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Crystallographic Quaternions

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Abstract: Symmetry transformations in crystallography are traditionally represented as equations and matrices, which can be suitable both for orthonormal and crystal reference systems. Quaternion representations, easily constructed for any orientations of symmetry operations, owing to the vector structure based on the direction of the rotation axes or of the normal vectors to the mirror plane, are known to be advantageous for optimizing numerical computing. However, quaternions are described in Cartesian coordinates only. Here, we present the quaternion representations of crystallographic point-group symmetry operations for the crystallographic reference coordinates in triclinic, monoclinic, orthorhombic, tetragonal, cubic and trigonal (in rhombohedral setting) systems. For these systems, all symmetry operations have been listed and their applications exemplified. Owing to their concise form, quaternions can be used as the symbols of symmetry operations, which contain information about both the orientation and the rotation angle. The shortcomings of quaternions, including different actions for rotations and improper symmetry operations, as well as inadequate representation of the point symmetry in the hexagonal setting, have been discussed.

Keywords: symmetry operations; quaternion representation; crystallography; non-Cartesian systems; Cayley table

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1. Introduction

The algebra of quaternions was invented nearly two centuries ago [1–4] and it is often used for technical and scientific applications involving various rotations, as well as in computer graphics [5–8]. In crystallography, quaternions have been applied for positioning diffractometer shafts [9,10], describing disorientations between crystal lattices [11,12], refining orientation matrix during diffraction measurements [13] and rotating and comparing molecules [14–17]. However, the applications of quaternions for representing symmetry operations are scarce and, like most of the quaternion calculations, they are limited to the orthonormal reference systems [18,19]. Owing to the easy and appealing algebra of quaternions, their application for transforming vectors described in crystallographic reference systems can be presented in a simple intuitive manner. A limitation is that all applications of quaternions in crystallography presented in the literature are described for Cartesian systems [20]. Presently, we discuss the application of quaternions for representing symmetry operations of vectors described in the reference axes of crystallographic systems. In this project, we aimed at investigating the applicability of quaternions representing point-symmetry operations for non-Cartesian reference systems of crystals, describing the transformations of vectors by using quaternions as well as generating new symmetry operations from others by combining (multiplying) their quaternion representations. While the quaternions were originally constructed for the orthogonal space, the crystallographic systems are, in general, non-Cartesian. For this reason, we have undertaken to derive quaternions representing symmetry operations in traditional crystallographic systems.

It will be shown that the quaternion representation of symmetry operations in crystallographic reference systems can be more concise than the equivalent matrices. Therefore, apart from the consequent simplicity of the notation and reduced number of arithmetic calculations, the direct connection of quaternions with the symmetric directions and the angle of rotation in crystallographic systems can make them more appealing for illustrating and teaching symmetry and point-group concepts. Another purpose of the present study was to investigate the limitations of adopting classical quaternions ($q = s + ui + vj + wk$) for the complete representation of all symmetry operations in non-Cartesian crystallographic reference systems. These limitations can be considered to be the stumbling blocks hindering the common use of quaternions in crystallography. To emphasize our intention to employ the quaternions to crystallographic systems, both the Schönflies and Hermann–Mauguin notations will be used for the symmetry elements and operations.

2. Discussion

2.1. Basic Definitions

Hereafter, the quaternion will be defined as $q = s + ui + vj + wk$, where s, u, v and w are scalars, all $s, u, v, w \subset R$, whereas i, j and k are imaginary versors fulfilling the conditions $i^2 = j^2 = k^2 = ijk = -1$ [2–4]. The quaternion is a four-dimensional version of complex numbers, where s is the real and u, v and w are the imaginary components. Quaternion q can represent a rotation by angle φ about vector $\boldsymbol{v} = [u, v, w]$ in the three-dimensional orthogonal space, when it is written in the following form:

$$q(\varphi,\boldsymbol{v}) = [\cos(\varphi/2) + \boldsymbol{n}\cdot\sin(\varphi/2)] \quad (1)$$

where the unit vector along the axis of rotation is $\boldsymbol{n} = \boldsymbol{v}/|\boldsymbol{v}|$.

2.2. Rotations

Equation (1), directly connecting quaternions with rotations, is well known and it can be generally applied for representing the symmetry operations in orthogonal systems [2–8]. For performing a rotation of a real-space vector $\boldsymbol{r} = [x\ y\ z]$, it should be projected onto the three-dimensional imaginary subspace of four-dimensional quaternions; this projection will be further represented by the same symbol, but with round brackets: $\boldsymbol{r} = (ix + jy + kz)$. Its image $\boldsymbol{r'}$ after the rotation by angle φ about vector $\boldsymbol{v}$, described by quaternion $q(\varphi,\boldsymbol{v})$ (Equation (1)), is equal to

$$\boldsymbol{r'} = q(\varphi,\boldsymbol{v})\cdot\boldsymbol{r}\cdot q^*(\varphi,\boldsymbol{v}) \quad (2)$$

where $q^*(\varphi,\boldsymbol{v})$ is the conjugate of $q(\varphi,\boldsymbol{v})$: $q^*(\varphi,\boldsymbol{v}) = q(\varphi,-\boldsymbol{v})$. Equation (2) is generally applicable for orthonormal (Cartesian) coordinates. Several such rotations are exemplified below.

Let us rotate vector $\boldsymbol{r} = [211]$ by 180° about the plane-diagonal vector [110] in a cubic system. This rotation is represented by the quaternion (Equation (1))

$$q\left(180^\circ, [110]\right) = \left(i/\sqrt{2} + j/\sqrt{2}\right).$$

According to Equation (2),

$$\boldsymbol{r}' = \left(i/\sqrt{2} + j/\sqrt{2}\right)\cdot(2i + 1j + 1k)\cdot\left(-i/\sqrt{2} - j/\sqrt{2}\right) = (i + 2j - k).$$

Thus, the vector components after the 180° rotation about direction [110] are $\boldsymbol{r'} = [1\ 2\ -1]$.

The rotation C_3 of vector $\boldsymbol{r} = [1, 0, 1]$, which in crystallographic coordinates corresponds to $\boldsymbol{r}_c = [1, 1/2, 1]$, about axis [z] can be performed by quaternion $q(120^\circ,[001])$, which according to Equation (1) is $q(120^\circ,[001]) = (1/2 + k\sqrt{3}/2)$. The rotated vector according to Equation (2) is

$$\boldsymbol{r}' = \left(1/2 + k\sqrt{3}\,/2\right)\cdot(1i + 0j + 1k)\cdot\left(1/2 - k\sqrt{3}\,/2\right) = \left(-1/2i + \sqrt{3}\,/2j + k\right).$$

Thus, the vector components after the rotation by 60° about the [001] axis are $\boldsymbol{r}'$ = [−1/2, $\sqrt{3}$/2, 1].

2.3. Efficiency of Quaternions

The quaternion representation of rotations and symmetry operations can be advantageous compared to other representations in certain applications. The most apparent and frequently cited advantage is the easiness of constructing performing any rotation from the rotation axis and angle, as defined in Equations (1) and (2). The matrix representation in a general case requires that the rotation be composed of the Euler rotations about the orthogonal axes:

$$\boldsymbol{R}_{\mathrm{x}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varepsilon_1 & -\sin\varepsilon_1 \\ 0 & \sin\varepsilon_1 & \cos\varepsilon_1 \end{pmatrix},\ \boldsymbol{R}_{\mathrm{y}} = \begin{pmatrix} \cos\varepsilon_2 & 0 & -\sin\varepsilon_2 \\ 0 & 1 & 0 \\ \sin\varepsilon_2 & 0 & \cos\varepsilon_2 \end{pmatrix},\ \boldsymbol{R}_{\mathrm{z}} = \begin{pmatrix} \cos\varepsilon_3 & -\sin\varepsilon_3 & 0 \\ \sin\varepsilon_3 & \cos\varepsilon_3 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

where the aligning angles ε_i (i = 1, 2, 3) can be calculated by using the trigonometric functions. Several variants are possible, for example, first, the rotation axis $\boldsymbol{v}$ can be rotated by angle ε_3 about axis $\boldsymbol{z}$ to bring it to the $\boldsymbol{xz}$ plane (matrix $\boldsymbol{R}_z$ multiplied by $\boldsymbol{v}$); subsequently, this new position of $\boldsymbol{v}$ can be rotated by angle ε_2 about axis $\boldsymbol{y}$ by matrix $\boldsymbol{R}_{\mathrm{y}}$, to overlie vector $\boldsymbol{v}$ with axis $\boldsymbol{x}$. For the so-aligned $\boldsymbol{v}$ axis, the rotation by angle φ is performed by the rotation matrix

$$\boldsymbol{R}_x(\varphi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & \sin\varphi & \cos\varphi \end{pmatrix}$$

Subsequently, the system should be rotated back by the reverse matrices of $\boldsymbol{R}_{\mathrm{z}}$ and $\boldsymbol{R}_{\mathrm{y}}$; hence, the matrix rotation of vector $\boldsymbol{r}$ by angle φ around vector $\boldsymbol{v}$ can be written as

$$\boldsymbol{r}' = \boldsymbol{R}_{\mathbf{z}}{}^{-1}\cdot\boldsymbol{R}_{\mathrm{x}}{}^{-1}\cdot\boldsymbol{R}_{\mathbf{x}}(\varphi)\cdot\boldsymbol{R}_{\mathbf{x}}\cdot\boldsymbol{R}_{\mathbf{z}}\cdot\boldsymbol{r}$$

Only the cubic system is consistent with the Cartesian reference system, as the unit cell parameters fulfil the orthonormal conditions $a = b = c$ and $\alpha = \beta = \gamma = 90°$. Crystallographic systems—tetragonal, hexagonal, trigonal, orthorhombic, monoclinic and triclinic—gradually depart from the orthonormal setting, with the most 'skew' being the triclinic system, where all a, b, and c are different in length and all α, β and γ divert from 90°.

Before using the Euler matrices, any non-Cartesian system should be orthogonalized. The most general case is for a triclinic crystal. Its unit cell parameters, a, b, c, α, β and γ, can be used for constructing a lower-triangular orthogonalization matrix $\boldsymbol{L}$ [21]:

$$\boldsymbol{L} = \begin{pmatrix} a\cdot\sin\beta\cdot\sin\gamma* & 0 & 0 \\ -a\cdot\sin\beta\cdot\cos\gamma* & b\cdot\sin\alpha & 0 \\ a\cdot\sin\beta & b\cdot\cos\alpha & c \end{pmatrix},$$

where $\cos\gamma^* = (\cos\alpha\cdot\cos\beta - \cos\gamma)/(\sin\alpha\cdot\sin\beta)$ and $\sin\gamma^* = (1 - \cos^2\gamma^*)^{1/2}$. The $\boldsymbol{L}$ matrix above would not generally preserve the crystal symmetric direction; for example, in a monoclinic system, the crystal symmetry direction [010], in the orthogonalized coordinates, would become [0, $b\sin\alpha$, $b\cos\beta$]. Thus, the rotation axis vector $\boldsymbol{v}$ requires orthogonalization, too. For returning to the crystallographic reference system, the rotation of the vector should

be transformed back by multiplying by the reverse of the orthogonalization matrix, $\boldsymbol{L}^{-1}$, so the formula above further complicates to

$$\boldsymbol{r}' = \boldsymbol{L}^{-1}\cdot\boldsymbol{R_z}^{-1}\cdot\boldsymbol{R}_{\mathrm{x}}{}^{-1}\cdot\boldsymbol{R_x}(\varphi)\cdot\boldsymbol{R_x}\cdot\boldsymbol{R_z}\cdot\boldsymbol{L}\cdot\boldsymbol{r}$$

The quaternion representation of this rotation by angle φ about vector $\boldsymbol{v}$, as defined in Equations (1) and (2), is straightforward and more concise. While there is no doubt about the concise form of the quaternion representation in Cartesian reference systems, to our knowledge direct quaternion transformations in non-Cartesian systems have not been explored, and the purpose of this work is to check the possibility of using the quaternion representations of point-group symmetry operations directly in crystallographic coordinates. The strength of matrix representations, commonly used in crystallography, is that the step transformations can be easily combined through the multiplication of matrices, which would reduce the above formula to $\boldsymbol{r}' = \boldsymbol{T}(\varphi)\cdot\boldsymbol{r}$, where $\boldsymbol{T}(\varphi) = \boldsymbol{L}^{-1}\cdot\boldsymbol{R_z}^{-1}\cdot\boldsymbol{R}_{\mathrm{x}}{}^{-1}\cdot\boldsymbol{R_x}(\varphi)\cdot\boldsymbol{R_x}\cdot\boldsymbol{R_z}\cdot\boldsymbol{L}$. Depending on the type of rotation, the comparison of the number of arithmetic operations can be more or less advantageous for the matrix and quaternion representations.

For example, finding a rotation about the 3-fold axis along direction [111] in a trigonal *R* lattice through the Euler rotations about the axes of orthogonalized reference system requires hundreds of arithmetic operations, including trigonometric functions, but as indicated above, they can be reduced to the matrix equation

$$\begin{pmatrix} y \\ z \\ x \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

The quaternion equation can be straightforwardly written following Equations (1) and (2):

$$(1 + i + j + k)(xi + yj + zk)(1 - i - j - k) = yi + zj + xk.$$

The reduced matrix representation requires 9 multiplications and 6 additions, while the quaternion representation requires 48 multiplications and 16 additions.

In another example, a rotation about the 2-fold axis along direction [100] is described by the following matrix equation, corresponding to just one Euler rotation about axis [$\boldsymbol{x}$]:

$$\begin{pmatrix} x \\ -y \\ z \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

and the quaternion equation $i(xi + yj + zk)(-i) = -i + yj + zk$ requires 9 multiplications and 6 additions, compared to 6 multiplications and no additions, respectively. It can be concluded that the advantages of the matrix and quaternion representations depend on the particular problem, its complication and possible optimization procedures for computations. In many crystallographic considerations, the symmetry operations or other calculations can be performed directly in the reference system of crystal axes, which is preferential, require less computer power, is more precise and easier than the procedures resorting to the orthogonalization. Undoubtedly, for the purpose of efficiently comparing the performance of matrix and quaternion representations in crystal reference systems, both these representations in non-Cartesian systems are required. Therefore, it is the purpose of this article to investigate the suitability of quaternions for symmetry operations directly in crystallographic reference systems.

2.4. Quaternion Identity and Inversion

Equation (1) can be used for deriving the identity quaternion, corresponding to the 360° rotation:

$$q(360^\circ,\boldsymbol{v}) = [\cos(180^\circ) + \boldsymbol{n}\cdot\sin(180^\circ)] = -1 \quad (3)$$

In this case, the $q(360^\circ,\boldsymbol{v})$ quaternion has only the scalar component different from zero, and the pre- and post-multiplications can be reduced to the multiplication by 1. It can be noted that Equation (3) can be extended by including an integer n of multiple full rotations:

$$q(n\cdot360^\circ,\boldsymbol{v}) = \cos(n\cdot180^\circ) + \boldsymbol{n}\sin(n\cdot180^\circ) = \begin{cases} -1 \text{ for } n \text{ odd} \\ 1 \text{ for } n \text{ even} \end{cases} \quad (3a)$$

Because $\boldsymbol{r'} = q\,\boldsymbol{r}q^*$ for all n, Equation (3a) is reduced to $\boldsymbol{r'} = 1\boldsymbol{r}$, i.e., the identity operation. Further, we shall assume as the definition of the inversion centre that for any vector $\boldsymbol{r}$ its inversion image is $-\boldsymbol{r}$. Consequently, the quaternion representation of the inversion centre can be defined as

$$\boldsymbol{r'} = -q(360^\circ,\boldsymbol{v})\cdot\boldsymbol{r}\cdot q^*(360^\circ,\boldsymbol{v}) \quad (4)$$

which can be simplified to the operation equivalent to the centre of inversion, C_i:

$$\boldsymbol{r'} = -1\cdot\boldsymbol{r} \quad (5)$$

2.5. Quaternion Mirror Plane

Quaternions are ideally suited for representing mirror-plane (C_s, m) symmetry operations. The mirror plane perpendicular to a given direction can be considered as a combination of a 2-fold rotation (by 180°) about the normal to a plane and the inversion centre at the intersection of the plane and the 2-fold axis. Following the above discussion, the mirror plane can be represented as the product

$$\boldsymbol{r'} = -q(180^\circ,\boldsymbol{n})\cdot\boldsymbol{r}\cdot q^*(180^\circ,\boldsymbol{n}) \quad (6)$$

where vector $\boldsymbol{n}$ is perpendicular to the mirror plane and fulfils the normalization condition as defined in Equation (1). It can be noted that for all quaternions with real part $s = 0$, Equation (6) can be reduced to a simpler form:

$$\boldsymbol{r'} = q\cdot\boldsymbol{r}\cdot q \quad (7)$$

This includes any quaternion $q(180^\circ,\boldsymbol{n})$, because $\cos(90^\circ) = 0$, which applies to all mirror planes, represented as their normal-direction vector $\boldsymbol{n}$ projected into the imaginary space.

For example, the reflection of vector $\boldsymbol{r} = [211]$ in the mirror plane perpendicular to vector $\boldsymbol{v} = [110]$ can be performed by Equation (6) for quaternion $q(180^\circ,[110])$ defined in Equation (1). In this example, $q(180^\circ,[110]) = (i + j)/\sqrt{2}$. According to Equation (6), $\boldsymbol{r'} = (i/\sqrt{2} + j/\sqrt{2})\cdot(2i + j + k)\cdot(i/\sqrt{2} + j/\sqrt{2}) = (-i - 2j + k)$, corresponding to the real-space vector $\boldsymbol{r'} = [-1\ -2\ 1]$.

2.6. Inverse Rotations

We shall further consider inverse rotations, which are the same as the symmetry operations of *inverse axes* (also termed *improper axes*) in crystallography. Originally, Schoenflies distinguished only one inverse rotation, which he termed *Spiegelachse* and denoted as S_4; according to Schönflies, axis S_4 was derived as a combination of a 4-fold rotation (C_4) with a perpendicular mirror plane (C_s). Symbol S in S_4 and subscript s − in C_s − are derived from the German word *Spiegel*, meaning *mirror* in English. Schönflies described combinations of the mirror plane with other rotation axes, denoted with symbols C_1, C_2, C_3, C_6, as C_i, C_s, $C_{3\mathrm{i}}$, and $C_{3\mathrm{h}}$, respectively. Since then, symbols S_1 (Hermann–Mauguin symbol m), S_2 ($\overline{1}$), S_3 ($\overline{6}$), S_4 ($\overline{4}$) and S_6 ($\overline{3}$) have been used, too (Hermann–Mauguin symbols are given in brackets). Hermann and Mauguin, in turn, combined natural 1-, 2-, 3-, 4- and 6-fold rotations with the centre of inversion, and the derived products were inversion axes denoted as $\overline{1}$, m, $\overline{3}$, $\overline{4}$ and $\overline{6}$.

Thus, the improper rotations $\bar{1}$, m, $\bar{3}$, $\bar{4}$ and $\bar{6}$ can be generated either (i) by combining the mirror plane with natural axes 2, 1, 6, 4 and 3, respectively, or (ii) by combining the inversion centre with natural axes 1, 2, 3, 4 and 6, respectively. For the first approach (i) of generating the inverse rotations by combining the rotations with the mirror plane, Equations (2) and (7) give

$$\boldsymbol{r'} = q(\varphi,\boldsymbol{n})\cdot q(180^\circ,\boldsymbol{n})\cdot\boldsymbol{r}\cdot q(180^\circ,\boldsymbol{n})\cdot q^*(\varphi,\boldsymbol{n}),$$

which can be reduced to

$$\boldsymbol{r'} = -q(\varphi,\boldsymbol{n})^*\cdot\boldsymbol{r}\cdot q(\varphi,\boldsymbol{n}) \quad (8)$$

The second approach (ii), i.e., the combination of a natural rotation axis with the inversion centre, gives

$$\boldsymbol{r'} = -q(\varphi,\boldsymbol{n})\cdot\boldsymbol{r}\cdot q^*(\varphi,\boldsymbol{n}) \quad (9)$$

The combinations with the mirror plane (Equation (8)) and with the inverse centre (Equation (9)) result in the opposite sense of the improper rotations.

For example, the symmetry operations for improper axis $\bar{4}$ around axis [z] can be based on the quaternion

$$q\left(90^\circ,\boldsymbol{n}\right) = \left[\cos\left(45^\circ\right) + \boldsymbol{n}\cdot\sin\left(45^\circ\right)\right] = (1+k)/\sqrt{2}.$$

Let us transform vector $\boldsymbol{r}$ = [1 1 1], so $\boldsymbol{r} = (i + j + k)$, according to Equation (8) (plane m plus the natural rotation 4)

$$\boldsymbol{r'} = -i + j - k,$$

which corresponds to the axis $\bar{4}$ (S_4) rotation rightward (when looking from the origin in the positive direction of axis [z]), while according to Equation (9) (inversion centre plus the natural rotation), we obtain

$$\boldsymbol{r'} = i - j - k,$$

corresponding to the operation of the improper rotation axis $\bar{4}$ performed leftward. Further in this paper, we will use the second approach (Equation (9)) for the improper rotations.

2.7. Crystal Reference Systems

Quaternions are generally described in Cartesian reference systems, i.e., orthogonal axes with versors equal in length. For certain non-Cartesian reference systems, it can be shown that quaternions can genuinely represent symmetry operations of crystallographic point groups. The quaternion representations of symmetry operations, as specified in Equations (1)–(9), can be directly applied to vectors described in the crystal reference sets of axes for the crystallographic systems, as specified in Tables 1–5. Thus, the symmetry operations of identity C_1 and inversion C_i have simple quaternion representations that are valid in the triclinic system (Table 1). These quaternion representations of C_1 and C_i can be applied in all crystallographic systems. Table 2 lists the symmetry operations C_1, C_i, C_2 and C_s valid in the monoclinic system. In this case, we have applied the IUCr convention to the monoclinic symmetry direction along [$\boldsymbol{y}$]. The symmetry operations characteristic of orthorhombic (Table 3) and tetragonal (Table 4) systems are valid in these non-Cartesian systems, too. The crystallographic reference axes of the cubic system are Cartesian; hence, the quaternion representations of all cubic symmetry operations, specified in Table 5, are valid.

It can be noted that the proper and improper rotations involving the same quaternion q can be achieved either through transformation type $\boldsymbol{r'} = q\cdot\boldsymbol{r}\cdot q^*$ (Equation (2)) or through transformation type $\boldsymbol{r'} = -q\cdot\boldsymbol{r}\cdot q^*$ (Equation (9)), respectively. For the identity and inversion centre, these transformation types simplify to $\boldsymbol{r'} = 1\cdot\boldsymbol{r}$ (Equation (3a)) and $\boldsymbol{r'} = -1\cdot\boldsymbol{r}$ (Equation (5)), respectively; for mirror planes, the simplification $\boldsymbol{r'} = q\cdot\boldsymbol{r}\cdot q$ (Equation (7)) is obtained. These main types of transformations as well as their simplifications have been indicated in Tables 1–5.

Table 1. Symmetry elements described in the Hermann–Mauguin notation for the triclinic system, the symmetry operations represented as quaternions and the transformation type for vector $\boldsymbol{r}$.

Symmetry Element	Quaternion (q)	Quaternion Action
1	1	$q\boldsymbol{r}$
$\overline{1}$	-1	$q\boldsymbol{r}$

Table 2. Symmetry elements for the monoclinic system and quaternion representations of their symmetry operations.

Symmetry Element	Quaternion (q)	Quaternion Action
1	1	$q\boldsymbol{r}$
$\overline{1}$	-1	$q\boldsymbol{r}$
$2_{[010]}$	k	$q\boldsymbol{r}q^*$
$m_{[010]}$	k	$q\boldsymbol{r}q$

Table 3. Symmetry elements for the orthorhombic system and the corresponding quaternion representations.

Symmetry Element	Quaternion (q)	Quaternion Action
1	1	$q\boldsymbol{r}$
$\overline{1}$	-1	$q\boldsymbol{r}$
$2_{[100]}$	i	$q\boldsymbol{r}q^*$
$2_{[010]}$	j	$q\boldsymbol{r}q^*$
$2_{[001]}$	k	$q\boldsymbol{r}q^*$
$m_{[100]}$	i	$q\boldsymbol{r}q$
$m_{[010]}$	j	$q\boldsymbol{r}q$
$m_{[001]}$	k	$q\boldsymbol{r}q$

Table 4. Symmetry operations for the tetragonal system, their quaternion representations and actions.

Symmetry Operation	Quaternion (q)	Quaternion Action
1	1	$q\boldsymbol{r}$
$\overline{1}$	-1	$q\boldsymbol{r}$
$2_{[100]}$	i	$q\boldsymbol{r}q^*$
$2_{[010]}$	j	$q\boldsymbol{r}q^*$
$2_{[001]}$	k	$q\boldsymbol{r}q^*$
$2_{[110]}$	$(i+j)/\sqrt{2}$	$q\boldsymbol{r}q^*$
$2_{[\bar{1}10]}$	$(-i+j)/\sqrt{2}$	$q\boldsymbol{r}q^*$
$4_{[001]}$	$(1+k)/\sqrt{2}$	$q\boldsymbol{r}q^*$
$4^2_{[001]}$	k	$q\boldsymbol{r}q^*$
$4^3_{[001]}$	$(-1+k)/\sqrt{2}$	$q\boldsymbol{r}q^*$
$\overline{4}_{[001]}$	$(1+k)/\sqrt{2}$	$-q\boldsymbol{r}q^*$
$\overline{4}^2_{[001]}$	k	$-q\boldsymbol{r}q^*$
$\overline{4}^3_{[001]}$	$(-1+k)/\sqrt{2}$	$-q\boldsymbol{r}q^*$
$m_{[100]}$	i	$q\boldsymbol{r}q$
$m_{[010]}$	j	$q\boldsymbol{r}q$
$m_{[001]}$	k	$q\boldsymbol{r}q$
$m_{[110]}$	$(i+j)/\sqrt{2}$	$q\boldsymbol{r}q$
$m_{[\bar{1}10]}$	$(-i+j)/\sqrt{2}$	$q\boldsymbol{r}q$

For non-Cartesian trigonal and hexagonal crystallographic systems (the hexagonal family), the quaternion representations of symmetry operations are not generally valid for the crystallographic reference axes. The quaternion representations of the symmetry operations can be applied for the Cartesian system. For example, the inverse rotation $\overline{3}$

of vector **r** = [1,0,1] about axis [z] can be performed for quaternion $q(120^\circ,[001])$ equal to $(1 + k\sqrt{3})/2$. According to Equation (9),

$$\boldsymbol{r}' = -\left(1 + k\sqrt{3}\right)\cdot(i + k)\cdot\left(1 - k\sqrt{3}\right)/4 = \left(i/2 - j\sqrt{3}/2 - k\right).$$

Thus, the ***r'*** vector components after the symmetry operation of improper rotation $\bar{3}$ about direction [001] is $[1/2 - \sqrt{3}/2 - 1]$, which is the $\bar{3}$ rotation performed for the orthogonal Cartesian system. However, for the crystallographic reference axes of the hexagonal unit cell, this cannot be performed. Only the symmetry operations for the trigonal point groups described in the *R* lattice can be represented as quaternions, as listed in Table 6.

Table 5. Symmetry operations for the cubic system, their quaternion representations and actions. For the sake of brevity, of all 40 proper and improper 3- and 4-fold axes, only the full set of operations has been listed for axes $3_{[111]}$; for the remaining ones, the power indices $\alpha = 1, 2$ and $\beta = 1, 2, 3$ have been introduced (cf. Table 4).

Symmetry Operation	Quaternion (q)	Quaternion Action
1	1	qr
$\bar{1}$	-1	qr
$2_{[100]}$	i	qrq^*
$2_{[010]}$	j	qrq^*
$2_{[001]}$	k	qrq^*
$2_{[110]}$	$(i + j)/\sqrt{2}$	qrq^*
$2_{[\bar{1}10]}$	$(-i + j)/\sqrt{2}$	qrq^*
$2_{[101]}$	$(i + k)/\sqrt{2}$	qrq^*
$2_{[\bar{1}01]}$	$(-i + k)/\sqrt{2}$	qrq^*
$2_{[011]}$	$(j + k)/\sqrt{2}$	qrq^*
$2_{[0\bar{1}1]}$	$(-j + k)/\sqrt{2}$	qrq^*
$3^1_{[111]}$	$(1 + i + j + k)/2$	qrq^*
$3^2_{[111]}$	$(-1 + i + j + k)/2$	qrq^*
$(3_{[\bar{1}11]})^\alpha$	$[(1 - i + j + k)/2]^\alpha$	qrq^*
$(3_{[1\bar{1}1]})^\alpha$	$[(1 + i - j + k)/2]^\alpha$	qrq^*
$(3_{[11\bar{1}]})^\alpha$	$[(1 + i + j - k)/2]^\alpha$	qrq^*
$(\bar{3}_{[111]})^\alpha$	$[(1 + i + j + k)/2]^\alpha$	$-qrq^*$
$(\bar{3}_{[\bar{1}11]})^\alpha$	$[(1 - i + j + k)/2]^\alpha$	$-qrq^*$
$(\bar{3}_{[1\bar{1}1]})^\alpha$	$[(1 + i - j + k)/2]^\alpha$	$-qrq^*$
$(\bar{3}_{[11\bar{1}]})^\alpha$	$[(1 + i + j - k)/2]^\alpha$	$-qrq^*$
$(4_{[100]})^\beta$	$[(1 + i)/\sqrt{2}]^\beta$	qrq^*
$(4_{[010]})^\beta$	$[(1 + j)/\sqrt{2}]^\beta$	qrq^*
$(4_{[001]})^\beta$	$[(1 + k)/\sqrt{2}]^\beta$	qrq^*
$(\bar{4}_{[100]})^\beta$	$[(1 + i)/\sqrt{2}]^\beta$	$-qrq^*$
$(\bar{4}_{[010]})^\beta$	$[(1 + j)/\sqrt{2}]^\beta$	$-qrq^*$
$(\bar{4}_{[001]})^\beta$	$[(1 + k)/\sqrt{2}]^\beta$	$-qrq^*$
$m_{[100]}$	i	qrq
$m_{[010]}$	j	qrq
$m_{[001]}$	k	qrq
$m_{[110]}$	$(i + j)/\sqrt{2}$	qrq
$m_{[\bar{1}10]}$	$(-i + j)/\sqrt{2}$	qrq
$m_{[101]}$	$(i + k)/\sqrt{2}$	qrq
$m_{[\bar{1}01]}$	$(-i + k)/\sqrt{2}$	qrq
$m_{[011]}$	$(j + k)/\sqrt{2}$	qrq
$m_{[0\bar{1}1]}$	$(-j + k)/\sqrt{2}$	qrq

Table 6. Symmetry operations in trigonal point groups described in the rhombohedral Bravais lattice *R*, their quaternion representations and actions.

Symmetry Operation	Quaternion (*q*)	Quaternion Action
1	1	qr
$\bar{1}$	-1	qr
$2_{[1\bar{1}0]}$	$(i-j)/\sqrt{2}$	qrq^*
$2_{[01\bar{1}]}$	$(j-k)/\sqrt{2}$	qrq^*
$2_{[\bar{1}01]}$	$(-i+k)/\sqrt{2}$	qrq^*
$3_{[111]}$	$(1+i+j+k)/2$	qrq^*
$3^2_{[111]}$	$(-1+i+j+k)/2$	qrq^*
$\bar{3}_{[111]}$	$(1+i+j+k)/2$	$-qrq^*$
$\bar{3}^2_{[111]}$	$(-1+i+j+k)/2$	$-qrq^*$
$m_{[1\bar{1}0]}$	$(i-j)/\sqrt{2}$	qrq
$m_{[01\bar{1}]}$	$(j-k)/\sqrt{2}$	qrq
$m_{[\bar{1}01]}$	$(-i+k)/\sqrt{2}$	qrq
$m_{[100]}$	i	qrq
$m_{[010]}$	j	qrq
$m_{[001]}$	k	qrq
$m_{[110]}$	$(i+j)/\sqrt{2}$	qrq
$m_{[\bar{1}10]}$	$(-i+j)/\sqrt{2}$	qrq

2.8. Quaternion Symbols of Symmetry Operations

Quaternions representing the operations in certain symmetry classes are concise and therefore they can be considered as a convenient method for writing symbols of symmetry operations and elements. The two main multiplication types for obtaining point-group symmetry operations of (i) natural axes 1, 2, 3, 4 and 6 are executed through multiplication qrq^* (Equation (2)) and (ii) improper rotation axes $\bar{1}$, m, $\bar{3}$, $\bar{4}$ and $\bar{6}$ are performed through multiplication $-qrq^*$ (Equation (9)). We propose that the quaternion symbol q be used for coding the natural rotations and the negative sign before quaternion, $-q$, for the improper rotations. As pointed before, other multiplication types are also possible, but they are simplifications of Equations (2) and (9); for example, the simplification qrq applies to the quaternion operations consisting of imaginary components only (Equation (7)).

It should be noted that the multiplications of quaternions representing natural rotations yield either 1 or -1 (cf. Equation (3a). For example, the double rotation of the multiplication q(180°,[z])·q(180°,[z]) equals -1. However, this negative sign of the combined quaternion would compensate in the transformation (Equation (2)); hence, it can be ignored in the multiplication table. It illustrates that the quaternions cannot be considered separately from their transformation types.

Figure 1 and Table 7 illustrate the informative concise quaternions applied as operation symbols used in the multiplication table for symmetry class *mmm* (Schönflies symbol D_{2h}). Below, by using various symmetry operations in the quaternion representation, the Miller indices of orthorhombic bipyramid faces have been indexed. Instead of general Miller indices (*hkl*), in order to avoid their confusion with the quaternion symbols, we transformed unit face (1 1 1) to complete its family of planes $\{1\,1\,1\}$:

$i(i+j+k)(-i) = (-1+k-j)(-i) = i-j-k$, corresponding to face $(1\,\bar{1}\,\bar{1})$;
$i(i+j+k)(i) = (-1+k-j)(i) = -i+j+k$, corresponding to face $(\bar{1}\,1\,1)$;
$j(i+j+k)(-j) = (-k-1+i)(-j) = -i+j-k$, corresponding to face $(\bar{1}\,1\,\bar{1})$;
$j(i+j+k)(j) = (-k-1+i)(j) = i-j+k$, corresponding to face $(1\,\bar{1}\,1)$;
$k(i+j+k)(-k) = (j-i-1)(-k) = -i-j+k$, corresponding to face $(\bar{1}\,\bar{1}\,1)$;
$-1(i+j+k) = -i-j-k$, corresponding to face $(\bar{1}\,\bar{1}\,\bar{1})$;
$-1(-i-j+k) = i-j-k$, corresponding to face $(1\,1\,\bar{1})$.

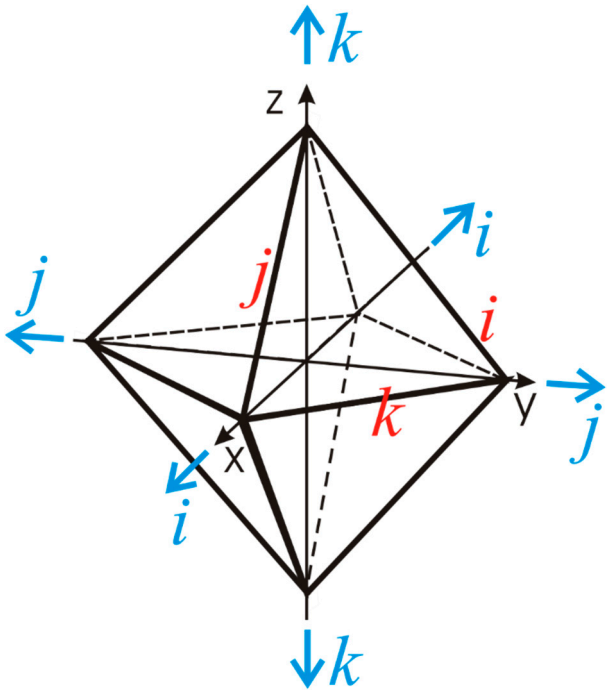

Figure 1. An orthorhombic bipyramid with its symmetry elements indicated as quaternions: 2-fold axes arrows and quaternions (indicated in blue); the mirror-plane quaternions (perpendicular to [x], [y] and [z]) running along the edges of the bipyramid are indicated in red (cf. Table 7).

Table 7. Multiplication table for the symmetry operations of point group *mmm*. Hermann–Mauguin symbols of symmetry operations with their directions in the indices are listed in the top row and left column, and their products are represented as quaternions in the table body. The proper rotations are positive (Equation (2) should be used), while the negative sign indicates improper rotations (Equation (9)).

Symmetry Operation	1	$\bar{1}$	$2_{[100]}$	$2_{[010]}$	$2_{[001]}$	$m_{[100]}$	$m_{[010]}$	$m_{[001]}$
1	1	-1	i	j	k	$-i$	$-j$	$-k$
$\bar{1}$	-1	1	$-i$	$-j$	$-k$	i	j	k
$2_{[100]}$	i	$-i$	1	k	j	-1	$-k$	$-j$
$2_{[010]}$	j	$-j$	k	1	i	$-k$	-1	$-i$
$2_{[001]}$	k	$-k$	j	i	1	$-j$	$-i$	-1
$m_{[100]}$	$-i$	i	-1	$-k$	$-j$	1	k	j
$m_{[010]}$	$-j$	j	$-k$	-1	$-i$	k	1	i
$m_{[001]}$	$-k$	k	$-j$	i	-1	j	i	1

The corresponding matrix operations are

$$\begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 1 \\ -1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix},$$
$$\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ -1 \\ -1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix},$$
$$\begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}.$$

Each of the quaternion operations requires either six or three quaternion multiplications, whereas all the vector-by-matrix multiplications above require nine scalar multiplications and six additions.

The quaternion symbols become somewhat more complicated for the 4-fold rotations and the symmetry elements of the diagonal directions, as exemplified for point group $\bar{4}2m$ in Figure 2 and the multiplication of its quaternions in Table 8. However, the information explicitly contained in the quaternion symbol is comparable or higher than in other notations. For example, the symbols of 2-fold axis 2[110] and quaternion $(i + j)/\sqrt{2}$ contain a similar number of alphanumerical symbols, but the quaternion symbols could be further simplified by applying abbreviations, such as $p = 1/\sqrt{2}$ for normalizing diagonal planes or $s = 1/2$ (see Tables 4–6). So, quaternion symbol $(i + j)/\sqrt{2}$ can be shortened to $(i + j)p$.

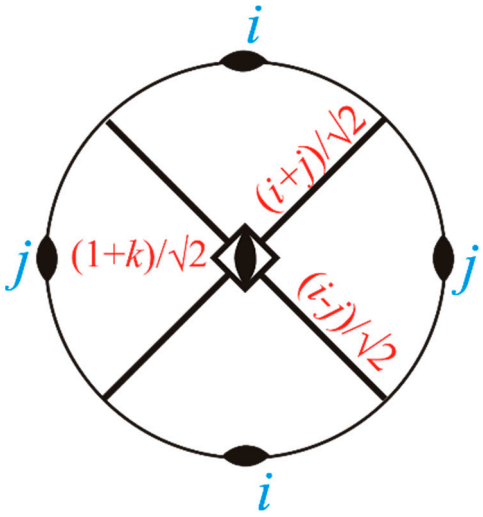

Figure 2. Cyclographic projection of point group $\bar{4}2m$ with indicated quaternion representations of the symmetry elements: proper rotations are blue and improper rotations are red (cf. Table 8). The conventional orientation of the reference system (axis [***y***] across the page and [*x*] down) is is apparent from the quaternion symbols.

Table 8. Multiplication table of symmetry operations in point group $\bar{4}2m$, with the Hermann–Mauguin symbols in the left column multiplied by this from the top row, e.g., $2_{[100]}\cdot\bar{4}^1{}_{[001]}$ is $-(i + j)/\sqrt{2}$ and $\bar{4}^1{}_{[001]}\cdot 2_{[100]}$ is $-(i - j)/\sqrt{2}$ in this non-Abelian point group. Quaternion representations of the symmetry operations are in the table body; the quaternions representing improper operations are marked by the minus sign.

Symmetry Operation	1	$\bar{4}^1{}_{[001]}$	$\bar{4}^2{}_{[001]}$	$\bar{4}^3{}_{[001]}$	$2_{[100]}$	$2_{[010]}$	$m_{[110]}$	$m_{[\bar{1}10]}$
1	1	$-\frac{1+k}{\sqrt{2}}$	k	$-\frac{k-1}{\sqrt{2}}$	i	j	$-\frac{i+j}{\sqrt{2}}$	$-\frac{i-j}{\sqrt{2}}$
$\bar{4}^1{}_{[001]}$	$-\frac{1+k}{\sqrt{2}}$	k	$-\frac{k-1}{\sqrt{2}}$	1	$-\frac{i-j}{\sqrt{2}}$	$-\frac{i+j}{\sqrt{2}}$	i	j
$\bar{4}^2{}_{[001]}$	k	$-\frac{k-1}{\sqrt{2}}$	1	$-\frac{1+k}{\sqrt{2}}$	j	i	$-\frac{i-j}{\sqrt{2}}$	$-\frac{i+j}{\sqrt{2}}$
$\bar{4}^3{}_{[001]}$	$-\frac{k-1}{\sqrt{2}}$	1	$-\frac{1+k}{\sqrt{2}}$	k	$-\frac{i+j}{\sqrt{2}}$	$-\frac{i-j}{\sqrt{2}}$	j	i
$2_{[100]}$	i	$-\frac{i+j}{\sqrt{2}}$	j	$-\frac{i-j}{\sqrt{2}}$	1	k	$-\frac{1+k}{\sqrt{2}}$	$-\frac{1-k}{\sqrt{2}}$
$2_{[010]}$	j	$-\frac{i-j}{\sqrt{2}}$	i	$-\frac{i+j}{\sqrt{2}}$	k	1	$-\frac{1-k}{\sqrt{2}}$	$-\frac{1+k}{\sqrt{2}}$
$m_{[110]}$	$-\frac{i+j}{\sqrt{2}}$	j	$-\frac{i-j}{\sqrt{2}}$	$-j$	$-\frac{1-k}{\sqrt{2}}$	$-\frac{1+k}{\sqrt{2}}$	1	k
$m_{[\bar{1}10]}$	$-\frac{i-j}{\sqrt{2}}$	i	$-\frac{i+j}{\sqrt{2}}$	j	$-\frac{1+k}{\sqrt{2}}$	$-\frac{1-k}{\sqrt{2}}$	k	1

Below, the quaternion and matrix representations of the symmetry operations are compared for generating equivalent atomic positions in a molecule. We chose the S_4-symmetric molecule of pentaerythritol, $C(CH_2OH)_4$, located on the centre of the four-fold inversion axis in the crystal structure, of tetragonal space-group symmetry $I\bar{4}$ [22]. Atom C1 at special position [000] transforms into itself (hence its site occupation factor is ¼, cf. Figure 3), while the methanol group is located in the general position [*xyz*] and it transforms to the equivalent positions $[xyz]_A$, $[xyz]_B$ and $[xyz]_C$ through quaternion operation $\bar{4}^1{}_{[001]}$ according to Equation (6): $[xyz]_A = -(1 + k)\cdot[xi + yj + zk]\cdot(1 - k)/2 = j - i - k$ (cf. Table 8); operation $\bar{4}^2{}_{[001]}$ according to

Equation (2): $[xyz]_B = k\cdot[xi + yj + zk]\cdot(-k) = -i - j + k$; and operation $\bar{4}^3_{[001]}$ as $(1 - k)\cdot[xi + yj + zk]\cdot(1 + k)/2 - j + i - k$ or simpler $k\cdot[xi + yj + zk]_A\cdot(-k)$. The equivalent matrix representations of these $\bar{4}$ operations are

$$\bar{4}^1 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \bar{4}^2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \bar{4}^3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

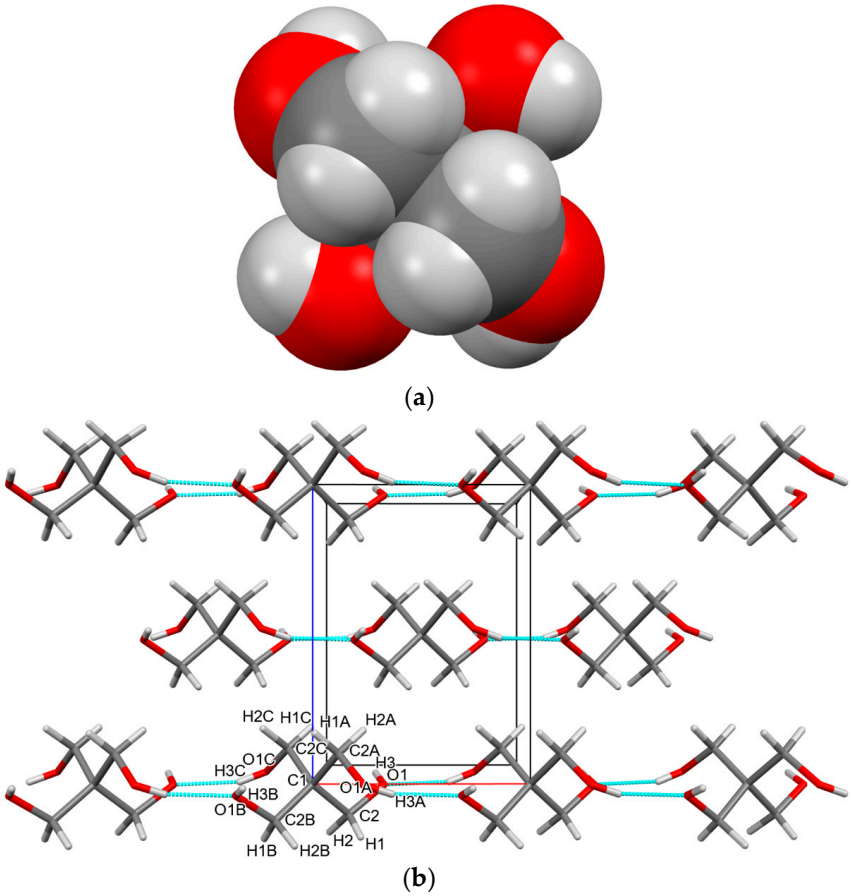

Figure 3. (**a**) Space-filling model of the pentaerythritol molecule viewed along its S_4 axis, as present in the crystal structure at 1.15 GPa [23]; code of colours: C, dark grey, H, light grey, O, red; (**b**) autostereographic projection [24] of the crystal structure, space group $I\bar{4}$, with atoms represented as capped sticks coloured as indicated above, hydrogen bonds OH···O are cyan; atomic labels C1 (C2 H1 H2 O1 H3) with no and with additional letters A, B and C indicate equivalent methanol substituents.

3. Conclusions

The quaternion representations of symmetry operations in crystallographic reference systems are attractive for several reasons, such as their easy intuitive construction, direct connections with the rotation axis orientation and rotation angles as well as the simplicity of performing arithmetic operations required for transforming vectors in both Cartesian and crystallographic reference systems. Most importantly, quaternions are an alternative to the matrix representation of symmetry operations, except the hexagonal reference system. The two different, matrix and quaternion, representations give the opportunity to choose the one more appropriate for performing crystallographic, diffractometric or any numerical calculations involving symmetry operations in triclinic, monoclinic, orthorhombic tetragonal, cubic and rhombohedral lattices. In these systems, owing to the simplicity of quaternions' notation, it can be used instead of symmetry operation symbols, for example, inmultiplication table of quaternions, analogous to Cayley tables of multiplied symmetry operations or for the symbols of cyclic crystallographic classes. Therefore, the direct application of quaternions for symmetry transformations of vectors in crystal reference systems appears very attractive.

However, there are important limitations of the quaternion representation of symmetry operations. In particular, the point-symmetry operations in the quaternion representation do not fulfil all requirements of the algebraic group, because two types of the multiplication actions are required for distinguishing proper and improper rotations. Moreover, the quaternion representations for the crystallographic hexagonal reference system have still not been resolved, and further studies aimed at the complete quaternion representations of all symmetry operations in crystallographic reference systems are required. The inadequacy of quaternions for generally representing the symmetry operations in all crystallographic reference systems is likely the main handicap for the common use of quaternions in crystallography [18,20], while they are thriving in other applications not requiring non-Cartesian reference systems [3–8]. Nonetheless, as presented in our study, even in the present incomplete compilation, the elegant form of quaternion rotations is appealing for their crystallographic applications.

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