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SYMMETRY OF ORTHORHOMBIC MATERIALS AND INTERACTIVE 3D VISUALIZATION IN GEOMETRIC ALGEBRA

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ABSTRACT

The *Space Group Visualizer* is the main software that we use in this work to show the symmetry of *orthorhombic* space groups as interactive computer graphics in three dimensions. For that it is necessary to know the features and the classification of orthorhombic point groups and space groups. For representing the symmetry transformations of point groups and space groups, we employ (Clifford) geometric algebra. This algebra results from applying the associative geometric product to the vectors of a vector space. Some major features of the software implementation are discussed. Finally a brief overview of interactive functions of the Space Group Visualizer is given.

1. INTRODUCTION

1.1 Orthorhombic Materials

Elements with orthorhombic lattice cell structures are gallium, black phosphorus, chlorine, bromine, iodine and rhombic sulfur [18]. More than 900 minerals are known to have orthorhombic structure. Important technical examples are *high temperature super conductors* $DyBa_2Cu_3O_{7-y}$ and $HoBa_2Cu_3O_{7-y}$, super conducting up to 86 K and 88 K, respectively [19].

Many orthorhombic materials display *piezoelectricity*, important for high voltage and power sources, sensors, actuators, frequency standards, piezoelectric motors and the reduction of vibrations [8].

Orthorhombic materials are technically highly relevant and their properties deserve a detailed structural investigation. The orthorhombic crystal class is fully characterized by its point symmetry group (leaving a selected vertex invariant) and each structure within an orthorhombic crystal class is sub-classified by its particular 3D space symmetry group.

We will use *geometric algebra* (GA) [10] to represent point groups [3,11,12] and space groups [4,5,13,14,15,16] in three dimensions (3D). Based on this new representation we develop the 3D interactive computer visualization of all 59 orthorhombic space groups.

1.2 Introduction to Geometric Algebra

Geometric algebras (GA) [10] are defined by applying the associative geometric product to vectors of a vector space.

In mathematics, a (Clifford) geometric algebra $G_n(V_n)$ is an algebra constructed over an inner product vector space V_n on which a geometric product is defined. For all multivectors (elements of the algebra, including real numbers and vectors of V_n) $A, B, C \in G_n(V_n)$ the geometric product has the following properties:

1. Closure of the geometric product of multivectors:

$$\forall A, B \in G_n : AB \in G_n. \quad (1)$$

2. Right and left distributivity over the addition of multivectors:

$$A(B+C) = AB + AC, \quad (2)$$
$$(A+B)C = AC + BC, \quad (3)$$

3. Associativity of both geometric multiplication and addition

$$(AB)C = A(BC) = ABC. \quad (4)$$
$$(A+B)+C = A+(B+C) = A+B+C. \quad (5)$$

4. Real unit (scalar) element:

$$1A = A. \tag{6}$$

5. Tensor contraction (quadratic form, square of length) of vectors

$$\forall \vec{a} \in V_n, \vec{a}^2 = \left|\vec{a}\right|^2 \in \mathrm{R}. \tag{7}$$

6. Commutativity of the product by a scalar $\lambda \in \boldsymbol{R}$

$$\lambda A = A\lambda. \tag{8}$$

Note that the first two properties of closure and distributivity are needed to form an algebra. The next two make it an associative, unital algebra. The distinctive point of our geometric algebra formulation is the natural correspondence between geometric entities and elements of the associative algebra. This comes from the fact that the geometric product of vectors is defined in terms of the dot product and the wedge product of vectors as

$$\forall \vec{a}, \vec{b} \in V_n:$$
$$\vec{a}\vec{b} = \vec{a} \cdot \vec{b} + \vec{a} \wedge \vec{b} = \left|\vec{a}\right|\left|\vec{b}\right|(\cos\alpha + I \sin\alpha), \tag{9}$$

where α is the angle between the vectors $\vec{a}$ and $\vec{b}$, and I is the oriented unit bivector area of the plane spanned by $\vec{a}$ and $\vec{b}$.
The dot product (or inner product) is symmetric. The outer product (or wedge product) is anti-symmetric. It was invented by H. Grassmann (1844).

$$\vec{a} \cdot \vec{b} = \vec{b} \cdot \vec{a}. \tag{10}$$
$$\vec{a} \wedge \vec{b} = -\vec{b} \wedge \vec{a}. \tag{11}$$

Dot and wedge products are therefore related to the geometric product by

$$\vec{a} \cdot \vec{b} = \frac{1}{2}(\vec{a}\vec{b} + \vec{b}\vec{a}) = \left|\vec{a}\right|\left|\vec{b}\right|\cos\alpha, \tag{12}$$

$$\vec{a} \wedge \vec{b} = \frac{1}{2}(\vec{a}\vec{b} - \vec{b}\vec{a}) = \left|\vec{a}\right|\left|\vec{b}\right| I \sin\alpha. \tag{13}$$

The wedge product (13) is illustrated in Fig. 1.
An important consequence is that under the geometric product parallel vectors commute

$$\vec{a} \parallel \vec{b} \Leftrightarrow \vec{a}\vec{b} = \vec{b}\vec{a}, \tag{14}$$

Because $\vec{a} \wedge \vec{b} = 0$ for $\vec{a} \parallel \vec{b}$, and perpendicular vectors anti-commute

$$\vec{a} \perp \vec{b} \Leftrightarrow \vec{a}\vec{b} = -\vec{b}\vec{a}, \tag{15}$$

because $\vec{a} \cdot \vec{b} = 0$ for $\vec{a} \perp \vec{b}$.

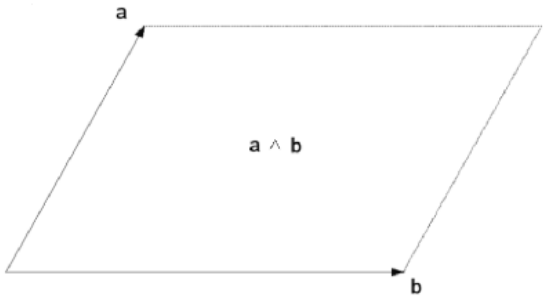

Fig. 1 Two vectors $\vec{a}$ and $\vec{b}$ define the bivector $\vec{a} \wedge \vec{b}$.

This in turn leads to the *reflection* formula (see Fig. 2) at a hyperplane with normal vector $\vec{a}$:

$$\vec{x}' = -\vec{a}^{-1}\vec{x}\vec{a}, \quad \vec{a}^{-1} = \frac{\vec{a}}{\vec{a}^2}, \quad \forall \vec{x} \in V_n \tag{16}$$

where $\vec{a}^{-1}$ is the multiplicative inverse of vector $\vec{a}$ w.r.t. the geometric product (9).

We can show Equ. (16) by a direct geometric computation:

$$\begin{aligned} \vec{x}' &= -\vec{x}_{\parallel} + \vec{x}_{\perp} = -\vec{a}^{-1}\vec{a}\vec{x}_{\parallel} + \vec{a}^{-1}\vec{a}\vec{x}_{\perp} \\ &= -\vec{a}^{-1}\vec{x}_{\parallel}\vec{a} - \vec{a}^{-1}\vec{x}_{\perp}\vec{a} = -\vec{a}^{-1}(\vec{x}_{\parallel} + \vec{x}_{\perp})\vec{a} \\ &= -\vec{a}^{-1}\vec{x}\vec{a}, \end{aligned} \tag{17}$$

where $\vec{x}_{\parallel} \parallel \vec{a}$ and $\vec{x}_{\perp} \perp \vec{a}$ can be computed from

$$\vec{x}_{\parallel} = (\vec{x} \cdot \vec{a})\vec{a}^{-1}, \quad \vec{x}_{\perp} = (\vec{x} \wedge \vec{a})\vec{a}^{-1}. \tag{18}$$

As a consequence of (16) the *rotation* (see Fig. 3) around the line of intersection of two hyperplanes with normal vectors $\vec{a}$, $\vec{b}$ by twice the angle between $\vec{a}$ and $\vec{b}$ is given by reflecting at planes perpendicular to $\vec{a}$ and $\vec{b}$:

$$\begin{aligned} &\forall \vec{x} \in V_n: \ \vec{x}' = (\vec{a}\vec{b})^{-1}\vec{x}\vec{a}\vec{b}, \\ &(\vec{a}\vec{b})^{-1} = \vec{b}^{-1}\vec{a}^{-1}, \end{aligned} \tag{19}$$

because

$$(\vec{b}^{-1}\vec{a}^{-1})(\vec{a}\vec{b}) = \vec{b}^{-1}(\vec{a}^{-1}\vec{a})\vec{b} = \vec{b}^{-1}\vec{b} = 1. \quad (20)$$

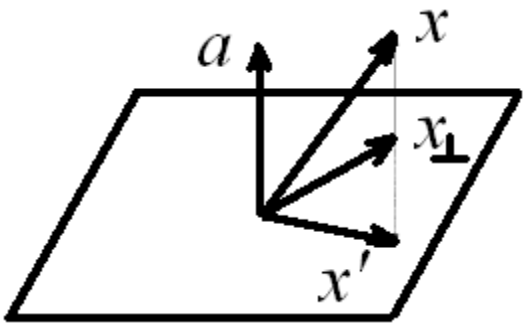

Fig. 2 Reflection of vector $\vec{x}$ through the plane with normal vector $\vec{a}$.

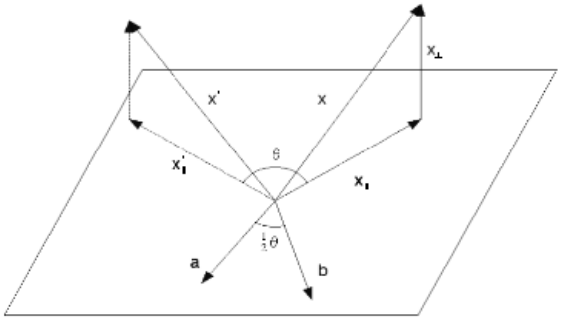

Fig. 3 Rotation of vector $\vec{x}$ through the angle θ around an axis perpendicular to vectors $\vec{a}$ and $\vec{b}$. Note that the rotation is through twice the angle $\theta/2$ between vectors $\vec{a}$ and $\vec{b}$.

2. POINT GROUPS

In mathematics, a point group is a group of geometric symmetries (isometries) leaving one selected point fixed and all lengths and angles invariant. Point groups have characteristic figures, e.g. polygons in two dimensions (2D) or polyhedrons in 3D, which they leave invariant as a whole. Point groups can exist in a Euclidean space of any dimension. In 2D a discrete point group is sometimes called a rosette group, and is used to describe the symmetries of an ornament.

2.1 Two-Dimensional Point Groups

Now we explain the two kinds of symmetry that can occur in a 2D point group.

- *Reflection* symmetries:

The simplest kind of geometric vector operator (versor) is a single vector, and the linear transformation that it generates according to (16) is called a reflection. The reflection (comp. Fig. 2) at a hyperplane (line in 2D) generated by the normal vector $\vec{a}$ has the form (17)

$$\vec{x}' = -\vec{a}^{-1}\vec{a}\vec{x} = \vec{x}_{\perp} - \vec{x}_{\parallel}, \quad (21)$$

where $\vec{x}_{\parallel}$ is the component of $\vec{x}$ along $\vec{a}$ (perpendicular to the hyperplane) and $\vec{x}_{\perp}$ is the component of $\vec{x}$ orthogonal to $\vec{a}$ (parallel to the hyperplane) as in (18).

- *Rotation* symmetries:

The product $\vec{a}\vec{b}$ of two vectors generates according to (19) a rotation (see Fig. 3)

$$\vec{x}' = (\vec{a}\vec{b})^{-1}\vec{x}(\vec{a}\vec{b}) = R^{-1}\vec{x}R, \quad (22)$$

through twice the angle between $\vec{a}$ and $\vec{b}$, with $R = \vec{a}\vec{b}$. For $\vec{a} \perp \vec{b}$ we get a 180° rotation, i.e. an inversion in 2D.

Two-dimensional symmetries of regular polygons with $n = 2,3,4$ and 6 corners characterize crystallographic point groups. $I = \vec{e}_1\vec{e}_2$ is the unit 2D area bivector, $\vec{e}_1, \vec{e}_2$ are two unit vectors with angle 90°, $\vec{a}, \vec{b}$ are vectors connecting vertexes, and the angle between $\vec{a}, \vec{b}$ is defined to be $180^\circ / n$. The vectors are finally attached to the invariant geometric center of each figure (Fig. 4). We obtain the following point groups, denoted by integers (1,2,3,4,6) without overbars (reflection groups) and with overbars (rotation groups).

1. For $n = 1$ (only one of the two vectors in an oblique or rectangular 2D cell),

   oblique: $\overline{1} = \{\vec{a}^2 = 1\}$, (23)

   rectangular: $1 = \{\vec{a}, \vec{a}^2 = 1\}$. (24)

   Point group $\overline{1}$ is the rotation subgroup of point group 1. ($\overline{1}$ contains only the identity transformation.) Note that the generators 1 and -1 both correspond to identity, because $\vec{x}' = (-1)\vec{x}(-1) = \vec{x}$.

2. For $n = 2$ (point pair connected by a line segment, corresponds to an oblique or rectangular 2D lattice cell), the angle $\angle(\vec{a}, b) = 180^\circ / 2 = 90^\circ$.

oblique: $\overline{2} = \{\vec{a}\vec{b}, (\vec{a}\vec{b})^2 = -1\}$, (25)

rectangular: $2 = \{\vec{a}, \vec{b}, \vec{a}\vec{b}, (\vec{a}\vec{b})^2 = -1\}$. (26)

$\overline{2}$ is the rotation subgroup of the reflection group 2. $\vec{a}$, $\vec{b}$ are the reflections across lines parallel to the sides, through the center of the rectangle.

3. For $n = 4$ (square shaped 2D cell),

$$4 = \{\vec{a}, \vec{b}, \vec{a}(\vec{a}\vec{b})^2, \vec{a}(\vec{a}\vec{b})^3, \vec{a}\vec{b}, (\vec{a}\vec{b})^2, (\vec{a}\vec{b})^3, (\vec{a}\vec{b})^4 = -1\}, \quad (27)$$

$$\overline{4} = \{\vec{a}\vec{b}, (\vec{a}\vec{b})^2, (\vec{a}\vec{b})^3, (\vec{a}\vec{b})^4 = -1\}. \quad (28)$$

$\overline{4}$ is the rotation subgroup of 4. $R = \vec{a}\vec{b}$ generates a 90° rotation around the geometric center of the square. $\vec{b}$ is a diagonal vector to the point next to the end point of $\vec{a}$, as shown in Fig. 4, $\vec{a}$ itself is a side vector.

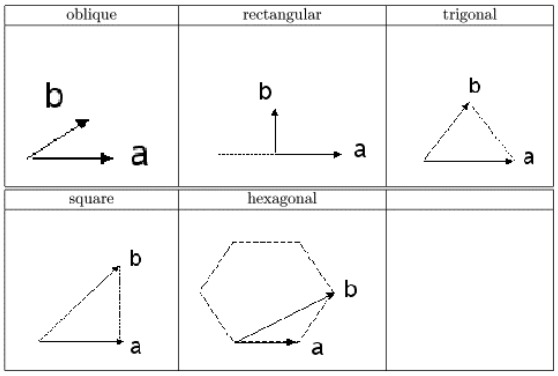

Fig. 4 An oblique cell and regular polygons for n =2,3,4,6 with vector generators $\vec{a}$, $\vec{b}$.

2.2 Three-Dimensional Point Groups

The three-dimensional (3D) discrete point groups are heavily used in chemistry and material science, especially to describe the symmetries of a molecule, of a cluster and of orbitals forming covalent bonds, and in this context they are also called molecular point groups. There are infinitely many discrete point groups in dimensions $n \geq 2$. However, only a finite number is compatible with the translational symmetry of a regular periodic lattice. This is stated in the crystallographic restriction theorem. In one dimension (1D) there are 2, in 2D 10, and in 3D 32 point groups, respectively. They are called crystallographic point groups.

In crystallography, a crystallographic point group is a set of symmetry operations, like rotations or reflections, that leave a central point fixed while moving each atom of the crystal to the position of an atom of the same kind. That is, a crystal cell would look exactly the same before and after any of the operations in its point group. In the classification of crystals, each point group corresponds to a crystal class. We list the first eight crystallographic 3D point groups in Table 1, according to their crystal system with point group symbol (international name [2], geometric name [1], Schoenflies symbol), and the geometric versor generators (products of the lattice vectors $\vec{a}$, $\vec{b}$, $\vec{c}$) [1].

Table 1 The first eight 3D point groups listed by crystal system, number (1-8) (from [2]), international (from [2]), geometric (from [1]) and Schonflies names, complete with a list of versor generators.

Crystal system	No.	Int. name	Geom. name	Schoenflies	Generators
Triclinic (anorthic)	1	1	$\overline{1}$	C_1	1
	2	$\bar{1}$	$\overline{22}$	C_i	a∧b∧c
Monoclinic	3	2	$\overline{2}$	C_2	a∧b
	4	m	1	C_s	a
	5	2/m	$\overline{2}2$	C_{2h}	a∧b, c
Orthorhombic	6	222	$\overline{22}$	D_2	ab, bc
	7	mm2	2	C_{2v}	a,b
	8	mmm	22	D_{2h}	a,b,c

3. SPACE GROUPS IN TWO AND THREE DIMENSIONS

Space groups are basically combinations of point group symmetries together with suitably chosen fractions of lattice (vertex to vertex) translations.

3.1 Two-Dimensional Space Groups

A 2D space group is a mathematical concept to classify repetitive designs on two-dimensional surfaces, such as wallpaper patterns or crystal planes, based on the symmetries in the pattern. Such patterns occur frequently in nature, architecture and decorative art. The mathematical study of such patterns reveals that no more than exactly 17 different types of patterns can occur. [9]

The unit cell of a primitive "p" lattice contains a single lattice point. The unit cell of a centered "c" lattice contains two points, one of them at the center of the 2D lattice cell. We explain the

various combinations of symmetries and the 17 2D space groups and their generators in Tables 2 and 3. Restricting $\vec{x}$ and $\vec{t}$ to the $\vec{a}$, $\vec{b}$ -plane, Table 2 lists symmetries of 2D space groups, hyperplanes are then simply lines. The expressions of Table 2 are also true for 3D space groups, with $\vec{x},\vec{t} \in \boldsymbol{R}^3$. In 3D the center of rotation simply becomes the axis of rotation perpendicular to the $\vec{a}$, $\vec{b}$ -plane, and the hyperplanes become ordinary 2D planes.

Table 2 Examples of various symmetries and combinations in Euclidean GA, and in the conformal GA model of Euclidean space with 3D vectors $\vec{a},\vec{b},\vec{t} \in \boldsymbol{R}^3$, and integers $k,l \in \boldsymbol{Z}$.

Euclidean	Conformal	Conf. operator	Symmetry and condition
$-\vec{a}^{-1}\vec{x}\vec{a}$	$-\vec{a}^{-1}X\vec{a}$	$\vec{a}$	reflection at hyperplane ($\perp \vec{a}$) located at origin
$(\vec{a}\vec{b})^{-1}\vec{x}(\vec{a}\vec{b})$	$(\vec{a}\vec{b})^{-1}X(\vec{a}\vec{b})$	$\vec{a}\vec{b}$	rotation in $\vec{a},\vec{b}$-plane by twice $\angle(\vec{a},\vec{b})$, rot. center at origin
$\vec{x}+\vec{t}$	$T_{\vec{t}}^{-1}XT_{\vec{t}}$	$T_{\vec{t}}$	translation by $\vec{t} \in \mathbb{R}^3$
		$\vec{a}T_{\frac{1}{2}\vec{b}}$	glide reflection ($\vec{a} \perp \vec{b}$) with hyperplane ($\perp \vec{a}$)
		$\vec{a}T_{k\vec{a}}$	reflection at hyperplane ($\perp \vec{a}$) located at $\frac{k}{2}\vec{a}$
		$\vec{a}T_{\frac{1}{2}\vec{b}}T_{k\vec{a}}$	glide reflection ($\vec{a} \perp \vec{b}$) with hyperplane ($\perp \vec{a}$) located at $\frac{k}{2}\vec{a}$
		$\vec{a}\vec{b}T_{k\vec{a}+l\vec{b}}$	180° rotation ($\vec{a} \perp \vec{b}$) located at $\frac{k}{2}\vec{a}+\frac{l}{2}\vec{b}$
		$T_{\vec{t}}^{-1}\vec{a}\vec{b}T_{\vec{t}}$	rotation in $\vec{a},\vec{b}$-plane by twice $\angle(\vec{a},\vec{b})$, rot. center at $\vec{t}$

Best suited for the inclusion of translations is the so-called conformal model of Euclidean space (in the GA of $\boldsymbol{R}^{4,1}$), which adds two null-vector dimensions for the origin $\vec{n}_0$ and infinity $\vec{n}_\infty$

$$X = \vec{x} + \frac{1}{2}\vec{x}^2\vec{n}_\infty + \vec{n}_0, \tag{29}$$

$$\vec{n}_0^2 = \vec{n}_\infty^2 = X^2 = 0, \tag{30}$$

$$X \cdot \vec{n}_\infty = -1. \tag{31}$$

The inner product of two conformal points gives their Euclidean distance and therefore the mid plane of two points *A, B* as

$$X \cdot A = -\frac{1}{2}(\vec{x}-\vec{a})^2, X \cdot B = -\frac{1}{2}(\vec{x}-\vec{b})^2 \Rightarrow X \cdot (A-B) = 0, \tag{32}$$

$$m = A - B \propto \vec{p} + d\vec{n}, \quad m^2 = 1, \tag{33}$$

where $\vec{p}$ is a unit normal to the mid plane and *d* its signed scalar distance from the origin. Reflecting at two parallel planes *m*, *m'* with Euclidean distance $\vec{t}/2$ we get the translation (by $\vec{t}$) operator *T*

$$X' = m'mXmm' = T_{\vec{t}}^{-1}XT_{\vec{t}}, \tag{34}$$

with

$$T_{\vec{t}} = 1 + \frac{1}{2}\vec{t}\vec{n}. \tag{34a}$$

Reflection at two non-parallel planes *m*, *m'* yields the rotation around the *m*, *m'* line of intersection (axis) by twice the angle between *m* and *m'*.

Table 3 The 17 2D space groups and their generators listed by crystal system, with numbers (1-17) [2], international [2] and geometric [1] names. The always present pure lattice translations T_a and T_b are not listed.

	No.	Int. Notation	Geom. Notation	Generators
Oblique (anorthic)	1	p1	p1	1
	2	p2	p2	a∧b
Rectangular	3	pm	p1	a
	4	pg	p_g1	$aT_b^{1/2}$
	5	cm	c1	a ,$T_{a+b}^{1/2}$
	6	pmm	p2	a,b
	7	pmg	p_g2	$aT_b^{1/2}$,b
	8	pgg	p_g2_g	$aT_b^{1/2}$,$bT_a^{1/2}$
	9	cmm	c2	a,b,$T_{a+b}^{1/2}$
Square	10	p4	p4	ab
	11	p4m	p4	a,b
	12	p4g	p_g4	$aT_{b-a}^{1/2}$,b
Trigonal	13	p3	p3	ab
	14	p3m1	p3	a,b
	15	p31m	h3	a,b,$T_{a+b}^{1/3}$
Hexagonal	16	p6	p6	ab
	17	p6m	p6	a,b

Now both general translations and rotations are represented by geometric products of vectors (so-called versors). To study combinations of versors it is useful to know that

$$T_{\vec{t}}\vec{a} = \vec{a}T_{\vec{t}'}, \quad \vec{t}' = -\vec{a}^{-1}\vec{t}\vec{a}. \tag{35}$$

3.2 Three-Dimensional Space Groups

The 3D space groups are used to describe symmetry in 3D crystal structures. The symmetry operations that generate the groups are translations, reflections, glide reflections, inversions, rotations, screws and rotary inversions. There are 230 kinds of 3D space groups in all, and all 3D periodic translation symmetric crystals belong to exactly one of them. This applies to both natural and artificial crystals.

3.2.1 From Point Groups to Space Groups

Some of the symmetry operations involved in the space groups are not contained in the corresponding point group or Bravais lattice. Frequently occurring examples are compound symmetry operations called glide reflection and screw.

- *Glide reflection* symmetries:

A glide reflection is a reflection in a plane (21), followed by a translation (34) parallel to that plane. This is denoted with the help of an index *a*, *b*, *c*, *n* or *d* in the space group symbol, depending on the direction of the glide translation.

- *Screw* symmetries:

A screw is a rotation (22) about an axis, followed by a translation parallel to the axis. Screws are denoted by an indexed number k_t to describe the angle of rotation 360°/*k*, the index *t* indicates how often the axial translation needs to be repeated to finally obtain an integer multiple of a full lattice translation.

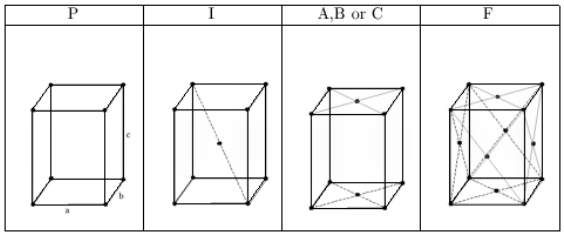

Fig.5 Orthorhombic Bravais lattices, with $|\vec{a}| \neq |\vec{b}| \neq |\vec{c}| \neq |\vec{a}|$, and with $\vec{a} \perp \vec{b} \perp \vec{c} \perp \vec{a}$. A, B or C indicate a base-centered Bravais lattice, with the extra general element located in the A side ($\perp \vec{a}$), B side ($\perp \vec{b}$), or C side ($\perp \vec{c}$).

3.2.2 Orthorhombic Space Groups

In crystallography, the orthorhombic crystal system is one of the seven major lattice systems. Orthorhombic lattices result from stretching a cubic lattice along two of its mutually orthogonal lattice vectors by two different factors, resulting in a rectangular prism with a rectangular base $\vec{a}$ by $\vec{b}$, ($\vec{b}$ different in length from $\vec{a}$), and height $\vec{c}$ ($\vec{c}$ is different in length from $\vec{a}$ and $\vec{b}$). All three basis vectors intersect at 90° angles. The three lattice vectors remain mutually orthogonal.

Table 4 Orthorhombic 3D space groups related to point groups No. 6 ($\overline{22}$), and No. 7 (2) listed with IT numbers [2], international [2] and geometric [1] symbols, and all versor generators, except the always present lattice translations T_a, T_b, T_c.

	Int. Notation	Geom. Notation	Space Group generators
16	P222	P$\bar{2}\bar{2}\bar{2}$	ab, bc
17	P222$_1$	P$\bar{2}_1\bar{2}\bar{2}$	ab$T_c^{1/2}$, bc
18	P2$_1$2$_1$2	P$\bar{2}_1\bar{2}_1\bar{2}$	ab$T_c^{1/2}$, bc$T_a^{1/2}$
19	P2$_1$2$_1$2$_1$	P$\bar{2}_1\bar{2}_1\bar{2}_1$	ab$T_c^{1/2}$, bc$T_a^{1/2}T_b^{1/2}$
20	C222$_1$	C$\bar{2}_1\bar{2}\bar{2}$	ab$T_c^{1/2}$, bc
21	C222	C$\bar{2}\bar{2}\bar{2}$	ab, bc
22	F222	F$\bar{2}\bar{2}\bar{2}$	ab, bc
23	I222	I$\bar{2}\bar{2}\bar{2}$	ab, bc
24	I2$_1$2$_1$2$_1$	I$\bar{2}\bar{2}_1\bar{2}_1$	ab, bc$T_a^{1/2}$
25	Pmm2	P2	a, b
26	Pmc2$_1$	P2$_c$	a, b$T_c^{1/2}$
27	Pcc2	P$_c$2$_c$	a$T_c^{1/2}$, b$T_c^{1/2}$
28	Pma2	P2$_a$	a, b$T_a^{1/2}$
29	Pca2$_1$	P$_c$2$_a$	a$T_c^{1/2}$, b$T_a^{1/2}$
30	Pnc2	P$_n$2$_c$	a$T_{b+c}^{1/2}$, b$T_c^{1/2}$
31	Pmn2$_1$	P2$_n$	a, b$T_{a+c}^{1/2}$
32	Pba2	P$_b$2$_a$	a$T_b^{1/2}$, b$T_a^{1/2}$
33	Pna2$_1$	P$_n$2$_a$	a$T_{b+c}^{1/2}$, b$T_a^{1/2}$
34	Pnn2	P$_n$2$_n$	a$T_{b+c}^{1/2}$, b$T_{a+c}^{1/2}$
35	Cmm2	C2	a, b
36	Cmc2$_1$	C2$_c$	a, b$T_c^{1/2}$
37	Ccc2	C$_c$2$_c$	a$T_c^{1/2}$, b$T_c^{1/2}$
38	Amm2	A2	a, b
39	Aem2	A$_b$2	a$T_b^{1/2}$, b
40	Ama2	A2$_a$	a, b$T_a^{1/2}$
41	Aea2	A$_b$2$_a$	a$T_b^{1/2}$, b$T_a^{1/2}$
42	Fmm2	F2	a, b
43	Fdd2	F$_d$2$_d$	a$T_{b+c}^{1/4}$, b$T_{a+c}^{1/4}$
44	Imm2	P2	a, b
45	Iba2	I$_b$2$_a$	a$T_b^{1/2}$, b$T_a^{1/2}$
46	Ima2	A2$_a$	a, b$T_a^{1/2}$

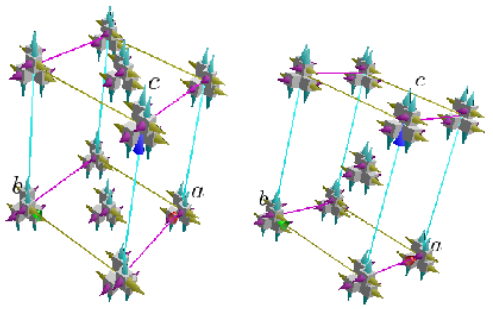

Fig. 6 Unit crystal cells (related to orthorhombic point group No. 6 ($\overline{22}$)) of the space groups No. 21 (C $\overline{222}$) and No. 23 (I $\overline{222}$), as displayed with the Space Group Visualizer [7].

There are four orthorhombic Bravais lattices (Fig. 5): primitive orthorhombic (P), base-centered orthorhombic (C), body-centered

orthorhombic (I), and face-centered orthorhombic (F).

3.2.3 Space Groups Associated with Orthorhombic Point Group No. 6 (Geometric: $\bar{2}2$)

Figure 6 shows crystal cells for the space groups No. 21 ($C\bar{2}22$) and No. 23 ($I\bar{2}22$) of the orthorhombic crystal system. The space groups associated with point group No. 6 have apart from translations only two types of symmetry generators: rotations and screws. Rotations for all three axis directions $\vec{a}$, $\vec{b}$ and $\vec{c}$ exist.

3.2.4 Space Groups Associated with Orthorhombic Point Group No. 7 (Geometric: 2)

Figure 7 shows crystal cells for the space groups No. 38 (A2) and No. 44 (I2) of the orthorhombic crystal system. Space groups associated with point group No. 7 have, apart from pure translations, four types of symmetry generators: rotations, screws, reflections, and glide reflections. The axial direction of the rotation can always be chosen as $\vec{c}$.

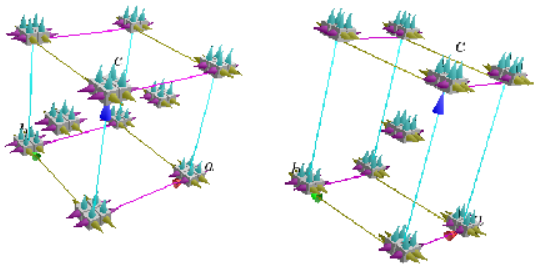

Fig. 7 Unit crystal cells related to orthorhombic point group No. 7 (2) of the space groups No. 38 (A2) and No. 44 (I2), as displayed with the Space Group Visualizer [7].

3.2.5 Space Groups Associated with Orthorhombic Point Group No. 8 (Geometric: 22)

Figure 8 shows crystal cells for the space groups No. 47 (P22) and No. 69 (F22) of the orthorhombic crystal system. There are three reflection generators in point group No. 8, and as a result inversion becomes also a symmetry. Rotation axis exist in all three directions $\vec{a}$, $\vec{b}$, and $\vec{c}$.

4. INTERACTIVE VISUALIZATION

The interactive Space Group Visualizer [5,7] is a script for the program CLUCalc. Each space group has its own XML input file.

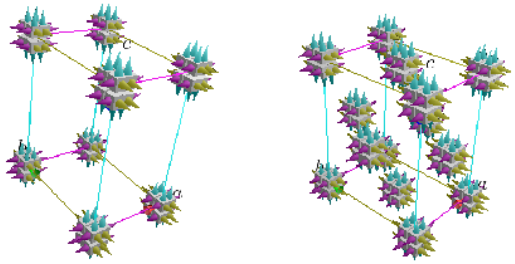

Fig. 8 Unit crystal cells related to orthorhombic point group No. 8 (22), of the space groups No. 47 (P22) and No. 69 (F22), as displayed with the Space Group Visualizer [7].

4.1 CLUCalc

The Open Source Software program CLUCalc [6] is an interactive visualisation tool, which is freely available. CLUCalc was initially developed to visualize Geometric Algebra. However, it has by now become a general visualisation tool, which is well suited to quickly develop algorithms, interactive visualisations and tutorials. Some of the most important features of CLUCalc are:

1. direct user interaction through mouse input, dialog elements and text links,
2. easy plotting of parametric surfaces,
3. automatic analysis and visualisation of Geometric Algebra entities,
4. simple texture mapping of basic geometric entities and arbitrary surface plots,
5. rendering and plotting or texture mapping of LaTex code,
6. reading, writing and manipulation of images in various formats,
7. preparation of presentations with interactive 3D-graphics.

All features of CLUCalc are described in an online manual that can be found on the homepage of CLUCalc [6].

4.2 What is XML?

The Extensible Markup Language (XML) is a W3C-recommended general-purpose markup language that supports a wide variety of

applications. XML languages or 'dialects' are easy to design and to process. XML is also designed to be reasonably human-legible, and to this end, terseness was not considered essential in its structure. XML is a simplified subset of the Standard Generalized Markup Language (SGML). Its primary purpose is to facilitate the sharing of data across different information systems, particularly systems connected via the Internet. Formally defined languages based on XML (such as RSS, MathML, XHTML, Scalable Vector Graphics, MusicXML and thousands of other examples) allow diverse software reliably to understand information formatted and passed in these languages. [8]
An *XML file example* is partly displayed below (for orthorhombic space group number 25, comp. Fig. 12). It serves as input for the purpose made CLUCalc script, called the Space Group Visualizer.

- orthorhombic geometric algebra vector basis

```
<basis>
    <vector id="a">
        <len value="0.7" fixed="0"/>
        <angle value="90" fixed="1"/>
    </vector>
    <vector id="b">
        <len value="1" fixed="0"/>
        <angle value="90" fixed="1"/>
    </vector>
    <vector id="c">
        <len value="1.2" fixed="0"/>
        <angle value="90" fixed="1"/>
    </vector>
</basis>
```

The mutual angles are defined and fixed ("1"), but the three lengths are not fixed ("0"), compare Fig. 9.

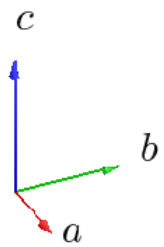

Fig. 9 Orthorhombic geometric algebra vector basis.

- geometric space group versor generator basis of Space group No. 25

```
<generator_basis>
    <generator id="a">
        <op type="ref" vec="a" />
    </generator>
    <generator id="b">
        <op type="ref" vec="b" />
    </generator>
    <generator id="Ta">
        <op type="trans" vec="a" factor="1"/>
    </generator>
    <generator id="Tb">
        <op type="trans" vec="b" factor="1"/>
    </generator>
    <generator id="Tc">
        <op type="trans" vec="c" factor="1"/>
    </generator>
</generator_basis>
```

For space group No. 25 (Fig. 12), the generator (versor) basis defined above has two reflections "ref" ($\vec{a}$ and $\vec{b}$) and the three translators "trans" (T_a , T_b , and T_c). This generator basis corresponds to column four of Table 4.

- Code for space group symmetry transformation versors of one unit cell generated by geometric products of the generator basis versors, for orthorhombic space group No. 25 (Fig. 12).

```
<symmetries>
    <generator>
        <op gen="a"/>
        <op gen="Ta" pow="0,1"/>
    </generator>
    <generator>
        <op gen="b"/>
        <op gen="Tb" pow="0,1"/>
    </generator>
    <generator>
        <op gen="a"/>
        <op gen="b"/>
        <op gen="Ta" pow="0,1"/>
        <op gen="Tb" pow="0,1"/>
    </generator>
</symmetries>
```

4.3 The Space Group Visualizer Script

Figure 10 shows a Space Group Visualizer [5] screen window. An explanation of its use is added below. Figure 11 is how the various

symmetries of a space group appear in the Space Group Visualizer. A free demo version of the space group visualizer with a representative selection of space groups can be downloaded from the Space group project homepage [7].

4.3.1 Selection of a Space Group

A space group is selected from a crystal system, by the associated point group number (1…32), and its space group number (1…230).

4.3.2 Display Functions

The development version of the Space Group Visualizer has the following major display functions located in the left browser panel below the space group selection section.

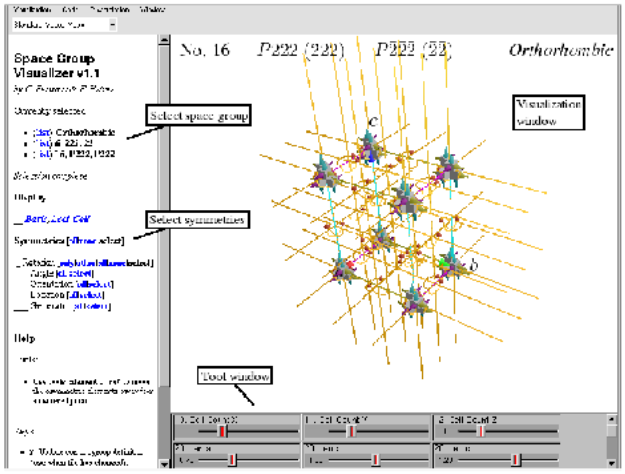

Fig.10 Space Group Visualizer main screen window for space group No. 16 (development version).

- Basis:

If this is selected the generator basis vectors are drawn and labelled $\vec{a}$, $\vec{b}$ and $\vec{c}$. These vectors need in general (e.g. in the hexagonal crystal system) not to be identical with the lattice basis. They only form the vectors from which the symmetry generators are constructed by geometric products. The basis vectors can be toggled on and off.

- Loci (asymmetric units in general positions):

If this is selected, asymmetric elements are drawn at the loci (locations) generated by the space group symmetries. In real crystals there are molecules or ions at these positions. An asymmetric element is necessary to show the symmetry relation to one general initial element, which is located near the origin of the cell vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$. The loci can also be toggled on and off.

- Cell contours:

If selected a wire frame lattice is drawn.
The *current* SGV Demo version 2.0 implements these functions through an interactive top icon bar.

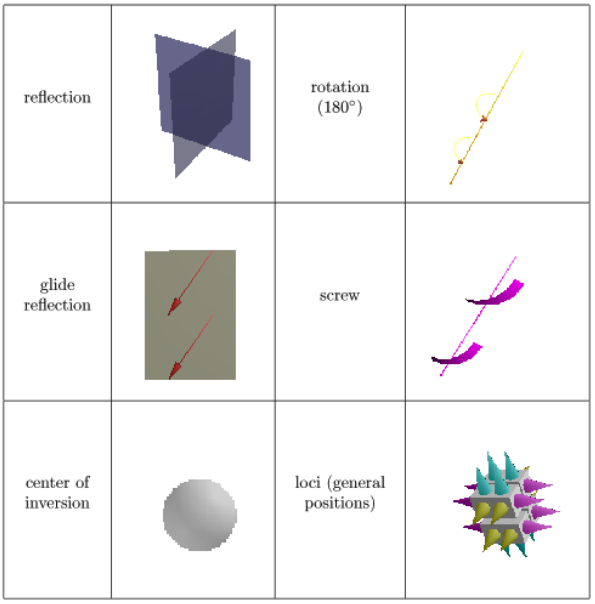

Fig.11 How symmetries appear in the Space Group Visualizer, and the general asymmetric objects (loci). One gray cube with three colored cones represents e.g. a molecule.

4.3.3 Tool Window Functions

- Cell Count:

The three cell count tools allow to select how many crystal cells or layers are drawn in the three lattice directions. This even allows to draw the point group symmetries or the 2D space group symmetries by choosing e.g. cell counts (0,1,1), (1,0,1), or (1,1,0).

- Len:

The number of these sliders depends again on the space group currently selected. They control

the length of the lattice basis vectors. For example, in the orthorhombic crystal system the lengths of all three basis vectors can be chosen arbitrarily, while in other systems certain lengths may be fixed.

- Plane Size in %:

The size of the planes of reflection and glide reflection can be changed in percent values. The default is 100 %, i.e. all plane parts are shown without gaps.

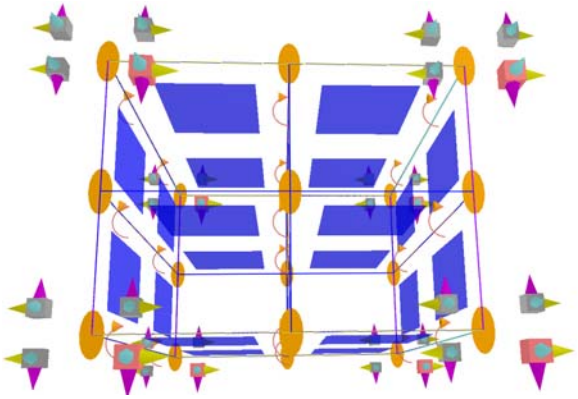

Fig. 12 All symmetries of one cell of space group No. 25 in the Space Group Visualizer [7].

- Cell Type:

Whether different lattice types are available depends on the space group currently displayed. Select here the lattice that you wish to display. If e.g. the geometric algebra cell definition [1] and the international cell [2] differ, one can choose between the two.

- Color Scheme:

Here a color scheme can be selected. For example, the *White Background* color scheme is useful to store visualisations for printing on paper. Default is the *Black Background* color scheme.

5. CONCLUSION

We succeeded in the visualization of all symmetries of the 59 orthorhombic space groups using the Space Group Visualizer. This visualization in three dimensions will definitely be of great advantage for the study and research of orthorhombic materials, because seeing the structure of orthorhombic crystals becomes now easily possible with the Space Group Visualizer. Indeed the precise space group sub-classification of many orthorhombic minerals is still unknown or uncertain [20].

Our future aim is to make the visualization of all space groups complete. It is further possible to create a molecule maker toolbox in the future to facilitate the comparison with the crystal of an actual material. Further possibilities include extensions for sub-periodic and magnetic crystal lattices.

A *color* version of this paper will be available online at [17].

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