf{e}_{2} + 0.5\mathbf{e}_{3}))^{*}$
= $-\mathbf{e}_{1} - 0.382\mathbf{e}_{2},$

here this result is equal to the quaternionic definition of 18th vertex as well.

The reflection operations can be also defined by the Clifford algebra elements. According to the xz-plane, the reflection of 10th vertex with Clifford algebra is

$$\mathbf{R}' = \sigma_{\mathbf{x}\mathbf{z}} \mathbf{R}_{10} \sigma_{\mathbf{x}\mathbf{z}}^{-1}$$
(48)
= $\mathbf{e}_{13}(\mathbf{e}_2 + 0.382\mathbf{e}_3)\mathbf{e}_{13}$
= $-\mathbf{e}_2 + 0.382\mathbf{e}_3,$

where σ_{xz}^{-1} is the inverse of σ_{xz} operation. The reflection of 10th vertex on the xz-plane is equal to the 13th vertex. After this reflection of the 10th vertex on the xz-plane, the reflection of 13th vertex on the xy-plane can be written as

$$\mathbf{R}'' = \sigma_{\mathbf{xy}} \mathbf{R}' \sigma_{\mathbf{xy}}^{-1}$$

$$= \sigma_{\mathbf{xy}} (\sigma_{\mathbf{xz}} \mathbf{R}_{10} \sigma_{\mathbf{xz}}^{-1}) \sigma_{\mathbf{xy}}^{-1}$$

$$= (\sigma_{\mathbf{xy}} \sigma_{\mathbf{xz}}) \mathbf{R}_{10} (\sigma_{\mathbf{xy}} \sigma_{\mathbf{xz}})^{-1}$$

$$= (-\mathbf{e}_{23}) (\mathbf{e}_{2} + 0.382 \mathbf{e}_{3}) (-\mathbf{e}_{32})$$

$$= -\mathbf{e}_{2} - 0.382 \mathbf{e}_{3}.$$

$$(49)$$

This result is equal to the quaternionic definition of 14th vertex in Table 3.

5 Conclusions

The geometrical methods and matrices are used for the investigation of symmetry operations of the symmetric solid. Clifford algebras are algebras of geometries and quaternions are hypercomplex numbers. In this study, Clifford algebra and quaternions are used for the symmetry operations. When these operations are made with Clifford algebra and quaternions, it is obvious that the calculations are easy and compact. The quaternions and Clifford algebra are much simpler to apply to the symmetry operations than the conventional methods of molecular symmetry. This method can be applied to the more complex structures. Also the computer programming of this calculations with Clifford algebra and quaternions may be easier than the usual methods.

References

- M. Kline: Mathematical Though from Ancient to Modern Times. Oxford University Press, Oxford (1972)
- [2] W.K. Clifford: Am. J. Math 1 (1878) 350
- [3] S.L. Altmann: Rotations, quaternions, and double groups. Clarendon Press, Oxford (1994)
- [4] J. Funda, R.P. Paul: in Proc. of 1988 IEEE Int. Conference on Robotics and Automation , Philadelphia (1988), p.886
- [5] M. Tanışlı: Acta Phys. Slov. 53 (2003) 253
- [6] O. Rodriques: Journal de Mathématiques Pures et Appliquées 5 (1840) 380
- [7] P. Lounesto: Lectures on Clifford Geometric Algebras. TTU Press, Cookeville, TN, USA (2002)
- [8] A. Pokorny, P. Herzig, S.L. Altman: Spectrochimica Acta A 57 (2001) 1931
- [9] H.P. Fritzer: Spectrochimica Acta A 57 (2001) 1919