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Groupoid analysis of pyroxenes

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Abstract

The structure and space-group symmetry of modular structures can be obtained from the knowledge of the structure and subperiodic symmetry of the modules and of the structure-building operations. This leads to a space groupoid, which contains all the partial operations relating any pairs of modules. Those partial operations that possess a continuation in the whole crystal space are global operations that show up in the space group of the structure. We present the whole procedure through the example of pyroxenes. The modular structure of these minerals has already been analysed in the past, but the groupoid construction has been only synthetically described. In this paper we present the full step-by-step process, which is largely unknown in the crystallographic community.

1. Introduction

Pyroxenes are rock-forming minerals occurring in a wide range of temperature and pressure, under which they present several polymorphs, monoclinic and orthorhombic, with a relatively complex series of phase transitions ([1] and references therein). The thermobarometry of monoclinic pyroxenes is used by mining industries, in particular in the prospection of diamonds, as well as to obtain data on pressure and temperature of the magma that can be used to propose detailed models of the lithosphere and mantle [2]. Extraterrestrial pyroxenes are known as well. In meteorites, the composition of pyroxenes is close to MgSiO_3 , members of the clinoenstatite-clinohypersthene series are common, calcium-rich and aluminium-rich pyroxenes are rare, and the jadeitic varieties are absent. In some meteorites, shock effects have resulted in the inversion of orthopyroxene to clinopyroxene of essentially the same composition [3]. On Mars, pyroxene minerals formed at

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depth in the crust [4]. In the Shergotty meteorite, a basalt body ejected 175 million years ago from Mars, the inner cores of pyroxenes are enriched in soluble trace elements when compared to the outer rims, suggesting that water was present in pyroxenes at depth but was largely lost as pyroxenes were carried to the surface during magma ascent [5].

The crystal structure of pyroxenes is monoarchetypal modular. This means that the structure of every pyroxene polymorph can be ideally decomposed into a series of isostructural building blocks (the *modules*) obtained from a single archetypal structure, mapped onto each other by different isometries in the different polymorphs. We remind the reader that two structures are called *isostructural* (or *isotypical*) if 1) they have the same space-group type or belong to a pair of enantiomorphic space-group types; and 2) the occupied Wyckoff positions, occupied either fully or partially at random, are the same in both structures [6]. Applied to subperiodic structures, this means that 1) the modules have the same type of subperiodic group, or belong to a pair of enantiomorphic subperiodic types¹; however, because a module can actually undergo some desymmetrization in the different modular structures, due to atomic ordering or substitutions or to small changes in the atomic fractional coordinates, their subperiodic groups can also be in direct group-subgroup relation; 2) a one-to-one correspondence between occupied atomic sites in the modules exists, with a comparable variability in the atomic coordinates. The cell parameters along the direction(s) of periodicity, as well and the thickness(es) along the direction(s) of missing periodicity, and the chemical composition of the modules may slightly differ in the different polymorphs.

In the case of pyroxenes, the modules are layers obtained from the high clinopyroxene polymorph, whose space group is of type $C2/c$, considered as archetypal structure. The cell parameters at a given temperature and pressure, which define the different space groups of the same type, depend on the chemical composition. Because we are here interested in the space groupoid of the pyroxenes, which depends on the type of subperiodic group of the layer and on the structure-

¹ To be noted that enantiomorphic types occur for rod groups, not layer groups.

building operations, rather than in their structure, we abstract from the chemical composition, 51
which has been dealt with in our previous publication [7]. The module is obtained by retaining the 52
atoms in the interval $x \in [-1/4, +1/4]$. The symmetry group of the module is therefore the diperiodic 53
group $P(1)2/c1$ (OD (Order-Disorder) notation after [8]). Volume E of the International Tables for 54
Crystallography use the symbol $p12/a1$ [9], which implies an exchange of the a and c axes with 55
respect to the standard setting of high pyroxenes, because Volume E assumes that the plane of the 56
layer is ab , although nothing prevents the user to adopt a different choice, which would lead to 57
 $p12/c1$ [10], where the stacking direction is however not explicitly shown. For this reason we prefer 58
to adopt the OD symbol. The archetypal structure is then obtained back by stacking this module 59
with the C -centring translation, or any operation in the coset obtained by applying this translation to 60
the $P(1)2/c(1)$ symmetry of the module [11]. The module-mapping isometries are not, in general, 61
global operations: this means that they act only on the subspace of the crystal space occupied by the 62
modules they map. These isometries are termed *partial operations* and are usefully classified into 63
partial operations *sensu stricto*, if they map two different modules, and *local operations*, if they map 64
a module to itself. The latter build the subperiodic groups of the modules. The whole set of partial 65
operations builds an algebraic structure more general than a group, known as a groupoid, in the 66
sense of Brandt [12], i.e. an algebraic structure differing from a group in that it is not closed under 67
composition. 68

Nespolo and Aroyo [7] have analyzed the modular structure of pyroxenes, showing that mapping 69
the fractional atomic coordinates of the module obtained from the archetype to the coordinate 70
system of a given polymorph, and applying the partial operation(s) mapping that module to the 71
other module(s) in the same polymorph one obtains a structural model whose fractional atomic 72
coordinates are very close to those of the refined structure. They also presented a groupoid analysis 73
of the three main polymorphs, but because of the limited space available and of the mineralogical 74
audience that part of the analysis was abridged. We believe that an in-depth analysis is worth 75

presenting, considering the further developments of the groupoid analysis of crystal structures 76
presented in the following years [13], [14], [15]. 77

After a general reminder of the construction of a groupoid and how to identify the global operations 78
that build the space group of the structure, we present a detailed analysis of the groupoids of 79
pyroxene polymorphs. In the appendix, we present a reminder of some crystallographic symbols 80
seldom used in the description of space groups. 81

2. Construction of the space groupoid of a modular crystal structure 82

The symmetry group of a module is a subperiodic group: diperiodic group if the module is a layer, 83
monoperiodic group if the module is a rod, or non-periodic group if the module is a brick. We 84
emphasize the difference between *non-periodic* and *aperiodic*: the former is a point group, 85
considered as the limit of subperiodic groups to non-periodic structures, while the latter refers to a 86
structure which is not periodic in the three-dimensional space but can be described by a d- 87
dimensional ($d > 3$) space group. These structures occur in incommensurate crystals, quasi-crystals 88
or composite crystals whose components have periodicities which are one incommensurate to the 89
other in at least one direction. 90

A monoarchetypal modular structure is composed of identical (congruent or enantiomorphic) 91
modules. One considers first of all a single module as well as all the partial operations mapping the 92
other modules to it. The sense of mapping is here important: if the module under consideration is 93
identified with an index p , then the partial operations φ_{pq} map the q -th module to the p -th module 94
but not vice-versa. Because modules in pyroxenes are layers, let us indicate the module as L_p : the 95
operations φ_{pq} map L_q to L_p . In symbols: $\varphi_{pq}L_q = L_p$. The special case $q = p$ identifies the local 96
operations that map L_p to itself: $\varphi_{pp}L_p = L_p$. The set of local operations $N_p = \{\varphi_{pp}\}$ constitutes the 97
subperiodic group of L_p . The set $\Phi_{pq} = \{\varphi_{pq}\}$, $p \neq q$, contains all the partial operations mapping L_q to 98
 L_p . By choosing one of them as representative and labeling it as ϕ_{pq} , the set Φ_{pq} can be expressed as 99
a right coset of N_p : $\Phi_{pq} = N_p\phi_{pq}$. The union of sets $\cup_q \Phi_{pq} = \cup_q \{\varphi_{pq}\}$ contains all the partial operations 100

mapping any module L_q to L_p , including L_p itself, and constitutes the *mixed group* M_p of L_p . The name is somewhat unfortunate because it does not contain the inverse of the partial operations *sensu strictu* (M_p contains ϕ_{pq} but not $\phi_{qp} = \phi_{pq}^{-1}$) and therefore it is a not group. It is, however, a well established term in the literature (e.g. [16]), since the introduction of its German version *Mischgroup* in 1927 [17]. N_p is called the *nucleus* of the mixed group M_p . If the number of modules, up to lattice translations, is n , numbering the modules from 0 to $n-1$, the mixed group can be explicitly written as follows:

N_p	$N_p\phi_{p0}$	$N_p\phi_{p1}$...	$N_p\phi_{pn-1}$
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The expression above can be read as the right coset decomposition of M_p in terms of N_p . If one makes p too running on all the modules, then the set of inverse operations $\Phi_{pq} = \{\phi_{pq}^{-1}\}$ shows up in the mixed group M_q , whose nucleus is:

$$N_q = \{\phi_{qq}\} = \{\phi_{qp}\phi_{pp}\phi_{pq}\} = \{\phi_{pq}^{-1}\phi_{pp}\phi_{pq}\} = \phi_{pq}^{-1}\{\phi_{pp}\}\phi_{pq} = \phi_{pq}^{-1}N_p\phi_{pq}.$$

In other words, the nucleus N_q of L_q is conjugated to the nucleus N_p of L_p by the partial operations mapping q to p , as one should expect from the fact that the structure is monoarchetypal and the subperiodic groups of all the modules are necessarily of the same type. The combination of a partial operation mapping L_r to L_q and L_q to L_p is another partial operation mapping L_r to L_p . The partial operations mapping L_r to L_q can therefore be written as follows:

$$\Phi_{qr} = N_q\phi_{qr} = \phi_{pq}^{-1}N_p\phi_{pq}\phi_{qr} = \phi_{pq}^{-1}N_p\phi_{pr}$$

so that the mixed group of L_q can be written as a function of the mixed group of L_p :

$$M_q = \cup_r \Phi_{rq} = \cup_r N_q\phi_{qr} = \cup_r \phi_{pq}^{-1}N_p\phi_{pr}$$

Without loss of generality one can take $p = 0$ and build a matrix containing all the mixed groups:

N_0	$N_0\phi_{01}$	$N_0\phi_{02}$...	$N_0\phi_{0n-1}$
$\phi_{01}^{-1}N_0$	$\phi_{01}^{-1}N_0\phi_{01}$	$\phi_{01}^{-1}N_0\phi_{02}$...	$\phi_{01}^{-1}N_0\phi_{0n-1}$
$\phi_{02}^{-1}N_0$	$\phi_{02}^{-1}N_0\phi_{01}$	$\phi_{02}^{-1}N_0\phi_{02}$...	$\phi_{02}^{-1}N_0\phi_{0n-1}$
...
$\phi_{0n-1}^{-1}N_0$	$\phi_{0n-1}^{-1}N_0\phi_{01}$	$\phi_{0n-1}^{-1}N_0\phi_{02}$...	$\phi_{0n-1}^{-1}N_0\phi_{0n-1}$

The p -th line of the table is the p -th mixed group M_p and the table is the space groupoid of the modular structure. The diagonal terms are all of the form $\phi_{0p}^{-1}N_0\phi_{0p} = N_p$, so that the space groupoid can be rewritten as follows:

N_0	$N_0\phi_{01}$	$N_0\phi_{02}$...	$N_0\phi_{0n-1}$
$\phi_{01}^{-1}N_0$	N_1	$\phi_{01}^{-1}N_0\phi_{02}$...	$\phi_{01}^{-1}N_0\phi_{0n-1}$
$\phi_{02}^{-1}N_0$	$\phi_{02}^{-1}N_0\phi_{01}$	N_2	...	$\phi_{02}^{-1}N_0\phi_{0n-1}$
...
$\phi_{0n-1}^{-1}N_0$	$\phi_{0n-1}^{-1}N_0\phi_{01}$	$\phi_{0n-1}^{-1}N_0\phi_{02}$...	N_{n-1}

Some of the partial operations of the groupoid have a continuation into different subspaces. This means that these operations are simply the restrictions of the same global isometry to the subspace spanned by the modules on which they act; their matrix representations have the same linear part whereas their translation part differs only by lattice translations.

The operation that always has a continuation to the whole space is the identity, which does not possess a geometric element. The other operations may or may not have continuation. Those which have a continuation to the whole space of the modular structure occur in each and every mixed group, modulo a lattice translation. Each set $\phi_{0p}^{-1}N_0\phi_{0q} = N_p\phi_{pq}$ is a coset of M_q with respect to N_p ; because cosets are by definition disjoint sets, an operation occurs at most once in each mixed group M_q . To identify the space group of a modular structure coincides therefore to locate those operations of its space groupoid which occur in each mixed group modulo a lattice translation.

2. Construction of the space groupoids of the pyroxene polymorphs

The structural relations between modules in the pyroxene polymorphs were suggested by Brown et al. [18], on the basis of the displacement of the SiO_3 chains, which can be either $+c/3$ or $-c/3$ along the a axis of the monoclinic polymorph. By indicating these displacement as $+$ and $-$ respectively,

the three main polymorphs correspond to the sequences ++ (clinopyroxenes), +- (protopyroxenes) and ++-- (orthopyroxenes), in their respective unit cells. These relations are shown in Figs 1-3. The diperiodic group of the module is $P(1)2/c1$: the twofold rotation about $0y\frac{1}{4}$, the inversion at the origin and the c -glide at $x0z$ are local operations for the module. This means that in the coordinate system of the diperiodic groups; the inversion centers and the twofold rotation axes are located on a direction at the center of the module: therefore, the module spans the subspace from $-a/2n$ to $+a/2n$ of the clinopyroxene space, where n is then number of layers defining the period along the stacking direction (Fig. 1).

The operations mapping the two modules in the structure of clinopyroxenes are those obtained by decomposing the $C2/c$ space group into cosets of $P2/c$. As representative operation, one can choose the C -centering translation of $C2/c$. The operation mapping the two modules in the structure of protopyroxenes is a b -glide reflection acting at the interface between the two modules (Fig. 2). Finally, for orthopyroxene, built by four modules, the partial operations are those of the two other polymorphs as well as their combination (Fig. 3a). In the following, the operations are written in the Seitz notation, to make the comparison easier [19]. Layers are hereafter indicated as L_0, L_1 etc., as in the figures. On the negative side of the a axis, they are indicated as L_{-1}, L_{-2} etc.

2.1 Clinopyroxenes

In the conventional setting of the space group, the structure of clinopyroxenes contains two modules related by the C -centering translation. The groupoid is shown in Table 1. The upper half shows the construction of the groupoid, where the partial operation ϕ_{01} is $t(\frac{1}{2}\frac{1}{2}0)$. The lower half shows the result.

Beyond the identity, the continuation scheme is shown in Table 2.

Local operations occur in pairs: they fix different layers and are one the continuation of the other. Partial operations *sensu stricto* do not fix any layer: each of them is the continuation of itself. All these operation are therefore promoted to global operations and the space group containing them is

of type $C2/c$, as one should expect from the fact that the partial operation $\{1|\frac{1}{2}\frac{1}{2}0\}$ applied to the module actually gives back the archetype structure from which that module has been obtained.

2.1 Protopyroxenes

The structure of protopyroxenes contains two modules related by a b -glide reflection about a plane located at the interface between the two modules. The coordinate system is obtained by the transformation $\mathbf{a}+\mathbf{c}/2, \mathbf{b}, \mathbf{c}$ applied to the coordinate system of clinopyroxenes. Because the first module spans the space between $-a/4$ and $+a/4$, the geometric element of the b -glide is at $\frac{1}{4}yz$. In the construction of the groupoid the operation ϕ_{10} is therefore $\{m_{100}|\frac{1}{2}\frac{1}{2}0\}^{-1} = \{m_{100}|\frac{1}{2}\overline{1}\frac{1}{2}0\}$. The construction of the groupoid is shown in Table 3. The nuclei N_0 and N_1 are exactly the same as those of clinopyroxenes.

The eight operations in the groupoid all have continuation in the whole space (Table 4) and build a space group of type $Pbcn$, which is indeed the space-group type of protopyroxenes.

2.3 Orthopyroxenes

The structure of orthopyroxenes is obtained from the common module by applying the translation that builds the structure of clinopyroxenes, the b -glide that builds that of protopyroxenes, as well as their combination. The unit cell spans four modules so that the coordinate system is obtained by doubling that a axis for protopyroxenes, or by the transformation $2\mathbf{a}+\mathbf{c}, \mathbf{b}, \mathbf{c}$ applied to the coordinate system of clinopyroxenes. In this setting, the module L_0 spans the subspace between $-x/8$ and $x/8$, the translation mapping L_1 to L_0 becomes $t(\frac{1}{4}\frac{1}{2}\frac{1}{4})$, the b -glide mapping L_3 to L_0 is located at $\frac{3}{8}yz$; finally, the operation mapping L_2 to L_0 is the combination of the last two operations, i.e. a g -glide at $\frac{1}{4}yz$ with glide component $00\frac{1}{4}$. The construction of the groupoid is shown in Table 5, which is divided into three parts because of the need of a shift of the origin. The upper part shows the construction scheme. The middle part is the result, with the global operations in bold. Fig. 3b is a modification of Fig. 3a where the global operations are shown in black, the partial operations *sensu*

strictu in red and the local operations in blue. The global operations, that occur in each and every mixed group, are the following.

- Twofold screw rotations at $x0\frac{1}{8}$, both components $a/2$ and $-a/2$ present. The combination with the lattice translations generates other twofold screw rotations at $x\frac{1}{2}\frac{1}{8}$, $x0\frac{5}{8}$, and $x\frac{1}{2}\frac{5}{8}$.
- Twofold screw rotations at $\frac{1}{8}y\frac{1}{8}$ and $\frac{5}{8}y\frac{1}{8}$, both components $b/2$ and $-b/2$ present. The combination with the lattice translations generates other twofold screw rotations at $\frac{1}{8}y\frac{5}{8}$, $\frac{5}{8}y\frac{1}{8}$ and $\frac{5}{8}y\frac{5}{8}$.
- Twofold screw rotations at $\frac{3}{8}\overline{1}4z$ and $\frac{3}{8}\frac{1}{4}z$, only the component $c/2$ present. The combination with the lattice translations generates the $-c/2$ as well as other twofold screw rotations at $\frac{3}{8}\frac{3}{4}z$, $\frac{7}{8}\frac{1}{4}z$ and $\frac{7}{8}\frac{3}{4}z$.
- Inversion centers at $\frac{1}{8}\frac{1}{4}\overline{1}\frac{7}{8}$ and $\frac{1}{8}\overline{1}\frac{1}{4}\frac{7}{8}$. The combination with the lattice translations generates other inversion centers at $\frac{1}{8}\frac{1}{4}\frac{3}{8}$, $\frac{5}{8}\frac{1}{4}\frac{3}{8}$, $\frac{1}{8}\frac{3}{4}\frac{3}{8}$, $\frac{5}{8}\frac{3}{4}\frac{3}{8}$, $\frac{1}{8}\frac{1}{4}\frac{7}{8}$, $\frac{5}{8}\frac{1}{4}\frac{7}{8}$, $\frac{1}{8}\frac{3}{4}\frac{7}{8}$ and $\frac{5}{8}\frac{3}{4}\frac{7}{8}$.
- *b*-glide reflections at $\frac{3}{8}yz$, both components $b/2$ and $-b/2$ present. The combination with the lattice translations generates other *b*-glide reflections at $\frac{7}{8}yz$.
- *c*-glide reflections are $x0z$ and $x\frac{1}{2}z$, only the $c/2$ component present. The combination with the lattice translations generates the $-c/2$ component.
- *a*-glide reflections at $xy\frac{1}{8}$, both components $a/2$ and $-a/2$ present, as well as the co-planar glide reflections $g(\overline{1}\frac{1}{2}10)$ and $g(\overline{1}\frac{1}{2}10)$. The combination with the lattice translations generates other *a*-glide reflections at $xy\frac{5}{8}$.

The full Hermann-Mauguin symbol of the space group is $P2_1/b2_1/c2_1/a$, but the origin is not on the inversion center.

The partial operations without continuation to global operations are the following.

- Screw rotation $2\frac{1}{2}$ at $x\frac{1}{4}\overline{1}\frac{1}{4}$. The component $a/4$ maps L_1 to L_2 , whereas the component $-a/4$ does the opposite mapping. The combination with the global lattice translations generates screw rotations of the same type at $x\frac{3}{4}\overline{1}\frac{1}{4}$, $x\frac{1}{4}\frac{1}{4}$, $x\frac{3}{4}\frac{1}{4}$.

- Screw rotations $2_{3/2}$ at $x\overline{1/4}0$. The component $3a/4$ maps L_0 to L_3 , whereas the component $3a/4$ does the opposite mapping. 217
218
- Twofold rotations at $0y^{1/4}$, $^{1/4}y0$, $^{1/2}y0$ and $^{3/4}y^{1/4}$. These are local operations of L_0 , L_1 , L_2 and L_3 respectively. The combination with the global lattice translations generates local twofold rotations at $0y^{3/4}$, $^{1/4}y^{1/2}$, $^{1/2}y^{1/2}$ and $^{3/4}y^{3/4}$. 219
220
221
- Twofold screw rotation $2_{1/2}$ at $^{1/2}0z$, mapping L_3 to L_1 ; the coaxial screw rotation $2_{3/2}$ does the opposite mapping. The combination with the global lattice translations generates the same screw rotations at $0^{1/2}z$, $^{1/2}^{1/2}z$ and $00z$. 222
223
224
- Twofold screw rotation $2_{1/2}$ at $^{1/4}0z$, mapping L_0 to L_2 ; the coaxial screw rotation $2_{3/2}$ does the opposite mapping. The combination with the global lattice translations generates the same screw rotations at $^{1/4}^{1/2}z$, $^{3/4}^{1/2}z$ and $^{3/4}0z$. 225
226
227
- The inversions at 000 , $^{1/4}^{1/2}\overline{1/4}$, $^{1/2}0\overline{1/4}$ and $^{3/4}^{1/2}0$ are local operations of L_0 , L_1 , L_2 and L_3 respectively. The combination with the global lattice translations generates inversions at every half period from the four local inversion centers above. 228
229
230
- A glide reflection by $c/4$ and $-c/4$ at $^{1/4}yz$ maps L_2 to L_0 and vice-versa. The combination with the global lattice translations generates a glide reflection by $c/4$ and $-c/4$ at $^{3/4}yz$, which maps L_2 to L_4 and vice-versa. 231
232
233
- A glide reflection by $c/4$ and $-c/4$ at $^{1/2}yz$ maps L_3 to L_1 and vice-versa. The combination with the global lattice translations generates a glide reflection by $c/4$ and $-c/4$ at $0yz$, which maps L_1 to L_{-1} and vice-versa. 234
235
236
- A glide reflection $d(^{1/4}0^{1/4})$ at $x^{1/4}z$ maps L_0 to L_1 ; the opposite mapping is obtained by a glide reflection $d(\overline{1/4}0\overline{1/4})$ about the same plane. 237
238
- A glide reflection $d(\overline{1/4}0^{1/4})$ at $x\overline{1/4}z$ maps L_3 to L_2 ; the opposite mapping is obtained by a glide reflection $d(^{1/4}0\overline{1/4})$ about the same plane. 239
240

- A glide reflection $g(\overline{1/4}1/20)$ about $xy0$ maps L_2 to L_1 ; the opposite mapping is obtained by a glide reflection $g(\overline{1/4}1/20)$ about the same plane.
- A glide reflection $g(\overline{3/4}1/20)$ about $xy1/4$ maps L_3 to L_1 ; the opposite mapping is obtained by a glide reflection $g(\overline{3/4}1/20)$ about the same plane.

To obtain the standard setting of the space group, a translation by $1/8\overline{1/4}1/8$, which bring the origin on an inversion center, is necessary. The groupoid after the shift of the origin is shown in the bottom part of Table 5. The continuation scheme for the global operations is shown in Table 6.

5. Other pyroxene structures

A few pyroxenes crystallize in space groups different from those presented above. The unit cell is spanned by two modules only, related by a single independent stacking operation. Also in these cases, the groupoids degenerate to groups.

Low clinopyroxenes are low-symmetry versions of clinopyroxenes where the space-group symmetry is reduced from $C2/c$ to $P2_1/c$ owing to distortions of every second SiO_3 chain. Formally, the symmetry of the modules is reduced to $P(1)n1$.

Protopyroxenes at high pressure occur in space groups of type $P2_1cn$, unconventional setting of $Pna2_1$, translationengleiche subgroups of $Pbcn$ with origin shift $01/40$. The layer group of the module is $P(1)c1$ and the stacking operation is $2_1 x00$ (with respect to the origin on $P2_1cn$). All the operations are global and the groupoid degenerates to a group.

$P2/n$ occurs in omphacites. Chemical ordering reduces the diperiodic group of the layer from $P(1)2/c1$ to its translationengleiche subgroup $P(1)21$, and the stacking operation $n x0z$ leads to $P2/n$.

6. Discussion

Modular structures are obtained by stacking or juxtaposing non-periodic, monoperiodic or diperiodic modules according to well-defined isometries: the structure-building operations. From the knowledge of the structure and symmetry of the modules and of the structure-building operations, one can easily obtain the idealized structure of any modular structure and from the

groupoid its space group. Some desymmetrization is possible in the real structure, which only implies to consider a subgroup of the group obtained in this way. This procedure has therefore a wide range of applications in material design and crystal engineering.

We have illustrated the method through the example of pyroxenes, that is sufficiently simple to present a complete detailed analysis. The space groups of pyroxenes can all be obtained through by applying the stacking operations to the diperiodic group of the layer which represents the building unit of all pyroxenes, abstracting from which cations occur in the coordination polyhedra of each pyroxene.

Orthopyroxenes have instead four layers in the period along the stacking direction, three types of stacking operation (two independent, the third obtained as combination of these two). Only a subset of the operations in the groupoid obtained by applying these operations to the diperiodic group of the layer have continuation to the whole crystal space and show up in the space group. All the other operations are partial and their occurrence is only revealed when the groupoid is analyzed.

Pyroxenes are a wide family of minerals, in which the cation sites host a large variety of atoms: Ca, Mg, Fe²⁺, Fe³⁺, Al, Mn, just to mention the most abundant ones. By neglecting the desymmetrization of layers, they could be considered configurational polytypes, i.e. the generalization of the category of polytypes to include members of variable chemical composition [20]. When interpreted as (configurational) polytypes, pyroxenes appear to be non-OD polytypes. Order-disorder (OD) polytypes [21] are a special class of polytypes, where pairs of adjacent layers are always geometrically equivalent. This means that members of an OD family are geometrically locally equivalent and, taking into account the short-range of interatomic interactions, also energetically equivalent. The modular interpretation of pyroxenes given here is not of the OD kind, because the two kinds of structure building operations, translation and *b*-glide reflection, lead to non-equivalent layer pairs (see Figs. 1–3). It is only by interpreting the interface between the modules as distinct layers that one can provide an OD interpretation of pyroxene polytypism, as done by Sedlacek et al.

[22]. These authors noted that the $[\text{SiO}_3]^{2-}$ part of the structure, which is located at the interface of the modules in the interpretation given here, can be considered as individual layers with $P(b)cm$ symmetry. The higher symmetry of these layers is then responsible for the stacking ambiguity. In fact, note that given L_0 in Figs. 1–3, the two possible orientations of L_1 are related by the m reflection of the $P(b)cm$ layer group. If interactions across the $[\text{SiO}_3]^{2-}$ chains are neglected, all pyroxene polytypes should therefore be of very similar energy. Since the OD interpretation is based on two distinct layers, the groupoid describing the partial symmetry is decomposed into two *connected components* of each kind of layer. Such groupoids are said to be of the Ehresmann type [23]. Our monoarchetypal interpretation allows to provide a simpler description in terms of Brandt groupoids, although it does not fit the definition of OD structures.

Appendix

A symmetry operation without intrinsic translational component leave invariant a proper subspace (point, direction, plane)², which is called the geometric element of that operation. The whole set of operations sharing the same geometric element is called an element set. For screw rotations and glide reflection, the geometric element is obtained by removing the intrinsic (screw, glide) component of the operation. The element set with the geometric element define the symmetry element. Among the operations of the element set, the one with the shortest positive (possible zero) translation is called the defining operation: it gives the name to the symmetry element. All the rotations and screw rotations sharing the same geometric element (direction) are called coaxial operations; all the reflections and glide reflections sharing the same geometric element (plane) are called co-planar operations.

The general symbol for a screw rotation is n_p , where n is the denominator of the fraction $2\pi/n$ giving the rotation component, and p is the numerator of the fraction p/n giving the screw component. n_0 is a pure rotation, always shortened to n . Coaxial screw rotations differ by an integer: they are

² We insist on the notion of proper subspace because the identity, which does not possess a geometric element, leave invariant the whole space, which is a trivial (not proper) subspace.

indicated as $n_p, n_{p+1}, n_{p+2}, n_{p+3}$ etc. Negative screw rotations are indicated as $n_{\bar{p}}, n_{\bar{p+1}}, n_{\bar{p+2}}, n_{\bar{p+3}}$. 315

Because the defining operation is used to name the symmetry element, only the symbol $n_p, p \in [0, n-1]$ is commonly used in the space-group notation [24]. Partial operations are not limited to integer 316

value of p so that unusual symbols may appear. For example, $2_{3/2}$ is a screw rotation with screw 317

component $(3/2)/2 = 3/4$. Two applications of the operation leads to a translation $3/2$, which is not a 318

lattice vector. This type of operation cannot therefore be a global operation, but it does occur as 319

partial operations. 320

Glide reflections are indicated as $g(pqr)$, where pqr are the fractional translations along the three 321

axes of the coordinate system. The most common glide reflections are indicated by a shortened 322

symbol $m = g(000)$, $a = g(1/200)$, $b = g(01/20)$, $c = g(001/20)$, n when the glide component is half of 323

the diagonal, d when the glide component is a quarter of the diagonal (only occurring in centered unit 324

cells), e when two glide component mutually perpendicular coexist (only occurring in centered unit 325

cells). Negative glide components are also indicated by the general symbol. For example, $g(1/200)$ 326

does not receive a special symbol, despite being of the same nature as a with only the sense of the 327

translation inverted. For the sake of brevity, in this manuscript we have differentiated $a_+ = g(1/200)$ 328

and $a_- = g(\bar{1}/200)$ (and the like for the b -glide) 329

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Figure captions 373

Figure 1. Schematic view of the modular structure of clinopyroxenes. The structure building 374
operation is the C -centering $t(\frac{1}{2}\frac{1}{2}0)$ translation mapping L1 to L0, which defines the second 375
coset of the first mixed group. The inverse C -centering $t(\frac{1}{2}\frac{1}{2}0)$ translation, mapping L0 to L1, defines the 376
first coset of the second mixed group. See Table 1. 377

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Figure 2. Schematic view of the modular structure of protopyroxenes. The structure building 379
operation is the b -glide reflection at $\frac{1}{4}yz$ mapping L1 to L0, which defines the second coset of the 380
first mixed group. The inverse operation, mapping L0 to L1, defines the first coset of the second 381
mixed group. See Table 3. 382

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Figure 3. (a) Schematic view of the modular structure of orthopyroxenes. The structure building 384
operations are the $t(\frac{1}{4}\frac{1}{2}\frac{1}{4})$ translation, mapping L1 to L0, which defines the second coset of the 385
first mixed group, the b -glide reflection at $\frac{3}{8}yz$ mapping L3 to L0, which defines the third coset of 386
the first mixed group, and their combination, a g -glide reflection $(00\frac{1}{4})$ at $\frac{1}{4}yz$, mapping L2 to L0, 387
which defines the fourth of the first mixed group. The inverse operations define the first coset of the 388
second, third and fourth mixed groups respectively. See Table 5. (b) The elements of the global 389
(black), local (blue) and partial *sensu strictu* (red) operations obtained from the groupoid analysis in 390
Table 5 (middle part, before applying the origin shift). The elements of the operations obtained by 391
combining them with lattice translations are not shown. Partial screw rotations with unusual screw 392
component $2\frac{1}{2}$ and $2\frac{3}{2}$, with screw components $\frac{1}{4}$ and $\frac{3}{4}$ respectively, which do not show up in the 393
space group, are shown with the conventional graphical symbol of screw rotations (half arrows) and 394
the p component of the p/n symbol explicitly given (see Appendix). The partial d -glide at $x\frac{1}{4}z$, 395
whose geometric element is the same as the co-planar g -glide reflections doing the opposite 396
mapping, is shown by a simplified symbol. 397

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Table 1. Space groupoid of clinopyroxenes obtained by applying the partial operation $t(\overline{1/2}1/20)$ to the subperiodic group of the layer. Operations are presented by their Seitz symbol. The upper half shows the construction of the groupoid, where $\phi_{10} = t(\overline{1/2}1/20)$. The lower half shows the result.

	Coset 1	Coset 2
Mixed group 1	$\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\overline{1} 000\}, \{m_{010} 00\frac{1}{2}\}$	$(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\overline{1} 000\}, \{m_{010} 00\frac{1}{2}\})\{1 \overline{1/2}1/20\}$
Mixed group 2	$\{1 \frac{1}{2}1/20\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\overline{1} 000\}, \{m_{010} 00\frac{1}{2}\})$	$\{1 \frac{1}{2}1/20\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\overline{1} 000\}, \{m_{010} 00\frac{1}{2}\})\{1 \overline{1/2}1/20\}$
Mixed group 1	$\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\overline{1} 000\}, \{m_{010} 00\frac{1}{2}\}$	$\{1 \overline{1/2}1/20\}, \{2_{010} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{\overline{1} \frac{1}{2}1/20\}, \{m_{010} \overline{1/2}\frac{1}{2}\frac{1}{2}\}$
Mixed group 2	$\{1 \frac{1}{2}1/20\}, \{2_{010} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{\overline{1} \frac{1}{2}1/20\}, \{m_{010} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\overline{1} 000\}, \{m_{010} 00\frac{1}{2}\}$

Table 2. Continuation scheme for the local and partial operations of the space groupoid of clinopyroxenes.

Number	Seitz symbol	Operation	Location	Layer invariant under the operation	Pairs of layers mapped by the operation	Continuation
1	$\{2_{010} 00\frac{1}{2}\}$	twofold rotation	$0y\frac{1}{4}$	L_0	$L_p \rightarrow L_{-p}$	2
2	$\{2_{010} 10\frac{1}{2}\}$	twofold rotation	$\frac{1}{2}y\frac{1}{4}$	L_1	$L_p \rightarrow L_{2-p}$	1
3	$\{\overline{1} 000\}$	inversion	000	L_0	$L_p \rightarrow L_{-p}$	4
4	$\{\overline{1} 110\}$	inversion	$\frac{1}{2}1/20$	L_1	$L_p \rightarrow L_{2-p}$	3
5	$\{m_{010} 00\frac{1}{2}\}$	<i>c</i> -glide reflection	$x0z$	L_0	$L_p \rightarrow L_{-p}$	6
6	$\{m_{010} 01\frac{1}{2}\}$	<i>c</i> -glide reflection	$x\frac{1}{2}z$	L_1	$L_p \rightarrow L_{2-p}$	5
7	$\{1 \frac{1}{2}1/20\}$	translation	---	---	$L_{p+1} \rightarrow L_p$	7
8	$\{1 \overline{1/2}1/20\}$	translation	---	---	$L_p \rightarrow L_{p+1}$	8
9	$\{2_{010} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	twofold screw rotation	$\frac{1}{4}y\frac{1}{4}$	---	$L_p \rightarrow L_{2-p}$	9
10	$\{2_{010} \frac{1}{2}1/2\frac{1}{2}\}$	twofold screw rotation	$\frac{1}{4}y\frac{1}{4}$	---	$L_p \rightarrow L_{2-p}$	10
11	$\{\overline{1} \frac{1}{2}1/20\}$	inversion	$\frac{1}{4}1/40$	---	$L_p \rightarrow L_{2-p}$	11
12	$\{m_{010} \overline{1/2}\frac{1}{2}\frac{1}{2}\}$	<i>n</i> -glide reflection	$x\frac{1}{4}z$	---	$L_p \rightarrow L_{2-p}$	12
13	$\{m_{010} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	<i>n</i> -glide reflection	$x\frac{1}{4}z$	---	$L_p \rightarrow L_{2-p}$	13

Table 3. Space groupoid of protopyroxenes obtained by applying the partial operation $b\frac{1}{4}yz$ to the subperiodic group of the layer. Operations are presented by their Seitz symbol. Same conventions as in Table 1.

	Coset 1	Coset 2
Mixed group 1	$\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\overline{1} 000\}, \{m_{010} 00\frac{1}{2}\}$	$(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\overline{1} 000\}, \{m_{010} 00\frac{1}{2}\})\{m_{100} \frac{1}{2}\overline{1/2}0\}$
Mixed group 2	$\{m_{100} \frac{1}{2}\frac{1}{2}0\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\overline{1} 000\}, \{m_{010} 00\frac{1}{2}\})$	$\{m_{100} \frac{1}{2}\frac{1}{2}0\}(\{1, 2_{010} 00\frac{1}{2}, \overline{1} 000, m_{010} 00\frac{1}{2}, m_{100} \frac{1}{2}\overline{1/2}0\})\{m_{100} \frac{1}{2}\overline{1/2}0\}$
Mixed group 1	$\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\overline{1} 000\}, \{m_{010} 00\frac{1}{2}\}$	$\{m_{100} \frac{1}{2}\overline{1/2}0\}, \{m_{001} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{2_{100} \overline{1/2}\frac{1}{2}\frac{1}{2}\}, \{2_{001} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
Mixed group 2	$\{m_{100} \frac{1}{2}\frac{1}{2}0\}, \{m_{001} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{2_{100} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{2_{001} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\overline{1} 000\}, \{m_{010} 00\frac{1}{2}\}$

Table 4. Continuation scheme for the local and partial operations of the space groupoid of protopyroxenes.

Number	Seitz symbol	Operation	Location	Layer invariant under the operation	Pairs of layers mapped by the operation	Continuation
1	$\{2_{010} 00\frac{1}{2}\}$	twofold rotation	$0y\frac{1}{4}$	L_0	$L_p \rightarrow L_{-p}$	2
2	$\{2_{010} 10\frac{1}{2}\}$	twofold rotation	$\frac{1}{2}y\frac{1}{4}$	L_1	$L_p \rightarrow L_{2-p}$	1
3	$\{\bar{1} 000\}$	inversion	000	L_0	$L_p \rightarrow L_{-p}$	4
4	$\{\bar{1} 110\}$	inversion	$\frac{1}{2}\frac{1}{2}0$	L_1	$L_p \rightarrow L_{2-p}$	3
5	$\{m_{010} 00\frac{1}{2}\}$	<i>c</i> -glide reflection	$x0z$	L_0	$L_p \rightarrow L_{-p}$	6
6	$\{m_{010} 01\frac{1}{2}\}$	<i>c</i> -glide reflection	$x\frac{1}{2}z$	L_1	$L_p \rightarrow L_{2-p}$	5
7	$\{m_{100} \frac{1}{2}\bar{2}0\}$	<i>b</i> -glide reflection	$\frac{1}{4}yz$	---	$L_{p+1} \rightarrow L_p$	7
8	$\{m_{100} \frac{1}{2}\frac{1}{2}0\}$	<i>b</i> -glide reflection	$\frac{1}{4}yz$	---	$L_p \rightarrow L_{p+1}$	8
9	$\{m_{00} \frac{1}{2}\bar{2}\frac{1}{2}\}$	<i>n</i> -glide reflection	$xy\frac{1}{4}$	---	$L_p \rightarrow L_{2-p}$	9
10	$\{m_{001} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	<i>n</i> -glide reflection	$xy\frac{1}{4}$	---	$L_p \rightarrow L_{2-p}$	10
11	$\{2_{100} \frac{1}{2}\bar{2}0\}$	twofold screw rotation	$x\frac{1}{4}0$	---	$L_p \rightarrow L_{2-p}$	11
12	$\{2_{100} \frac{1}{2}\frac{1}{2}0\}$	twofold screw rotation	$x\frac{1}{4}0$	---	$L_p \rightarrow L_{2-p}$	12
13	$\{2_{001} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	twofold screw rotation	$\frac{1}{4}\frac{1}{4}z$	---	$L_p \rightarrow L_{2-p}$	13

Table 5. Space groupoid of orthopyroxenes obtained by applying the partial operations $t(\frac{1}{4}\frac{1}{2}\frac{1}{4})$, b $\frac{3}{8}yz$ and their combination to the subperiodic group of the layer. Operations are presented by their Seitz symbol. The result of the construction of the groupoid is shown in the middle part of the table: operations common to all mixed groups, modulo a lattice translation, are written in bold. Only half of the operations have a continuation. The global operations define a non-standard setting of the space group, as can be seen from the fact that the inversion center is not at the origin, but at $\frac{1}{8}\frac{1}{4}\frac{1}{8}$ or $\frac{5}{8}\frac{1}{4}\frac{1}{8}$. By applying a shift of the origin $\frac{1}{8}\frac{1}{4}\frac{1}{8}$ the standard setting of the space group is obtained (bottom part of the table).

	Coset 1	Coset 2: $L_1 \rightarrow L_0$	Coset 3: $L_3 \rightarrow L_0$	Coset 4: $L_2 \rightarrow L_0$
Mixed group 1	$\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\}$	$\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\}\{1 \frac{1}{4}\frac{1}{2}\frac{1}{4}\}$	$\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\}\{m_{010} \frac{3}{4}\frac{1}{2}0\}$	$\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\}, \{m_{010} \frac{1}{2}0\frac{1}{4}\}$
Mixed group 2: $L_0 \rightarrow L_1$	$\{1 \frac{1}{4}\frac{1}{2}\bar{2}\frac{1}{4}\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$	$\{1 \frac{1}{4}\frac{1}{2}\bar{2}\frac{1}{4}\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$	$\{1 \frac{1}{4}\frac{1}{2}\bar{2}\frac{1}{4}\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$	$\{1 \frac{1}{4}\frac{1}{2}\bar{2}\frac{1}{4}\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$
Mixed group 3: $L_3 \rightarrow L_1$	$\{m_{010} \frac{3}{4}\bar{2}0\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$	$\{m_{010} \frac{3}{4}\bar{2}0\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$	$\{m_{010} \frac{3}{4}\bar{2}0\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$	$\{m_{010} \frac{3}{4}\bar{2}0\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$
Mixed group 4: $L_2 \rightarrow L_1$	$\{m_{010} \frac{1}{2}0\bar{2}\frac{1}{4}\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$	$\{m_{010} \frac{1}{2}0\bar{2}\frac{1}{4}\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$	$\{m_{010} \frac{1}{2}0\bar{2}\frac{1}{4}\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$	$\{m_{010} \frac{1}{2}0\bar{2}\frac{1}{4}\}(\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\})$
Mixed group 1	$\{1 000\}, \{2_{010} 00\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 00\frac{1}{2}\}$	$\{1 \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{2_{010} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{\bar{1} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{m_{010} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}$	$\{m_{001} \frac{3}{4}\frac{1}{2}0\}, \{m_{001} \frac{3}{4}\frac{1}{2}\frac{1}{2}\}, \{2_{100} \frac{3}{4}\frac{1}{2}0\}, \{2_{001} \frac{3}{4}\frac{1}{2}\frac{1}{2}\}$	$\{m_{100} \frac{1}{2}0\frac{1}{4}\}, \{m_{001} \bar{2}0\frac{1}{4}\}, \{2_{100} \frac{1}{2}0\frac{1}{4}\}, \{2_{001} \frac{1}{2}0\frac{1}{4}\}$
Mixed group 2	$\{1 \frac{1}{4}\frac{1}{2}\bar{2}\frac{1}{4}\}, \{2_{010} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{\bar{1} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{m_{010} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}$	$\{1 000\}, \{2_{010} \frac{1}{2}00\}, \{\bar{1} \frac{1}{2}1\frac{1}{2}\}, \{m_{010} 01\frac{1}{2}\}$	$\{m_{100} 11\frac{1}{4}\}, \{m_{001} \bar{2}1\frac{1}{4}\}, \{2_{100} \frac{1}{2}0\frac{1}{4}\}, \{2_{001} 10\frac{1}{4}\}$	$\{m_{100} \frac{3}{4}\frac{1}{2}0\}, \{m_{001} \bar{2}\frac{1}{4}0\}, \{2_{100} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{2_{001} \frac{3}{4}\frac{1}{2}\frac{1}{4}\}$
Mixed group 3	$\{m_{100} \frac{3}{4}\bar{2}0\}, \{m_{001} \frac{3}{4}\bar{2}\frac{1}{2}\}, \{2_{100} \frac{3}{4}\bar{2}0\}, \{2_{001} \frac{3}{4}\bar{2}\frac{1}{2}\}$	$\{m_{100} 11\frac{1}{4}\}, \{m_{001} \bar{2}1\frac{1}{4}\}, \{2_{100} \frac{1}{2}0\frac{1}{4}\}, \{2_{001} 10\frac{1}{4}\}$	$\{1 000\}, \{2_{010} 1\frac{1}{2}0\frac{1}{2}\}, \{\bar{1} 1\frac{1}{2}\bar{1}0\}, \{m_{010} 01\frac{1}{2}\}$	$\{1 \frac{1}{4}\bar{2}\frac{1}{4}\}, \{2_{010} 1\frac{1}{4}\bar{2}\frac{1}{4}\}, \{\bar{1} 1\frac{1}{4}\bar{2}\frac{1}{4}\}, \{m_{010} \frac{1}{4}\bar{2}\frac{1}{4}\}$
Mixed group 4	$\{m_{100} \frac{1}{2}0\bar{2}\frac{1}{4}\}, \{m_{001} \frac{1}{2}0\frac{1}{4}\}, \{2_{100} \frac{1}{2}0\bar{2}\frac{1}{4}\}, \{2_{001} \frac{1}{2}0\frac{1}{4}\}$	$\{m_{100} \frac{3}{4}\bar{2}0\}, \{m_{001} \frac{3}{4}\bar{2}\frac{1}{2}\}, \{2_{100} \frac{3}{4}\bar{2}0\}, \{2_{001} \frac{3}{4}\bar{2}\frac{1}{2}\}$	$\{1 \frac{1}{4}\frac{1}{2}\bar{2}\frac{1}{4}\}, \{2_{010} 1\frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{\bar{1} \frac{1}{4}\frac{1}{2}\bar{2}\frac{1}{4}\}, \{m_{010} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}$	$\{1 000\}, \{2_{010} 100\}, \{\bar{1} 10\frac{1}{2}\}, \{m_{010} 00\frac{1}{2}\}$
Mixed group 1	$\{1 000\}, \{2_{010} \frac{1}{4}0\frac{1}{4}\}, \{\bar{1} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{m_{010} 0\frac{1}{2}\frac{1}{2}\}$	$\{1 \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{2_{010} 0\frac{1}{2}\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} \frac{1}{4}0\frac{1}{4}\}$	$\{m_{100} \frac{1}{2}\frac{1}{2}0\}, \{m_{001} \frac{3}{4}\frac{1}{2}\frac{1}{4}\}, \{2_{100} \frac{1}{4}\bar{1}\frac{1}{4}\}, \{2_{001} \frac{1}{2}\bar{1}\frac{1}{2}\}$	$\{m_{100} \frac{1}{4}0\frac{1}{4}\}, \{m_{001} \bar{2}0\frac{1}{2}\}, \{2_{100} \frac{1}{2}\frac{1}{2}0\}, \{2_{001} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}$

Mixed group 2	$\{1 \frac{1}{4} \frac{1}{2}\bar{4}\}, \{2_{010} 0\frac{1}{2}\frac{1}{2}\}, \{\bar{1} 000\}, \{m_{010} 0\frac{1}{4}\frac{1}{4}\}$	$\{1 000\}, \{2_{010} \frac{1}{4}0\frac{1}{4}\}, \{\bar{1} \frac{1}{4}\frac{1}{2}\bar{4}\}, \{m_{010} 0\frac{1}{2}\frac{1}{2}\}$	$\{m_{100} \frac{3}{4}1\frac{1}{4}\}, \{m_{001} \frac{1}{2}1\frac{1}{2}\}, \{2_{100} \frac{1}{2}\frac{1}{2}0\}, \{2_{001} \frac{3}{4}\frac{1}{2}\frac{1}{4}\}$	$\{m_{100} \frac{1}{2}\frac{1}{2}0\}, \{m_{001} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{2_{100} \frac{1}{4}0\frac{1}{4}\}, \{2_{001} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
Mixed group 3	$\{m_{100} \frac{1}{2}\frac{1}{2}0\}, \{m_{001} \frac{3}{4}\frac{1}{2}\frac{3}{4}\}, \{2_{100} \frac{3}{4}1\frac{1}{4}\}, \{2_{001} \frac{1}{2}1\frac{1}{2}\}$	$\{m_{100} \frac{3}{4}1\frac{1}{4}\}, \{m_{001} \frac{1}{2}1\frac{1}{2}\}, \{2_{100} \frac{1}{2}\frac{1}{2}0\}, \{2_{001} \frac{3}{4}\frac{1}{2}\frac{3}{4}\}$	$\{1 000\}, \{2_{010} 1\frac{1}{4}0\frac{3}{4}\}, \{\bar{1} 1\frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{m_{010} 01\frac{1}{2}\frac{1}{2}\}$	$\{1 \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{2_{010} 1\frac{1}{2}\frac{1}{2}\}, \{\bar{1} 1\bar{1}0\}, \{m_{010} \frac{1}{4}1\frac{3}{4}\}$
Mixed group 4	$\{m_{100} \frac{1}{4}0\frac{1}{4}\}, \{m_{001} \frac{1}{2}0\frac{1}{2}\}, \{2_{100} \frac{1}{2}\frac{1}{2}0\}, \{2_{001} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}$	$\{m_{100} \frac{1}{2}\frac{1}{2}0\}, \{m_{001} \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{2_{100} \frac{1}{4}0\frac{1}{4}\}, \{2_{001} \frac{1}{2}0\frac{1}{2}\}$	$\{1 \frac{1}{4}\frac{1}{2}\frac{1}{4}\}, \{2_{010} 1\frac{1}{2}\frac{1}{2}\}, \{\bar{1} 1\bar{1}0\}, \{m_{010} \frac{1}{4}1\frac{1}{4}\}$	$\{1 000\}, \{2_{010} \frac{3}{4}0\frac{1}{4}\}, \{\bar{1} \frac{3}{4}\frac{1}{2}\frac{1}{4}\}, \{m_{010} 0\frac{1}{2}\frac{1}{2}\}$

Table 6. Continuation scheme for the local and partial operations of the space groupoid of orthopyroxenes.

Number	Seitz symbol	Operation	Location	Layer invariant under the operation	Pairs of layers mapped by the operation	Continuation
1	$\{2_{100} \frac{1}{2}\frac{1}{2}0\}$	twofold screw rotation $-a/2$	$x\bar{y}40$	---	L2→L0, L3→L1	2
2	$\{2_{100} \frac{1}{2}\frac{1}{2}0\}$	twofold screw rotation $a/2$	$x\bar{y}40$	---	L3→L1, L0→L2	1
3	$\{2_{010} 0\frac{1}{2}\frac{1}{2}\}$	twofold screw rotation $-b/2$	$0y\frac{1}{4}$	---	L1→L0	4,5
4	$\{2_{010} 0\frac{1}{2}\frac{1}{2}\}$	twofold screw rotation $b/2$	$0y\frac{1}{4}$	---	L0→L1	3,5
5	$\{2_{010} 1\frac{1}{2}\frac{1}{2}\}$	twofold screw rotation $-b/2$	$\frac{1}{2}y\frac{1}{4}$	---	L2→L3	3,4
6	$\{2_{010} 1\frac{1}{2}\frac{1}{2}\}$	twofold screw rotation $c/2$	$\frac{1}{2}y\frac{1}{4}$	---	L3→L2	7,8
7	$\{2_{001} \frac{1}{2}1\frac{1}{2}\}$	twofold screw rotation $c/2$	$\frac{1}{4}\bar{y}z$	---	L3→L0, L0→L3	6,8
8	$\{2_{001} \frac{1}{2}0\frac{1}{2}\}$	twofold screw rotation $c/2$	$\frac{1}{4}0z$	---	L2→L1, L1→L2	6,7
9	$\{\bar{1} 000\}$	inversion	0	---	L1→L0, L0→L1	10
10	$\{\bar{1} 1\bar{1}0\}$	inversion	$\frac{1}{2}\bar{y}0$	---	L2→L3, L3→L2	9
11	$\{m_{100} \frac{1}{2}\frac{1}{2}0\}$	b -glide reflection, $b/2$	$\frac{1}{4}yz$	---	L3→L0, L2→L3	12
12	$\{m_{100} \frac{1}{2}\frac{1}{2}0\}$	b -glide reflection, $-b/2$	$\frac{1}{4}yz$	---	L0→L3, L1→L2	11
13	$\{m_{010} 0\frac{1}{2}\frac{1}{2}\}$	c -glide reflection	$x\bar{y}4z$	L0, L2		14,15
14	$\{m_{010} 0\frac{1}{2}\frac{1}{2}\}$	c -glide reflection	$x\bar{y}4z$	L1		13,15
15	$\{m_{010} 01\frac{1}{2}\frac{1}{2}\}$	c -glide reflection	$x\bar{y}4z$	L3		13,14
16	$\{m_{001} \frac{1}{2}0\frac{1}{2}\}$	a -glide reflection, $-a/2$	$xy\frac{1}{4}$	---	L2→L0	17
17	$\{m_{001} \frac{1}{2}0\frac{1}{2}\}$	a -glide reflection, $a/2$	$xy\frac{1}{4}$	---	L0→L2	16
18	$\{m_{001} \frac{1}{2}1\frac{1}{2}\}$	g -glide reflection ($\frac{1}{2}10$)	$xy\frac{1}{4}$	---	L3→L1	19
19	$\{m_{001} \frac{1}{2}1\frac{1}{2}\}$	g -glide reflection ($\frac{1}{2}\bar{1}0$)	$xy\frac{1}{4}$	---	L1→L3	18

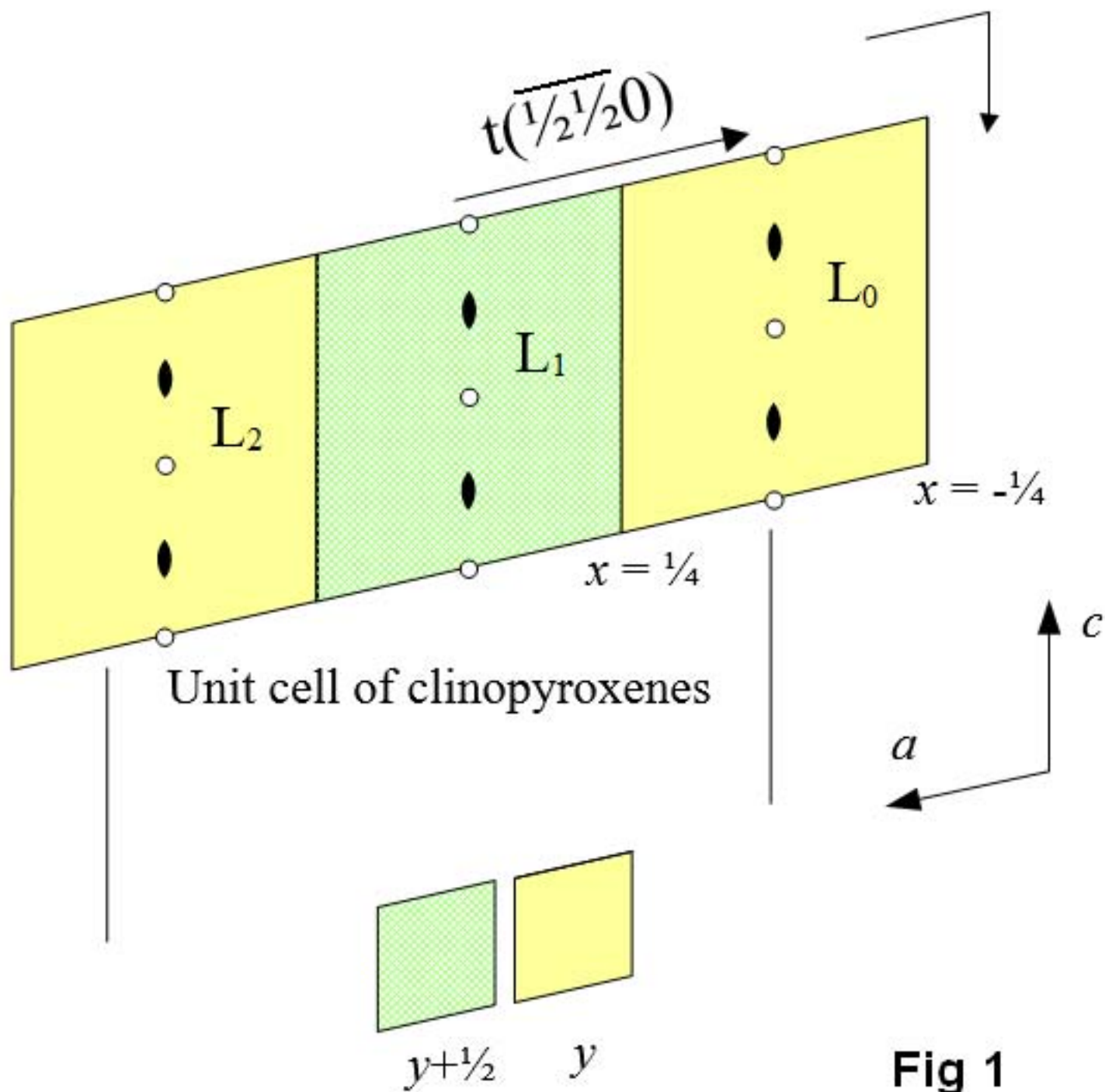


Fig 1

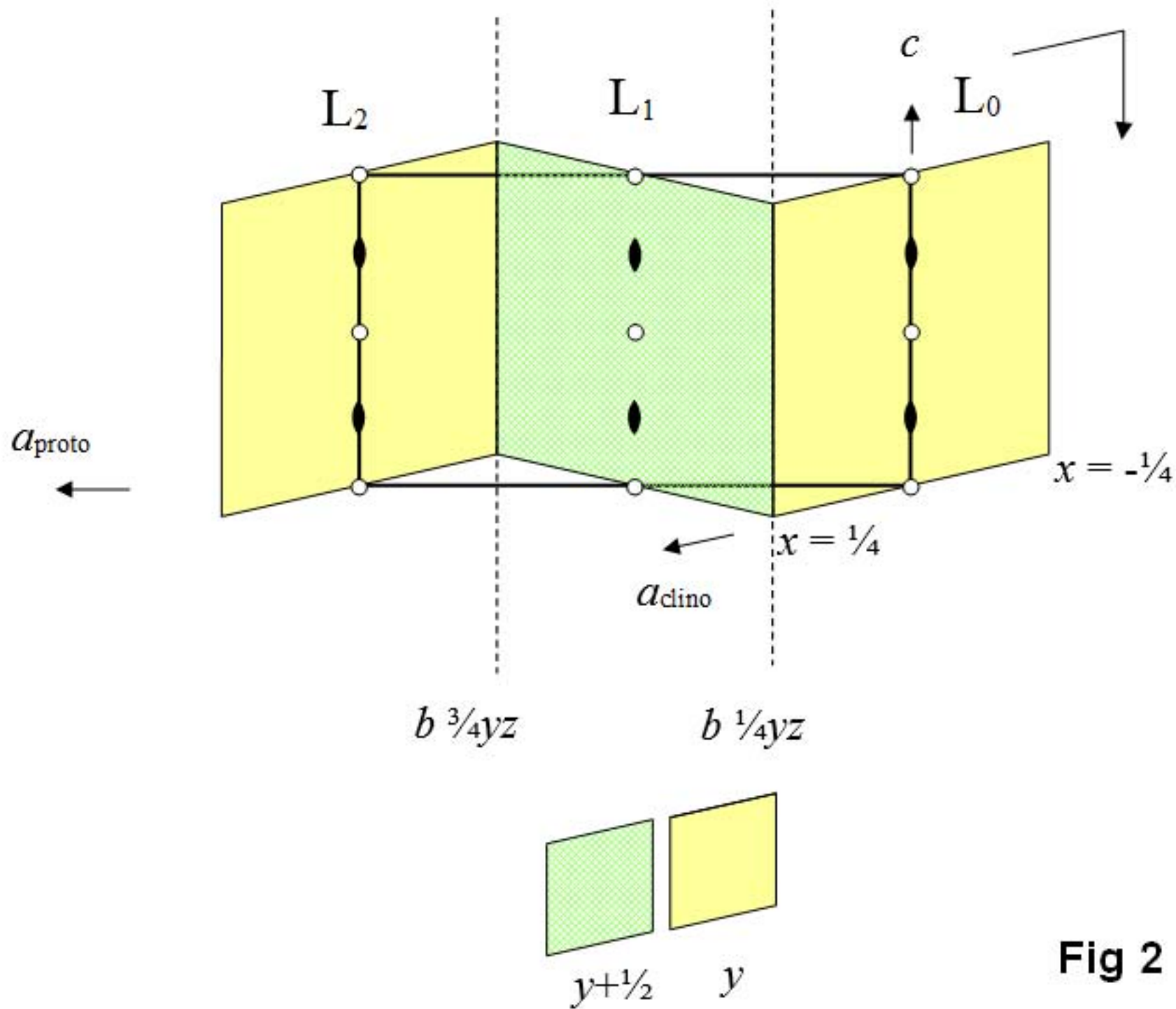
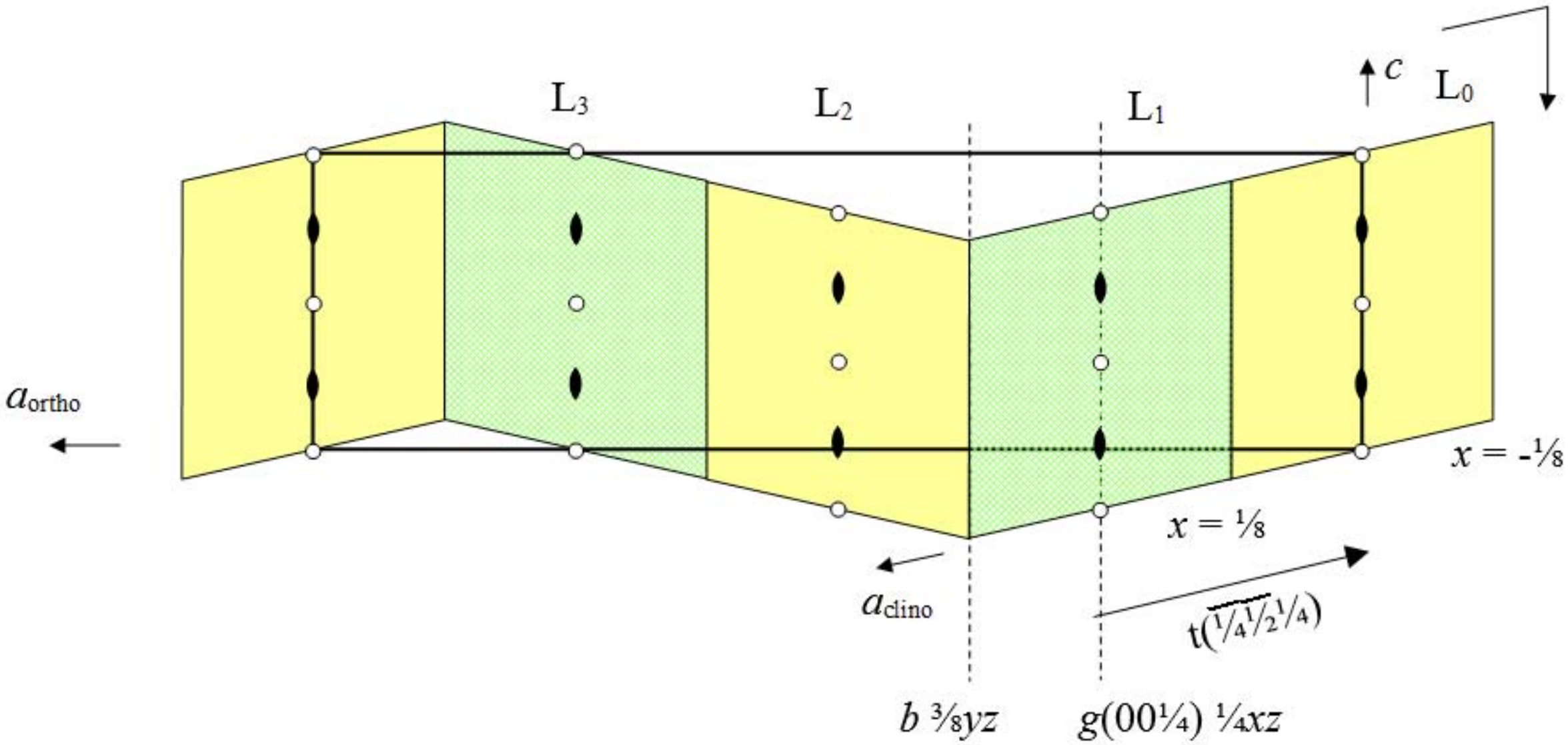


Fig 2



$L_1 \rightarrow L_0: t$

$L_3 \rightarrow L_0: b^{3/8}yz$

$L_2 \rightarrow L_0 = L_2 \rightarrow L_1 \rightarrow L_0: tb = g(00^{1/4})^{1/4}xz$

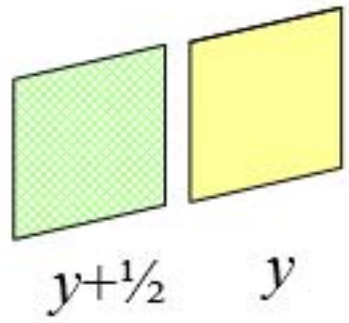


Fig 3a

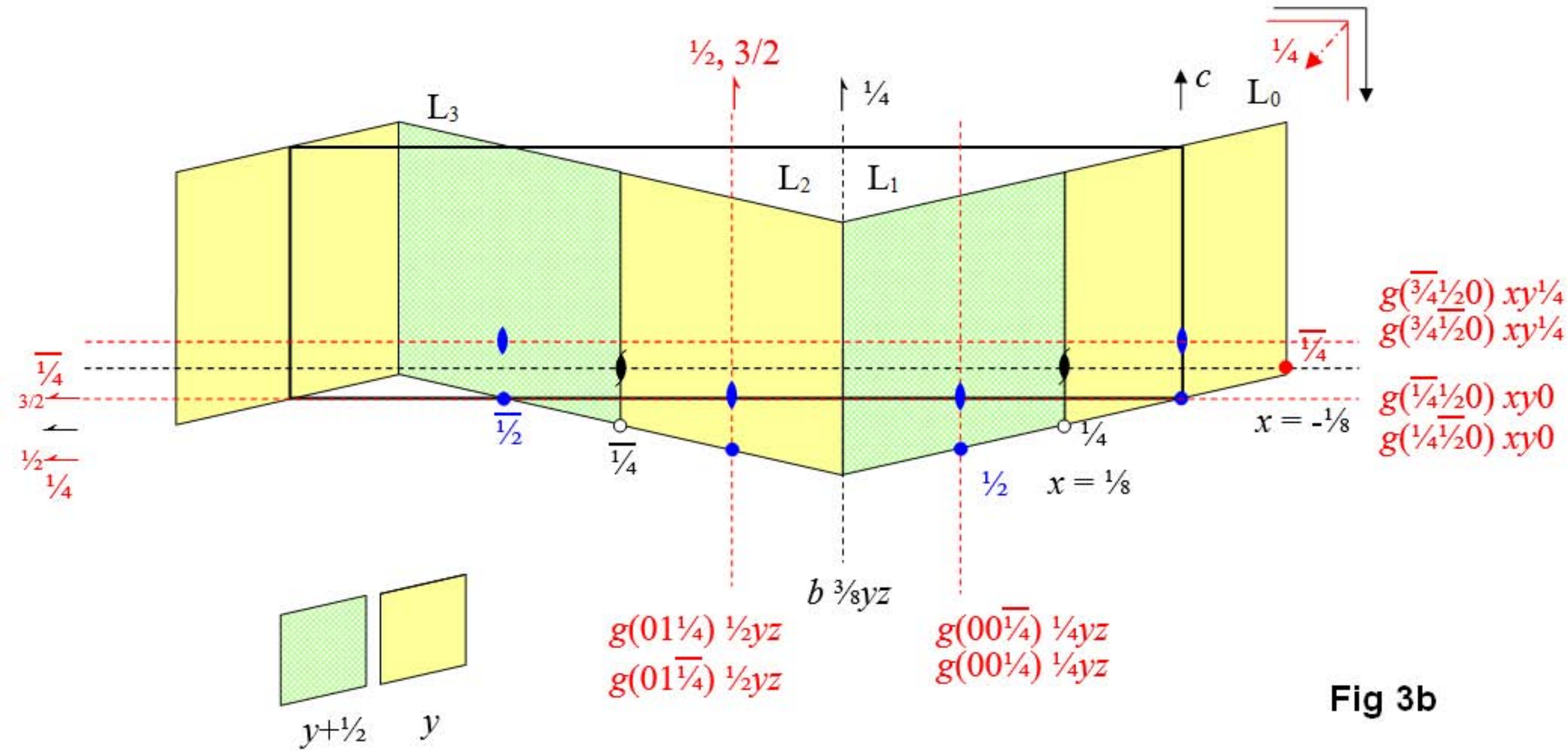


Fig 3b