# Algorithm for conversion between geometric algebra versor notation and conventional crystallographic symmetry-operation symbols

Eckhard Hitzer and Christian Perwass

June 13, 2009

## 1 Introduction

This paper establishes an algorithm for the conversion of conformal geometric algebra (GA) [3, 4] versor symbols of space group symmetry-operations [6–8, 10] to standard symmetry-operation symbols of crystallography [5]. The algorithm is written in the mathematical language of geometric algebra [2–4], but it takes up basic algorithmic ideas from [1]. The geometric algebra treatment simplifies the algorithm, due to the seamless use of the geometric product for operations like intersection, projection, rejection; and the compact conformal versor notation for all symmetry operations and for geometric elements like lines and planes.

The transformations between the set of three geometric symmetry vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$, used for generating multivector versors, and the set of three conventional crystal cell vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of [5] have already been fully specified in [8] complete with origin shift vectors. In order to apply the algorithm described in the present work, all locations, axis vectors and trace vectors must be computed and oriented with respect to the conventional crystall cell, i.e. its origin and its three cell vectors.

Section 2 reviews the notation for symmetry operations used in ITA2005 [5] together with representative sets of examples in tabulated form. Section 3 reviews the conformal geometric algebra description of points, affine points, lines and planes, their direction, location, parallelness, intersection (meet), as well as the projection of translation vectors. Section 4 introduces the notions of coordinate system, reciprocal coordinate vectors, coordinates, axis lines and basal planes. Section 5 shows how to determine the conventional crystallographic location points of lines and planes. Section 6 shows how to determine the crystallographic trace vectors of planes from intersections with basal coordinate planes. Section 7 explains how to obtain the crystallographic positive sense of a vector. Section 8 introduces to the choice of variable symbols $t \in \{x, y, z\}$ for parametrizing lines and planes. Finally Section 9 presents the full conversion algorithm.

## 2 Specification of symmetry-operations in ITA2005

In this section we review how the symmetry-operations of reflections, glide reflections, rotations, screw rotations, inversions and rotoinversions are specified in ITA2005, together with some concrete examples, similar to Wittgenstein's definition of the mean-

Table 1: Examples of reflections from ITA2005 [5].

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $m$ | $x,0,z$ | $m$ | $0,y,z$ | $m$ | $x,\frac{1}{4},z$ | $m$ | $x,y,0$ |
| $m$ | $x,x,z$ | $m$ | $x,\bar{x},z$ | $m$ | $x,2x,z$ | $m$ | $2x,x,z$ |
| $m$ | $x,y,y$ | $m$ | $x,y,x$ | $m$ | $x,y,\frac{1}{4}$ | $m$ | $x,y+\frac{1}{2},\bar{y}$ |
| $m$ | $\bar{x}+\frac{1}{2},y,x$ | $m$ | $x+\frac{1}{2},\bar{x},z$ | | | | |

ing of words by their use. How the relevant parameter values, location vectors, axis vectors, and trace vectors of planes can be derived from the geometric algebra versor representation will be explained in subsequent sections.

Here we only point out that in geometric algebra the determination of the coordinates of centers of (roto)inversion, and of rotation angles is straight forward, and is therefore not further explained.

## 2.1 Reflections

In ITA2005 [5] reflections are specified in the following way

$$m \quad t_1\mathbf{v}_{\text{Trace1}} + t_2\mathbf{v}_{\text{Trace2}} + \mathbf{v}_{\text{Locat}}, \tag{1}$$

where the parameters $t_1, t_2 \in \{x,y,z\}, t_1 \neq t_2$, and negative values are indicated by overbars

$$\bar{x} = -x, \quad \bar{y} = -y, \quad \bar{z} = -z. \tag{2}$$

The second part $\quad t_1\mathbf{v}_{\text{Trace1}} + t_2\mathbf{v}_{\text{Trace2}} + \mathbf{v}_{\text{Shift}}$ specifies the reflection plane. The determination of the trace vectors $\mathbf{v}_{\text{Trace1}}, \mathbf{v}_{\text{Trace2}}$, of the parameters $t_1, t_2$ and of the $\mathbf{v}_{\text{Locat}}$ will be explained in the following sections. Before explaining further details we give a set of examples in Table 1.

The first entry in Table 1 is composed of

$$t_1 = x,\ \mathbf{v}_{\text{Trace1}} = (1,0,0),\ \ t_2 = z,\ \mathbf{v}_{\text{Trace2}} = (0,0,1),\ \ \mathbf{v}_{\text{Locat}} = (0,0,0). \tag{3}$$

The second entry in column three of Table 1 is composed of

$$t_1 = x,\ \mathbf{v}_{\text{Trace1}} = (1,2,0),\ \ t_2 = z,\ \mathbf{v}_{\text{Trace2}} = (0,0,1),\ \ \mathbf{v}_{\text{Locat}} = (0,0,0). \tag{4}$$

The last entry in Table 1 is composed of

$$t_1 = x,\ \mathbf{v}_{\text{Trace1}} = (1,-1,0),\ \ t_2 = z,\ \mathbf{v}_{\text{Trace2}} = (0,0,1),\ \ \mathbf{v}_{\text{Locat}} = (\frac{1}{2},0,0). \tag{5}$$

## 2.2 Glide reflections

In ITA2005 [5] glide reflections are specified in the following way

$$r \quad t_1\mathbf{v}_{\text{Trace1}} + t_2\mathbf{v}_{\text{Trace2}} + \mathbf{v}_{\text{Locat}}, \tag{6}$$

with $r \in \{a,b,c\}$ for intrinsic (parallel to the glide plane) glide vectors $\mathbf{w}_g \in \{\mathbf{a}/2, \mathbf{b}/2, \mathbf{c}/2\}$, respectively (see Table 2). If the intrinsic glide vector does not equal half a crystallographic cell vector, instead the following notation is used

$$s \quad \mathbf{w}_g \quad t_1\mathbf{v}_{\text{Trace1}} + t_2\mathbf{v}_{\text{Trace2}} + \mathbf{v}_{\text{Locat}}, \tag{7}$$

Table 2: Examples of axial glide reflections from ITA2005 [5].

| glide vector $\mathbf{a}/2$ | glide vector $\mathbf{b}/2$ | glide vector $\mathbf{c}/2$ |
|---|---|---|
| $a \quad x,y,\frac{1}{4}$ | $b \quad x,y,\frac{1}{4}$ | $c \quad x,\frac{1}{4},z$ |

Table 3: Examples of glide reflections, diagonal glide reflections and two pairs of diamond glide reflections from ITA2005 [5].

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| $g$ | $(0,\frac{1}{2},\frac{1}{2})$ | $x,y,y$ | $n$ | $(\frac{1}{2},0,\frac{1}{2})$ | $x,0,z$ | $d$ | $(\frac{1}{4},\frac{1}{4},0)$ | $x,y,\frac{1}{8}$ |
| $g$ | $(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ | $x-\frac{1}{4},x,z$ | $n$ | $(\frac{1}{2},\frac{1}{2},0)$ | $x,y,0$ | $d$ | $(\frac{1}{4},\frac{3}{4},0)$ | $x,y,\frac{3}{8}$ |
| $g$ | $(-\frac{1}{4},\frac{1}{4},\frac{1}{2})$ | $x+\frac{1}{4},\bar{x},z$ | $n$ | $(0,\frac{1}{2},\frac{1}{2})$ | $0,y,z$ | $d$ | $(0,\frac{1}{4},\frac{1}{4})$ | $\frac{1}{8},y,z$ |
| $g$ | $(\frac{1}{2},-\frac{1}{4},\frac{1}{4})$ | $x,y+\frac{1}{4},\bar{y}$ | | | | $d$ | $(0,\frac{1}{4},\frac{3}{4})$ | $\frac{3}{8},y,z$ |

Table 4: Examples of rotations from ITA2005 [5].

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 2 | $0,y,0$ | $4^+$ | $0,0,z$ | $3^+$ | $0,0,z$ | $6^+$ | $0,0,z$ |
| 2 | $0,y,\frac{1}{4}$ | $4^-$ | $0,0,z$ | $3^-$ | $0,0,z$ | $6^-$ | $0,0,z$ |
| 2 | $\frac{1}{4},0,z$ | $4^+$ | $0,\frac{1}{2},z$ | $3^+$ | $x,x,x$ | | |
| 2 | $\frac{1}{4},\frac{1}{4},z$ | $4^-$ | $\frac{1}{2},0,z$ | $3^-$ | $x,x,x$ | | |
| | | $4^+$ | $\frac{1}{4},\frac{1}{4},z$ | $3^+$ | $\bar{x},x,\bar{x}$ | | |
| | | $4^-$ | $\frac{1}{4},\frac{1}{4},z$ | $3^-$ | $x,\bar{x},\bar{x}$ | | |

with $s = g$ for general glide vectors $\mathbf{w}_g$, $s = n$ for face diagonal glide vectors $\mathbf{w}_g$, and $s = d$ for socalled (pairs of) Diamond glide planes $\mathbf{w}_g$, which occur in centered cells only: orthorhombic $F$ space groups, tetragonal $I$ space groups, and in cubic $I$ and $F$ space groups. They always occur in pairs with alternating glide vectors, e.g. $\mathbf{w}_g = \frac{1}{4}(\mathbf{a} \pm \mathbf{b})$. The second power of a glide reflection $d$ always gives a centering vector. Or in other words: The glide vector $\mathbf{w}_g$ is always one half of a centering vector (see third column of Table 3).

The other entities $\mathbf{v}_{\text{Trace1}}, \mathbf{v}_{\text{Trace2}}$, $t_1, t_2$ and $\mathbf{v}_{\text{Locat}}$ specify the glide plane itself, exactly like in the specification of reflection planes in Section 2.1. Before explaining further details we give a set of examples in Tables 2 and 3.

## 2.3 Rotations

In ITA2005 [5] rotations are specified in the following way

$$n^{\pm} \quad t\,\mathbf{v}_{\text{Axis}} + \mathbf{v}_{\text{Locat}}, \tag{8}$$

where the number $n \in \{2,3,4,6\}$ specifies rotations by $\{360°/n\}$ around the axis, which is in turn specified by the straight line $t\mathbf{v}_{\text{Axis}} + \mathbf{v}_{\text{Locat}}$ with parameter $t \in \{x,y,z\}$. The upper index $+$ $(-)$ indicates whether the rotation is right-handed relative to the sense of $\mathbf{v}_{\text{Axis}}$ (or left-handed). The number $n = 2$ carries no $\pm$ index. The choice of $t$, $\mathbf{v}_{\text{Axis}}$, and $\mathbf{v}_{\text{Locat}}$ will be explained in the following sections. We now give some examples in Table 4.

Table 5: Examples of screw rotations from ITA2005 [5].

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 2 | $(0,\frac{1}{2},0)$ | $0,y,0$ | $3^+$ | $(0,0,\frac{1}{3})$ | $\frac{1}{3},\frac{1}{3},z$ | $6^-$ | $(0,0,\frac{5}{6})$ | $0,0,z$ |
| 2 | $(0,\frac{1}{2},0)$ | $0,y,\frac{1}{4}$ | $3^-$ | $(0,0,\frac{1}{3})$ | $\frac{1}{3},0,z$ | $6^+$ | $(0,0,\frac{1}{6})$ | $0,0,z$ |
| 2 | $(0,0,\frac{1}{2})$ | $\frac{1}{4},0,z$ | $3^-$ | $(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ | $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | $6^-$ | $(0,0,\frac{2}{3})$ | $0,0,z$ |
| $4^+$ | $(0,0,\frac{1}{4})$ | $0,\frac{1}{2},z$ | $3^+$ | $(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ | $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$ | $6^+$ | $(0,0,\frac{1}{3})$ | $0,0,z$ |
| $4^-$ | $(0,0,\frac{3}{4})$ | $\frac{1}{2},0,z$ | $3^+$ | $(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ | $x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$ | $6^-$ | $(0,0,\frac{1}{2})$ | $0,0,z$ |
| $4^+$ | $(0,0,\frac{1}{2})$ | $0,0,z$ | $3^-$ | $(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ | $\bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$ | $6^+$ | $(0,0,\frac{1}{2})$ | $0,0,z$ |
| $4^-$ | $(0,0,\frac{1}{2})$ | $0,0,z$ | $3^+$ | $(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ | $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ | | | |
| $4^+$ | $(0,0,\frac{1}{4})$ | $-\frac{1}{4},\frac{1}{4},z$ | $3^-$ | $(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})$ | $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | | | |
| $4^-$ | $(0,0,\frac{3}{4})$ | $\frac{1}{4},-\frac{1}{4},z$ | | | | | | |

For example the fourth entry in column 1 of Table 4 shows a 180° rotation around the axis given by

$$t = z, \quad \mathbf{v}_{\text{Axis}} = (0,0,1), \quad \mathbf{v}_{\text{Locat}} = (\frac{1}{4},\frac{1}{4},0). \tag{9}$$

The third entry in column 2 of Table 4 shows a right-handed 90° rotation around the axis given by

$$t = z, \quad \mathbf{v}_{\text{Axis}} = (0,0,1), \quad \mathbf{v}_{\text{Locat}} = (0,\frac{1}{2},0). \tag{10}$$

The 6th entry in column 3 of Table 4 shows a left-handed 120° rotation around the axis given by

$$t = x, \quad \mathbf{v}_{\text{Axis}} = (1,-1,-1), \quad \mathbf{v}_{\text{Locat}} = (0,0,0). \tag{11}$$

The first entry in column 4 of Table 4 shows a right-handed 60° rotation around the axis given by

$$t = z, \quad \mathbf{v}_{\text{Axis}} = (0,0,1), \quad \mathbf{v}_{\text{Locat}} = (0,0,0). \tag{12}$$

## 2.4 Screw rotations

In ITA2005 [5] screw rotations are specified in the following way

$$n^{\pm} \quad \mathbf{w}_g \quad t\,\mathbf{v}_{\text{Axis}} + \mathbf{v}_{\text{Locat}}, \tag{13}$$

where $\mathbf{w}_g$ specifies the intrinsic translation part of the screw rotation, parallel to the rotation axis $\mathbf{v}_{\text{Axis}}$. All other entities $n^{\pm}$, $t$, $\mathbf{v}_{\text{Axis}}$, and $\mathbf{v}_{\text{Locat}}$ specify the screw axis itself, exactly like in the specification of rotations in Section 2.3. Before explaining further details we give a set of examples in Table 5.

## 2.5 Inversions

In ITA2005 [5] inversions are specified in the following way

$$\bar{1} \quad \mathbf{v}_{\text{Locat}}, \tag{14}$$

where $\bar{1}$ is the symbol, and $\mathbf{v}_{\text{Locat}}$ the coordinate triplet of the center of inversion. Some examples are given in Table 6.

Table 6: Examples of inversions from ITA2005 [5].

| | | | | | |
|---|---|---|---|---|---|
| $\bar{1}$ | $0,0,0$ | $\bar{1}$ | $\frac{1}{4},\frac{1}{4},0$ | $\bar{1}$ | $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ |

Table 7: Examples of rotoinversions from ITA2005 [5].

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $\bar{3}^+$ | $0,0,z$ | ; | $0,0,0$ | $\bar{4}^+$ | $0,0,z$ | ; | $0,0,\frac{1}{4}$ |
| $\bar{3}^-$ | $0,0,z$ | ; | $0,0,0$ | $\bar{4}^-$ | $0,0,z$ | ; | $0,0,\frac{1}{4}$ |
| $\bar{3}^+$ | $\frac{1}{3},-\frac{1}{3},z$ | ; | $\frac{1}{3},-\frac{1}{3},\frac{1}{6}$ | $\bar{4}^+$ | $\frac{1}{2},-\frac{1}{4},z$ | ; | $\frac{1}{2},-\frac{1}{4},\frac{3}{8}$ |
| $\bar{3}^-$ | $\frac{1}{3},\frac{2}{3},z$ | ; | $\frac{1}{3},\frac{2}{3},\frac{1}{6}$ | $\bar{4}^-$ | $0,\frac{3}{4},z$ | ; | $0,\frac{3}{4},\frac{1}{8}$ |
| $\bar{3}^+$ | $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$ | ; | $0,\frac{1}{2},\frac{1}{2}$ | $\bar{6}^-$ | $0,0,z$ | ; | $0,0,\frac{1}{4}$ |
| $\bar{3}^-$ | $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ | ; | $0,0,\frac{1}{2}$ | $\bar{6}^+$ | $0,0,z$ | ; | $0,0,\frac{1}{4}$ |
| $\bar{3}^+$ | $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$ | ; | $-\frac{1}{8},\frac{1}{8},\frac{1}{8}$ | | | | |
| $\bar{3}^-$ | $x+1,\bar{x}-1,\bar{x}$ | ; | $\frac{1}{8},-\frac{1}{8},\frac{7}{8}$ | | | | |

## 2.6 Rotoinversions

First note, that rotoinversions (i.e. rotary inversions) do not occur in triclinic, monoclinic, and orthorhombic crystals. In ITA2005 [5] rotoinversions are specified in the following way

$$\overline{n}^{\pm} \quad t\,\mathbf{v}_{\text{Axis}} + \mathbf{v}_{\text{Locat}}\ ; \quad \mathbf{w}_{\text{Inv}} \tag{15}$$

where $\mathbf{w}_{\text{Inv}}$ specifies the center of inversion on the rotation axis $t\,\mathbf{v}_{\text{Axis}} + \mathbf{v}_{\text{Locat}}$. Alternatively $\mathbf{w}_{\text{Inv}}$ can be regarded as the intersection of the rotation axis with the reflection plane of an equivalent rotary reflection. The number $n \in \{3,4,6\}$ specifies rotations by $\{360^\circ/n\}$ around the rotation axis. The upper index $+$ $(-)$ indicates again whether the rotation is right-handed relative to the sense of $\mathbf{v}_{\text{Axis}}$ (or left-handed). The overbar of $\overline{n}^{\pm}$ distinguishes rotary inversions from pure rotations. All other entities $t$, $\mathbf{v}_{\text{Axis}}$, and $\mathbf{v}_{\text{Locat}}$ specify the screw axis itself, exactly like in the specification of rotations in Section 2.3. Before explaining further details we give a set of examples in Table 7.

For example the third entry on the left side of Table 7 shows a right-handed 120° rotoinversion given by

$$t = z, \quad \mathbf{v}_{\text{Axis}} = (0,0,1), \quad \mathbf{v}_{\text{Locat}} = (\frac{1}{3},-\frac{1}{3},0), \quad \mathbf{v}_{\text{Inv}} = (\frac{1}{3},-\frac{1}{3},\frac{1}{6}). \tag{16}$$

The last entry on the left side of Table 7 shows a left-handed 120° rotoinversion given by

$$t = x, \quad \mathbf{v}_{\text{Axis}} = (1,-1,-1), \quad \mathbf{v}_{\text{Locat}} = (1,-1,0), \quad \mathbf{v}_{\text{Inv}} = (\frac{1}{8},-\frac{1}{8},\frac{7}{8}). \tag{17}$$

The third on the right side of Table 7 shows a right-handed 90° rotoinversion given by

$$t = z, \quad \mathbf{v}_{\text{Axis}} = (0,0,1), \quad \mathbf{v}_{\text{Locat}} = (\frac{1}{2},-\frac{1}{4},0), \quad \mathbf{v}_{\text{Inv}} = (\frac{1}{2},-\frac{1}{4},\frac{3}{8}). \tag{18}$$

The fifth on the right side of Table 7 shows a left-handed 60° rotoinversion given by

$$t = z, \quad \mathbf{v}_{\text{Axis}} = (0,0,1), \quad \mathbf{v}_{\text{Locat}} = (0,0,0), \quad \mathbf{v}_{\text{Inv}} = (0,0,\frac{1}{4}). \tag{19}$$

# 3 Geometric algebra description of geometric elements and symmetry operations

In conformal geometric algebra a line is given by ($E = \boldsymbol{e}_\infty \wedge \boldsymbol{e}_0$)

$$Line = \boldsymbol{d} \wedge C \wedge \boldsymbol{e}_\infty = \boldsymbol{d} \wedge \boldsymbol{c}\,\boldsymbol{e}_\infty - \boldsymbol{d}E = \boldsymbol{d}\boldsymbol{c}_\perp \boldsymbol{e}_\infty - \boldsymbol{d}E, \tag{20}$$

where

$$C = \boldsymbol{c} + \frac{1}{2}\boldsymbol{c}^2 \boldsymbol{e}_\infty + \boldsymbol{e}_0, \tag{21}$$

is any conformal point on the line associated with the $\boldsymbol{c} \in \mathbb{R}^3$. $\boldsymbol{c}_\perp$ is the distance vector of the line from the origin, called $\mathbf{v}_{\text{Shift}}$ in [1]. The vector $\boldsymbol{d} \in \mathbb{R}^3$ is the unit direction vector of the line, called $\mathbf{v}_{\text{Axis}}$ in [1]. The condition for $C$ to be on the line (20) is

$$C \in Line \quad \Leftrightarrow \quad C \wedge Line = 0. \tag{22}$$

A plane is represented by

$$Plane = \mathbf{i} \wedge C \wedge \boldsymbol{e}_\infty = \mathbf{i} \wedge \boldsymbol{c}\,\boldsymbol{e}_\infty - \mathbf{i}E = \mathbf{i}\boldsymbol{c}_\perp \boldsymbol{e}_\infty - \mathbf{i}E, \tag{23}$$

where again $C$ is any conformal point on the plane associated with the $\boldsymbol{c} \in \mathbb{R}^3$. $\boldsymbol{c}_\perp$ is the distance vector of the plane from the origin, called $\mathbf{v}_{\text{Shift}}$ in [1]. The orientation of the plane is given by its unit bivector $\mathbf{i} \in Cl_{3,0}$. The condition for $C$ to be on the plane (23) is

$$C \in Plane \quad \Leftrightarrow \quad C \wedge Plane = 0. \tag{24}$$

In general the shortest distance $\mathbf{v}_{\text{Shift}}$ of a line (20) (or plane (23)) $F$ from the origin is calculated [9] by

$$\mathbf{v}_{\text{Shift}} = D^{-1}(F \wedge \boldsymbol{e}_0)E, \tag{25}$$

with

$$D = -F \cdot E = \begin{cases} \boldsymbol{d} & \text{for } F = Line \\ \mathbf{i} & \text{for } F = Plane \end{cases}. \tag{26}$$

This solution for $\mathbf{v}_{\text{Shift}}$ is general, constructive and algebraic, no system of linear equation needs to be solved. Note further that (26) is the general way how to extract the direction vector $\mathbf{v}_{\text{Axis}}$ from a line (20)

$$\mathbf{v}_{\text{Axis}} = \boldsymbol{d} = -Line \cdot E. \tag{27}$$

An equivalent way of representing a plane dually with its Euclidean normal vector

$$\boldsymbol{n} = \mathbf{i}\, i^{-1} = \frac{\boldsymbol{c}_\perp}{|\boldsymbol{c}_\perp|}, \qquad \boldsymbol{n} \in \mathbb{R}^3, \tag{28}$$

is[1]

$$\mu = Plane^\star = Plane\, I_5^{-1} = \boldsymbol{n} + d\boldsymbol{e}_\infty, \tag{29}$$

with oriented Euclidean distance of the plane from the origin

$$d = \boldsymbol{c}_\perp \cdot \boldsymbol{n}. \tag{30}$$

[1]The star symbol in $\mu = Plane^\star = Plane I_5^{-1}$ means multiplication by the inverse pseudoscalar of the conformal model of three-dimensional Euclidean space, i.e. multiplication by $I_5^{-1} = i^{-1}E = -iE$. This is the general method for calculating *dual* multivectors.

Now the condition for a conformal point $C$ to be on the plane $\mu$ is

$$C \in \mu \quad \Leftrightarrow \quad C \cdot \mu = 0, \tag{31}$$

because the inner product $\cdot$ is dual to the outer product $\wedge$.

**Remark 3.1** *Equation* (28) *assumes that the plane is in normal form, i.e. that the scalar factor* $\lambda \in \mathbb{R} \setminus \{0\}$ *of the equivalent plane* $\lambda Plane$ *is chosen such that the unit oriented right handed Euclidean pseudoscalar* $i = (\boldsymbol{c}_{\perp}/|\boldsymbol{c}_{\perp}|)\mathbf{i}$.

Parallel planes *Plane* (dual expression $\mu$) and *Plane*$'$ (dual expression $\mu'$) are characterized in GA by parallel bivector parts $\mathbf{i} = \lambda \mathbf{i}', \lambda \in \mathbb{R} \setminus 0$, or equivalently parallel normal vectors $\boldsymbol{n} = \lambda \boldsymbol{n}', \lambda \in \mathbb{R} \setminus 0$. An algebraic way of checking parallelness of planes is to verify the condition: $\boldsymbol{n}'\boldsymbol{n} = \boldsymbol{n}\boldsymbol{n}'$, or equivalently $\boldsymbol{n} \wedge \boldsymbol{n}' = 0$. Or because the outer product $\mu \wedge \mu' = \boldsymbol{n} \wedge \boldsymbol{n}' + (d'\boldsymbol{n}' - d\boldsymbol{n})\boldsymbol{e}_{\infty}$ we can also directly check parallelness by verifying if

$$(\mu \wedge \mu')\boldsymbol{e}_{\infty} = 0. \tag{32}$$

We similarly have that for a plane *Plane* (dual expression $\mu$) and a line *Line* (dual expression *Line*$^{\star}$) parallelness can be checked by

$$(\mu \wedge Line^{\star})\boldsymbol{e}_{\infty} = 0. \tag{33}$$

Given according to (26) the direction of a plane $D = \mathbf{i}$ and of a line $D = \boldsymbol{d}$, the translation part $\mathbf{w}$ of a symmetry operation is most easily split into parts parallel (intrinsic)

$$\mathbf{w}_g = (\mathbf{w} \cdot D)D^{-1}, \quad D^{-1} = \frac{D}{D^2}, \tag{34}$$

and perpendicular

$$\mathbf{w}_L = (\mathbf{w} \wedge D)D^{-1}, \tag{35}$$

to the plane or line.

In geometric algebra, like in Grassmann-Cayley algebra, the meet product (product symbol $\vee$) computes the common subspace blade of two blades. It can thus be applied in order to compute intersections like the intersection of a line and a plane, or of two planes. Computing the meet of a conformal line and a plane results either in the line itself, iff the line is part of the plane; or in an affine point, iff the line intersects the plane (but is not parallel to the plane); or the direction of the line wedge infinity ($\boldsymbol{d} \wedge \boldsymbol{e}_{\infty}$), iff the line is parallel to the plane (but not part of the plane).

An affine point is a point pair $C \wedge \boldsymbol{e}_{\infty}$ of a finite point like (21) and the point at infinity $\boldsymbol{e}_{\infty}$. The Euclidean part $\boldsymbol{c} \in \mathbb{R}^3$ of an affine point can be extracted with

$$\boldsymbol{c} = (C \wedge \boldsymbol{e}_{\infty} \wedge \boldsymbol{e}_0)E. \tag{36}$$

# 4 Coordinates

A crystallographic coordinate system is conventionally given by three coordinate axis vectors

$$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \in \mathbb{R}^3. \tag{37}$$

All details of converting between the geometric algebra choice of crystal cell with its symmetry vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$, as used e.g. in the Space Group Visualizer [10], and the crystallographic cell vectors $\mathbf{e}_1 = \mathbf{a}, \mathbf{e}_2 = \mathbf{b}, \mathbf{e}_3 = \mathbf{c}$ of [5] are given in [8] complete with origin shift vectors[2]. In the current work all results have to be finally represented in coordinates with respect to the conventional crystallographic cell [5] for the sake of obtaining the conventional crystallographic notation of symmetry operations.

The three corresponding reciprocal vectors are obtained by [2]

$$\mathbf{e}_1^* = \frac{\mathbf{e}_2 \wedge \mathbf{e}_3}{\mathbf{e}_1 \wedge \mathbf{e}_2 \wedge \mathbf{e}_3}, \quad \mathbf{e}_2^* = \frac{\mathbf{e}_3 \wedge \mathbf{e}_1}{\mathbf{e}_1 \wedge \mathbf{e}_2 \wedge \mathbf{e}_3}, \quad \mathbf{e}_3^* = \frac{\mathbf{e}_1 \wedge \mathbf{e}_2}{\mathbf{e}_1 \wedge \mathbf{e}_2 \wedge \mathbf{e}_3}. \tag{38}$$

The two systems of vectors are related by

$$\mathbf{e}_k \cdot \mathbf{e}_l^* = \delta_{k,l}, \quad k,l \in \{1,2,3\} \tag{39}$$

with the Kronecker symbol defined as

$$\delta_{k,l} = 0, \text{ if } k \neq l, \quad \delta_{k,l} = 1, \text{ if } k = l. \tag{40}$$

With the help of the reciprocal vectors $\{\mathbf{e}_1^*, \mathbf{e}_2^*, \mathbf{e}_3^*\}$ we can compute the coordinates $x_k, k = 1,2,3$ of any vector $\mathbf{x} \in \mathbb{R}^3$:

$$\mathbf{x} = \sum_{k=1}^{3} x_k \mathbf{e}_k, \quad x_k = \mathbf{x} \cdot \mathbf{e}_k^* \tag{41}$$

In some steps of the algorithm we obtain indexes $k \notin \{1,2,3\}$. These indexes are equivalent to $k \pm 3 : x_0 = x_3, x_4 = x_1, x_5 = x_2$.

Each conformal coordinate axis line (*Axis*) is given by

$$Axis_k = \boldsymbol{e}_0 \wedge C_k \wedge \boldsymbol{e}_\infty = \mathbf{e}_k E, \quad C_k = \mathbf{e}_k + \frac{1}{2}\mathbf{e}_k^2 \boldsymbol{e}_\infty + \boldsymbol{e}_0, \quad k = 1,2,3. \tag{42}$$

In order to check paralellness of a general plane $\mu$ to an axis $Axis_k$ we can either use (33) or simply check if

$$\mu \cdot \mathbf{e}_k = 0. \tag{43}$$

Basal planes (*BPlane*) of a coordinate system are given by the following conformal 4-blades

$$BPlane_1 = -\mathbf{e}_2 \wedge \mathbf{e}_3 E, \quad BPlane_2 = -\mathbf{e}_3 \wedge \mathbf{e}_1 E, \quad BPlane_3 = -\mathbf{e}_1 \wedge \mathbf{e}_2 E, \tag{44}$$

or (up to scale) alternatively in dual form (29) by the normal vectors

$$\mu_1 = \mathbf{e}_1^*, \quad \mu_2 = \mathbf{e}_2^*, \quad \mu_3 = \mathbf{e}_3^*, \tag{45}$$

which are exactly the reciprocal vectors of (38).

# 5 Direct determination of location points of lines and planes

A location point (called variable origin in [1]) of a line or plane is a point $\mathbf{v}_{\text{Locat}}$ on the line or plane conventionally chosen for parametrizing all other points on the line or plane as in (61) and (62).

In the following the combined *choice and direct computation* of location points for lines and planes using geometric algebra techniques is explained. In particular the meet product $\vee$ for computing intersections of geometric objects like lines and planes proves very useful.

[2]Please note that for monoclinic space groups with socalled (declared) unique axis $b$ ITA2005 [5] uses $\mathbf{e}_1 = \mathbf{c}, \mathbf{e}_2 = \mathbf{a}, \mathbf{e}_3 = \mathbf{b}$, which corresponds to the current SGV implementation at the time of writing this paper (i.e. June 2009).

## 5.1 Location points of lines

For lines (20) the conformal location point is given in affine point form [4]

1. $V_{\text{Locat}} \wedge \boldsymbol{e}_\infty = Line \vee BPlane_3$ if the result is an affine point,
2. else $V_{\text{Locat}} \wedge \boldsymbol{e}_\infty = Line \vee BPlane_1$ if the result is an affine point,
3. else $V_{\text{Locat}} \wedge \boldsymbol{e}_\infty = Line \vee BPlane_2$

where $\vee$ is the conformal meet product of geometric algebra.

**Remark 5.1** *It is evident from the description of the meet product of lines and planes in Section 3, that in the third row $Line \vee BPlane_2$ is always an affine point for both $Line \vee BPlane_3$ and $Line \vee BPlane_1$ not being affine points, because then the line Line will be parallel to both basal planes $BPlane_3, BPlane_1$ and therefore parallel to their line of intersection $Axis_2$. Using the dual form of the basal planes* (45)*, makes the computation of the meet $\vee$ in terms of the outer product $\wedge$ straight forward ($M^\star = M I_5^{-1}, M \in Cl_{4,1}$)*

*1. $V_{\text{Locat}} \wedge \boldsymbol{e}_\infty = (Line^\star \wedge \mathbf{e}_3^*)^\star$ if the result is an affine point,*

*2. else $V_{\text{Locat}} \wedge \boldsymbol{e}_\infty = (Line^\star \wedge \mathbf{e}_1^*)^\star$ if the result is an affine point,*

*3. else $V_{\text{Locat}} \wedge \boldsymbol{e}_\infty = (Line^\star \wedge \mathbf{e}_2^*)^\star$.*

The Euclidean part $\mathbf{v}_{\text{Locat}} \in \mathbb{R}^3$ can be directly extracted from the affine point $V_{\text{Locat}} \wedge \boldsymbol{e}_\infty$ by (36)

$$\mathbf{v}_{\text{Locat}} = (V_{\text{Locat}} \wedge \boldsymbol{e}_\infty \wedge \boldsymbol{e}_0)E. \tag{46}$$

## 5.2 Location points of planes

The affine location point of a plane (23) is determined similarly by the intersection of the plane with the conformal coordinate axis lines

1. $V_{\text{Locat}} \wedge \boldsymbol{e}_\infty = Plane \vee Axis_1$ if the result is an affine point,
2. else $V_{\text{Locat}} \wedge \boldsymbol{e}_\infty = Plane \vee Axis_2$ if the result is an affine point,
3. else $V_{\text{Locat}} \wedge \boldsymbol{e}_\infty = Plane \vee Axis_3$.

The Euclidean part of the affine location point of a plane (23) is again determined according to (36).

**Remark 5.2** *In the third line of the location point determination of a plane* (23)*, the plane is parallel to both $Axis_1$ and $Axis_2$, so that the intersection $Plane \vee Axis_3$ necessarily leads to a well-defined affine point.*

## 5.3 Algorithm for the determination of location points

### 5.3.1 Algorithm for location points of lines

1. If $AP_3 = Line \vee BPlane_3$ affine point: abort and return $\mathbf{v}_{\text{Locat}} = (AP_3 \wedge \boldsymbol{e}_0)E$.
2. Else if $AP_1 = Line \vee BPlane_1$ affine point: abort and return $\mathbf{v}_{\text{Locat}} = (AP_1 \wedge \boldsymbol{e}_0)E$.
3. Else abort and return $\mathbf{v}_{\text{Locat}} = [(Line \vee BPlane_2) \wedge \boldsymbol{e}_0]E$.

#### 5.3.2 Algorithm for location points of planes

1. If $AP_1 = Plane \vee Axis_1$ affine point: abort and return $\mathbf{v}_{\text{Locat}} = (AP_1 \wedge \boldsymbol{e}_0)E$.
2. Else if $AP_2 = Plane \vee Axis_1$ affine point: abort and return $\mathbf{v}_{\text{Locat}} = (AP_2 \wedge \boldsymbol{e}_0)E$.
3. Else abort and return $\mathbf{v}_{\text{Locat}} = [(Plane \vee Axis_1) \wedge \boldsymbol{e}_0]E$.

# 6 Direct determination of two trace vectors for each plane

## 6.1 Crystallographic trace vectors of planes in geometric algebra

The crystallographic conventions that apply are contained in rule C6 and Table 1 of [1].

For a plane $\mu$ *parallel to one of the three basal planes* $\mu_k$, $k \in \{1,2,3\}$, compare (32), the trace vectors are simply the coordinate axis vectors spanning the basal plane (see (44))

$$\begin{aligned}
(\mu \wedge \mu_1)\boldsymbol{e}_\infty = 0: &\quad \mathbf{v}_{\text{Trace1}} = \mathbf{e}_2, \mathbf{v}_{\text{Trace2}} = \mathbf{e}_3, \\
(\mu \wedge \mu_2)\boldsymbol{e}_\infty = 0: &\quad \mathbf{v}_{\text{Trace1}} = \mathbf{e}_3, \mathbf{v}_{\text{Trace2}} = \mathbf{e}_1, \\
(\mu \wedge \mu_3)\boldsymbol{e}_\infty = 0: &\quad \mathbf{v}_{\text{Trace1}} = \mathbf{e}_1, \mathbf{v}_{\text{Trace2}} = \mathbf{e}_2.
\end{aligned} \tag{47}$$

**Remark 6.1** *We observe that the indexes* $1,2,3$ *of* $\mu_1, \mathbf{e}_2, \mathbf{e}_3$*, appear in cyclic order in* (47)*. Therefore together with* ***cyclic permutation*** *we can restrict ourselves to the first line of* (47)

$$(\mu \wedge \mu_1)\boldsymbol{e}_\infty = 0: \quad \mathbf{v}_{\text{Trace1}} = \mathbf{e}_2, \mathbf{v}_{\text{Trace2}} = \mathbf{e}_3. \tag{48}$$

Planes $\mu$ *parallel to only one coordinate axis* $Axis_k$, $k \in \{1,2,3\}$, i.e. according to (43)

$$\begin{aligned}
&\mu \cdot \mathbf{e}_k = 0, \text{ for some fixed } k \in \{1,2,3\}, \\
&\mu \cdot \mathbf{e}_l \neq 0, \quad l \in \{1,2,3\}, \quad l \neq k,
\end{aligned} \tag{49}$$

have this parallel coordinate axis vector $\mathbf{e}_k$ as their first trace vector

$$\mathbf{v}_{\text{Trace1}} = \mathbf{e}_k. \tag{50}$$

The direction vector of the line of intersection with the basal plane $\mu_k = \mathbf{e}_k^*$ formed by the two other coordinate axis vectors gives the second trace vector

$$Line_{\text{Trace2}} = \mu \vee \mathbf{e}_k^*. \tag{51}$$

The trace vector (up to scale) can be extracted from (51) using (27) as

$$\mathbf{v}_{\text{Trace2}} = Line_{\text{Trace2}} \cdot E = (\mu \vee \mathbf{e}_k^*) \cdot E. \tag{52}$$

Only in case that the plane $\mu$ in question is *not parallel to any of the three coordinate axis vectors*, a special convention is made by rule C6 of [1]

$$\mathbf{v}_{\text{Trace1}} = (\mu \vee \mathbf{e}_3^*) \cdot E, \quad \mathbf{v}_{\text{Trace2}} = (\mu \vee \mathbf{e}_2^*) \cdot E. \tag{53}$$

In this case the following parameters are chosen

$$t_1 = x, \quad t_2 = z. \tag{54}$$

## 6.2 Algorithm for the determination of trace vectors

In abbreviated *algorithmic* form the two trace vectors of a plane can be calculated by (assuming $\mathbf{e}_4 = \mathbf{e}_1$, $\mathbf{e}_5 = \mathbf{e}_2$)

1. For $k = 1,2,3$
   If $(\mu \wedge \mu_k)\boldsymbol{e}_\infty = 0$:
   abort and return $\mathbf{v}_{\text{Trace1}} = \mathbf{e}_{k+1}$, $\mathbf{v}_{\text{Trace2}} = \mathbf{e}_{k+2}$.

2. Else for $k = 1,2,3$
   If $\mu \cdot \mathbf{e}_k = 0$:
   abort and return $\mathbf{v}_{\text{Trace1}} = \mathbf{e}_k$, $\mathbf{v}_{\text{Trace2}} = (\mu \vee \mathbf{e}_k^*) \cdot E$.

3. Else abort and return $\mathbf{v}_{\text{Trace1}} = (\mu \vee \mathbf{e}_3^*) \cdot E$, $\mathbf{v}_{\text{Trace2}} = (\mu \vee \mathbf{e}_2^*) \cdot E$, $t_1 = x$, $t_2 = z$.

# 7 Crystallographic positive sense of a vector

## 7.1 Definition of crystallographic positive sense of a vector

The crystallographic positive sense of a vector $\mathbf{x} \neq 0$ with respect to a coordinate system (37) is defined by the condition (compare C2 of [1])

$$s(\mathbf{x}) = \prod_{k=1}^{3} x_k, \quad s(\mathbf{x}) > 0. \tag{55}$$

**Remark 7.1** *The value of $s(\mathbf{x})$ is coordinate system specific.*

**Remark 7.2** *A vector $\mathbf{x}$ with $s(\mathbf{x}) < 0$ can always be reoriented to positive sense by*

$$\mathbf{x} \mapsto \operatorname{sgn}(s(\mathbf{x}))\mathbf{x}. \tag{56}$$

In case that $s(\mathbf{x}) = 0$ the vector $\mathbf{x}$ must lie in one of the basal planes (44). The sense of $\mathbf{x}$ is then chosen such that

$$\begin{aligned} x_1 > 0 \quad &\text{for} \quad x_3 = 0, \\ x_2 > 0 \quad &\text{for} \quad x_1 = 0, \\ x_3 > 0 \quad &\text{for} \quad x_2 = 0. \end{aligned} \tag{57}$$

**Remark 7.3** *The three conditions* (57) *express open half basal planes, where "open" means that the delimiting axis line is excluded. They are cyclically related by*

$$x_k > 0 \quad \textit{for} \quad x_{k-1} = 0, \quad k = 1,2,3. \tag{58}$$

**Remark 7.4** *A consequence of* (57) *is that pure multiples $x_k\mathbf{e}_k$, $x_k \neq 0$, $k = 1,2,3$ (no summation over k) of the three basis vectors are reoriented to $|x_k|\,\mathbf{e}_k$.*

## 7.2 Algorithm for reorientation of vectors to crystallographic positive sense

1. Precompute coordinates $x_k$ according to (41).

2. Compute $s(\mathbf{x})$ according to (55).

3. If $s(\mathbf{x}) \neq 0$ abort and return $\operatorname{sgn}(s(\mathbf{x}))\mathbf{x}$.
4. Else if $s(\mathbf{x}) = 0$ compute
$$t(\mathbf{x}) = \sum_{k=1}^{3} x_{k+1} x_{k-1}^2. \tag{59}$$
5. If $t(\mathbf{x}) \neq 0$, abort and return $\operatorname{sgn}(t(\mathbf{x}))\mathbf{x}$.
6. Else compute
$$u(\mathbf{x}) = \sum_{k=1}^{3} x_k, \tag{60}$$
abort and return $\operatorname{sgn}(u(\mathbf{x}))\mathbf{x}$.

# 8 Choice of variable symbols for parametrizing lines and planes

In crystallography [1, 5] standard orientation-location parts of geometric elements of symmetry operations are given in the form
$$t\mathbf{v}_{\text{Axis}} + \mathbf{v}_{\text{Locat}} \tag{61}$$
for lines and
$$t_1\mathbf{v}_{\text{Trace1}} + t_2\mathbf{v}_{\text{Trace2}} + \mathbf{v}_{\text{Locat}} \tag{62}$$
for planes. The question of this section is the conventional determination of the parameter variables $t$, $t_1$, $t_2$ for given coordinate form vectors $\mathbf{v}_{\text{Axis}}$, $\mathbf{v}_{\text{Trace1}}$, $\mathbf{v}_{\text{Trace2}}$. The axis vector of a line $\mathbf{v}_{\text{Axis}}$ is the coordinate form of the direction vector $\boldsymbol{d}$ of a line as given in (20). The trace vectors $\mathbf{v}_{\text{Trace1}}$ and $\mathbf{v}_{\text{Trace2}}$ of a plane (23) are the coordinate forms of direction vectors of two lines of intersection of the plane with basal planes (*BPlane*), compare (44) and (45). The conventional choice of the two lines of intersection from the (two or) three possible ones will also be explained in Section 6.

The vectors $\mathbf{v}_{\text{Axis}}$, $\mathbf{v}_{\text{Trace1}}$ and $\mathbf{v}_{\text{Trace2}}$ can all be expressed with respect to the coordinate system (37) in the form of (41)
$$\mathbf{v} = \sum_{k=1}^{3} v_k \mathbf{e}_k, \quad v_k = \mathbf{v} \cdot \mathbf{e}_k^*,\ k = 1,2,3. \tag{63}$$
The *conventional crystallographic parameter variables* are (compare (C3) of [1])
$$\begin{aligned} t = x \quad &\text{for} \quad v_1 \neq 0, \\ t = y \quad &\text{for} \quad v_1 = 0, v_2 \neq 0, \\ t = z \quad &\text{for} \quad v_1 = v_2 = 0, v_3 \neq 0, \end{aligned} \tag{64}$$
where $t \to t_1$ for $\mathbf{v}_{\text{Trace1}}$ and $t \to t_2$ for $\mathbf{v}_{\text{Trace2}}$.

# 9 Full algorithm for conversion of geometric algebra versor notation to crystallographic symmetry-operation notation

## 9.1 Algorithm for rotations, screw rotations and rotoinversions

1. Given the multivector versor expressions of rotations, screw rotations and rotoinversions, the axis line *Line* (20) can be easily computed.
2. According to Section 5.3.1 the location point of the line $\mathbf{v}_{\text{Locat}}$ is determined.
3. The direction vector $\mathbf{v}_{\text{Axis}}$ is determined according to (26).
4. The direction vector needs to be scaled, such that its three coordinates $v_k = \mathbf{v}_{\text{Axis}} \cdot \mathbf{e}_k^*, k = 1,2,3$ form relatively prime integers.
5. The direction vector needs to be oriented according to Section 7.2.
6. The variable symbol $t$ is chosen according to Section 8. Thus we arrive at the final (coordinate) form of the orientation-location part
$$t\,\mathbf{v}_{\text{Axis}} + \mathbf{v}_{\text{Locat}}. \tag{65}$$
7. For screw rotations the decomposition of translations of (34) leads to the intrinsic translation component (parallel to the axis).
8. The sense of the rotation axis is also important for the determination the correct crystallographic (left-handed = positive, or right-handed = negative) rotation angle $\alpha$, and its symbol $n^{\pm} = 360/\alpha$. The sign of $\alpha$ determines the upper $\pm$ index of $n^{\pm}$.

## 9.2 Algorithm for reflections and glide reflections

1. Given the multivector versor expressions of reflections and glide reflections, the reflection plane in vector form $\mu$ (29) can easily be determined.
2. According to Section 5.3.2 the location point of the line $\mathbf{v}_{\text{Locat}}$ is determined.
3. The two trace vectors $\mathbf{v}_{\text{Trace1}}$ and $\mathbf{v}_{\text{Trace2}}$ are determined according to Section 6.
4. Each trace vector needs to be scaled, such that its three coordinates $v_k = \mathbf{v}_{\text{Trace}} \cdot \mathbf{e}_k^*, k = 1,2,3$ form relatively prime integers.
5. Each trace vector needs to be oriented according to Section 7.2.
6. The variable symbols $t_1$, $t_2$ need to be chosen according to Section 8. Thus we arrive at the final (coordinate) form of the orientation-location part
$$t_1\,\mathbf{v}_{\text{Trace1}} + t_2\,\mathbf{v}_{\text{Trace2}} + \mathbf{v}_{\text{Locat}}. \tag{66}$$
7. For glide reflections the decomposition of translations of (34) leads to the intrinsic translation component $\mathbf{w}_g$ (parallel to the plane). This intrinsic translation component determines the choice of glide reflection symbol $r \in \{a,b,c\}$ for $\mathbf{w}_g \in \{\mathbf{a}/2, \mathbf{b}/2, \mathbf{c}/2\}$, or $s = n$ for face diagonal vectors $\mathbf{w}_g$, or $s = d$ for pairs of diamond glide vectors $\mathbf{w}_g$ (half of centering vectors). In all other cases the symbol is $s = g$. Compare Section 2.2.

## Acknowledgment

E. H. wishes to acknowledge God the creator: *Soli Deo Gloria*, as well as the loving support of his family. We gratefully acknowledge helpful discussions with M. Aroyo (Bilbao).

## References

[1] K. Stróż, *A systematic approach to the derivation of standard orientation-location parts of symmetry-operation symbols*, Acta Crystallographica Section A, A63, pp. 447–454, 2007.

[2] Doran, C. & Lasenby, A. (2003). *Geometric Algebra for Physicists*, CUP, Cambridge UK.

[3] Dorst, L. & Fontijne, D. & Mann, S. (2007). *Geometric Algebra for Computer Science: An Object-oriented Approach to Geometry*, Morgan Kaufmann Series in Computer Graphics, San Francisco.

[4] Li, H. (2008). *Invariant Algebras and Geometric Reasoning*, World Scientific, Singapore.

[5] Hahn, T. (2005). *Int. Tables for Crystallography*, 5th ed., Vol. A, Springer, Dordrecht.

[6] Hestenes, D. (2002). *Point groups and space groups in geometric algebra*, edited by L. Dorst et al., *Applications of Geometric Algebra in Computer Science and Engineering*, Birkhäuser, Basel, 3–34.

[7] Hestenes, D. & Holt, J. (2007). *The Crystallographic Space Groups in Geometric Algebra*, JMP, Vol. 48, 023514.

[8] E. Hitzer, C. Perwass, *Interactive 3D Space Group Visualization with CLUCalc and the Clifford Geometric Algebra Description of Space Groups*, accepted for Proc. 8th Int. Conf. on Clifford Algebras (ICCA8) and their Appl. in Math. Phys., 26-30 May 2008, Las Campinas, Brazil (2008).

[9] Hitzer, E. & Tachibana, K. & S. Buchholz, & Yu, I. (2009) *Carrier Method for the General Evaluation and Control of Pose, Molecular Conformation, Tracking, and the Like*, *Adv. appl. Clifford alg.*, Online First.

[10] C. Perwass, E. Hitzer, (2005). *Space Group Visualizer*, `www.spacegroup.info`.