

Representation of Crystallographic Subperiodic Groups by Geometric Algebra

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Acknowledgements

You answer us with awesome deeds of righteousness, O God our Savior, the hope of all the ends of the earth and of the farthest seas ...

Psalm 65:5 [8]

- I thank my wife, my children, my parents.
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Contents

- 1 Introduction
 - GA basics
 - Point Groups and Space Groups
- 2 Subperiodic Groups in GA
- 3 Frieze Groups
 - Table of Frieze groups
- 4 Rod groups
 - Table of rod groups
- 5 Layer groups
 - Table of layer groups
- 6 Conclusions



Introduction

- The 3D crystallographic **space groups represented in GA** (Hestenes 2002 [2], Hestenes & Holt 2007 [3]).
- Interactive 3D **Space Group Visualizer** created [5].
- For crystallographers the **subperiodic space groups** in 2D and 3D with only 1 or 2 degrees of freedom for translations are also of great interest [7].



- Clifford's associative **geometric product**

$$ab = a \cdot b + a \wedge b. \quad (1)$$

- Reflection** of vector x at hyperplane (through origin) with normal a

$$x' = -a^{-1}xa, \quad a^{-1} = \frac{a}{a^2}. \quad (2)$$

- The composition of two reflections yields a **rotation**

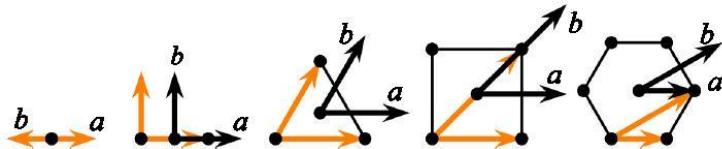
$$x' = (ab)^{-1}xab, \quad (ab)^{-1} = b^{-1}a^{-1}. \quad (3)$$

- Geometric product of k normal vectors (versor S) corresponds to **all symmetry transformations** of 2D, 3D crystal cell point groups

$$x' = (-1)^k S^{-1}xS. \quad (4)$$



- **2D point groups** are generated (cf. Table 1) by vectors subtending angles π/p



- **Example: Hexagonal** point group

$$6 = \{a, b, R = ab, R^2, R^3, R^4, R^5, R^6 = -1, aR^2, bR^2, aR^4, bR^4\}. \quad (5)$$

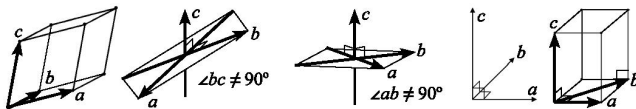
- **Rotation subgroup** (denoted with bar): $\bar{6}$.

Table: Geometric and international notation for 2D point groups.

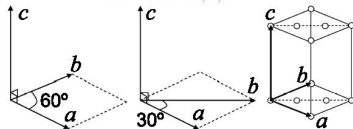
Crystal	Oblique		Rectangular		Trigonal		Square		Hexagonal	
geometric	$\bar{1}$	$\bar{2}$	1	2	3	$\bar{3}$	4	$\bar{4}$	6	$\bar{6}$
international	1	2	m	mm	3m	3	4m	4	6m	6



Selection of **three vectors** a, b, c from each crystal cell for generating **3D Point Groups**



Triclinic, monoclinic inclined, monoclinic orthogonal, orthorhombic, and tetragonal cell vectors a, b, c



trigonal (left), hexagonal (center) and hexagonally centered cell vectors a, b, c

Table: **Geometric 3D point group symbols** and generators with $\theta_{a,b} = \pi/p$, $\theta_{b,c} = \pi/q$, $\theta_{a,c} = \pi/2$, $p, q \in \{1, 2, 3, 4, 6\}$.

Symbol	1	$p \neq 1$	\bar{p}	pq	$\bar{p}q$	$p\bar{q}$	$\bar{p}\bar{q}$	$\bar{p}\bar{q}$
Generators	a	a, b	ab	a, b, c	ab, c	a, bc	ab, bc	abc



Space Groups

- Composition with translations best in **conformal model** of Euclidean space (in the GA of $\mathbb{R}^{4,1}$).
- A **plane** can be described by the vector

$$m = p - d e_{\infty}, \quad (6)$$

p is a unit normal to the plane, d its signed scalar distance from origin.

- Reflecting at 2 parallel planes m, m' with distance $t/2$ we get the **translation operator** (by $t \in \mathbb{R}^3$)

$$X' = m' m X m m' = T_t^{-1} X T_t, \quad T_t = 1 + \frac{1}{2} t e_{\infty}. \quad (7)$$

- Reflection at 2 non-parallel planes m, m' : **rotation** around m, m' -intersection by twice the angle subtended by m, m' .



Subperiodic groups – subgroups of space groups

- Subperiodic groups are subgroups of full 2D and 3D space groups.
- Frieze groups (7) are all subgroups of **2D space groups** with only **one DOF for translation**.
- Rod groups (75) are all subgroups of **3D space groups** with only **one DOF for translation**.
- Layer groups (80) are all subgroups of **3D space groups** with only **two DOF for translation**.



Notation

- One dot between the Bravais symbol ($\not\prec, p, c$) and index 1: **b is generator**.
- Two dots between the Bravais symbol ($\not\prec, p, c$) and index 1: **c is generator**.
- One dot between the Bravais symbol and index 2 (without or with bar): vectors **b, c are generators**.
- Two dots between the Bravais symbol and index 2 (without or with bar): vectors **a, c are generators**.
- Indexes a, b, c, n (and g for frieze groups) in 1st, 2nd, 3rd position after the Bravais symbol: reflections a, b, c (order!) change to **glide reflections**.
- Index n for **diagonal glide**.
- Dots also **position indicators**.
 Rod group 5: $\not\prec_c 1$ has glide reflection $aT_c^{1/2}$.
 Rod group 19: $\not\prec \cdot c 2$ has $bT_c^{1/2}$.
 Layer group 39: $p_b 2_a 2_n$ has $aT_b^{1/2}$, $bT_a^{1/2}$, and $cT_{a+b}^{1/2}$.
- \bar{n}_p : right handed **screw rotation** of $2\pi/n$ around \bar{n} -axis, with pitch $T_t^{p/n}$. t is shortest lattice translation vector parallel to axis, in screw direction.
 Layer group 21: $p\bar{2}\bar{2}_1\bar{2}_1$ has screw generators $bcT_a^{1/2}$ and $acT_b^{1/2}$.



Frieze Groups

Generating vectors a, b of oblique and rectangular cells for 2D Frieze groups.



Single translation direction a .



Tables of Crystallography (IUCr)

Depiction of Frieze group No. 7 in Int. Tables of Cryst. Vol. E. [7]

International Tables for Crystallography (2006). Vol. E, Frieze group 7, p. 36.

$\mu 2mg$

$2mm$

Rectangular

No. 7

$\mu 2mg$

Patterson symmetry $\mu 2mm$

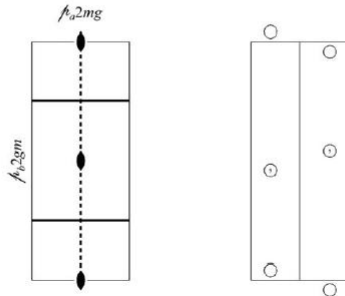




Table of Frieze groups

Geometric symbols for Frieze groups

The seven Frieze groups with **new geometric symbols and generators**. SG = space group, SGN = space group numbers, T_a is omitted.

Frieze Group #	Intern. Notat.	3D SG#	Intern. 3D SGN	Geom. 3D SGN	2D SG#	Intern. 2D SGN	Geom. 2D SGN	Geom. Notat.	Frieze Group Generators
Oblique									
F_1	$\not\parallel 1$	1	$P1$	$P\bar{1}$	1	$p1$	$p\bar{1}$	$\not\parallel \bar{1}$	
F_2	$\not\parallel 211$	3	$P2$	$P\bar{2}$	2	$p2$	$p\bar{2}$	$\not\parallel \bar{2}$	$a \wedge b$
Rectangular									
F_3	$\not\parallel 1m1$	6	Pm	$P1$	3	$pm(p1m1)$	$p1$	$\not\parallel 1$	a
F_4	$\not\parallel 11m$	6	Pm	$P1$	3	$pm(p11m)$	$p1$	$\not\parallel \cdot 1$	b
F_5	$\not\parallel 11g$	7	Pc	P_a1	4	$pg(p11g)$	p_g1	$\not\parallel \cdot g1$	$bT_a^{1/2}$
F_6	$\not\parallel 2mm$	25	$Pmm2$	$P2$	6	$p2mm$	$p2$	$\not\parallel 2$	a, b
F_7	$\not\parallel 2mg$	28	$Pma2$	$P2_a$	7	$p2mg$	$p2_g$	$\not\parallel 2_g$	$a, bT_a^{1/2}$

Rod Groups

Generating vectors a, b, c of triclinic, monoclinic inclined, monoclinic orthogonal, orthorhombic, tetragonal, trigonal, hexagonal and hexagonally centered (Bravais symbol: H or h) cells for 3D rod (and layer) groups. Single **translation direction** c .

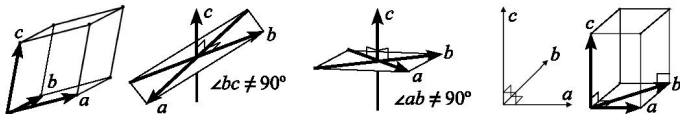


Fig. 3 From left to right: Triclinic, monoclinic inclined, monoclinic orthogonal, orthorhombic, and tetragonal cell vectors a, b, c for rod and layer groups.

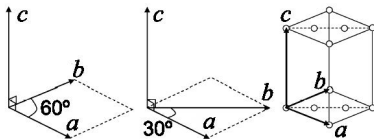


Fig. 4 Generating vectors a, b, c of trigonal (left), hexagonal (center) and hexagonally centered (right, Bravais symbol: H or h) cells for 3D rod and layer groups.

Tables of Crystallography (IUCr)

Depiction of rod group No. 75 in Int. Tables of Cryst. Vol. E. [7]

International Tables for Crystallography (2006). Vol. E, Rod group 75, pp. 214–217.

$\not\sim 6_3/mmc$

$6/mmm$

Hexagonal

No. 75

$\not\sim 6_3/m2/m2/c$

Patterson symmetry $\not\sim 6/mmm$

FIRST SETTING

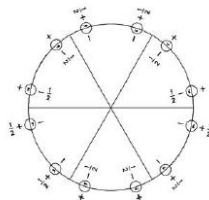
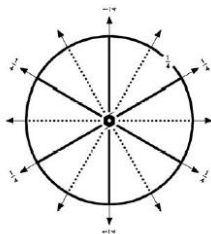




Table of rod groups

Triclinic and monoclinic rod groups. T_c is omitted.

Rod Group #	Intern. Notat.	3D Space Group #	Intern. 3D SGN	Geom. 3D SGN	Geom. Notat.	Rod Group Generators
Triclinic						
R_1	$\not\parallel 1$	1	$P1$	$P\bar{1}$	$\not\parallel \bar{1}$	
R_2	$\not\parallel 2$	2	$P\bar{1}$	$P2\bar{2}$	$\not\parallel 2\bar{2}$	$a \wedge b \wedge c$
Monoclinic/inclined						
R_3	$\not\parallel 211$	3	$P112$	$P\bar{2}$	$\not\parallel \bar{2}$	$b \wedge c$
R_4	$\not\parallel m11$	6	Pm	$P1$	$\not\parallel 1$	a
R_5	$\not\parallel c11$	7	Pc	$P_c 1$	$\not\parallel c 1$	$aT_c^{1/2}$
R_6	$\not\parallel 2/m11$	10	$P2/m$	$P2\bar{2}$	$\not\parallel 2\bar{2}$	$a, b \wedge c$
R_7	$\not\parallel 2/c11$	13	$P2/c$	$P_a 2\bar{2}$	$\not\parallel c 2\bar{2}$	$aT_c^{1/2}, b \wedge c$
Monoclinic/orthogonal						
R_8	$\not\parallel 112$	3	$P112$	$P\bar{2}$	$\not\parallel \bar{2}$	$a \wedge b$
R_9	$\not\parallel 112_1$	4	$P2_1$	$P\bar{2}_1$	$\not\parallel \bar{2}_1$	$(a \wedge b)T_c^{1/2}$
R_{10}	$\not\parallel 11m$	6	Pm	$P1$	$\not\parallel \dots 1$	c
R_{11}	$\not\parallel 112/m$	10	$P2/m$	$P\bar{2}\bar{2}$	$\not\parallel \bar{2}\bar{2}$	$a \wedge b, c$
R_{12}	$\not\parallel 112_1/m$	11	$P2_1/m$	$P\bar{2}_1 2$	$\not\parallel \bar{2}_1 2$	$(a \wedge b)T_c^{1/2}, c$



Table of rod groups

Orthorhombic rod groups. T_c is omitted.

Rod Group #	Intern. Notat.	3D Space Group #	Intern. 3D SGN	Geom. 3D SGN	Geom. Notat.	Rod Group Generators
Orthorhombic						
R_{13}	$\rho 222$	16	$P222$	$P\bar{2}\bar{2}\bar{2}$	$\rho\bar{2}\bar{2}\bar{2}$	ab, bc
R_{14}	$\rho 222_1$	17	$P222_1$	$P\bar{2}_1\bar{2}\bar{2}$	$\rho\bar{2}_1\bar{2}\bar{2}$	$abT_c^{1/2}, bc$
R_{15}	$\rho mm2$	25	$Pmm2$	$P2$	$\rho 2$	a, b
R_{16}	$\rho cc2$	27	$Pcc2$	P_c2_c	ρ_c2_c	$aT_c^{1/2}, bT_c^{1/2}$
R_{17}	$\rho mc2_1$	26	$Pmc2_1$	$P2_c$	$\rho 2_c$	$a, bT_c^{1/2}$
R_{18}	$\rho 2mm$	25	$Pmm2$	$P2$	$\rho .2$	b, c
R_{19}	$\rho 2cm$	28	$Pma2$	$P2_a$	$\rho ._c2$	$bT_c^{1/2}, c$
R_{20}	ρmmm	47	$Pmmm$	$P22$	$\rho 22$	a, b, c
R_{21}	ρccm	49	$Pccm$	P_c2_c2	ρ_c2_c2	$aT_c^{1/2}, bT_c^{1/2}, c$
R_{22}	ρmcm	51	$Pmma$	$P22_a$	$\rho 2_c2$	$a, bT_c^{1/2}, c$



Table of rod groups

Tetragonal rod groups. T_c is omitted.

Rod Group #	Intern. Notat.	3D Space Group #	Intern. 3D SGN	Geom. 3D SGN	Geom. Notat.	Rod Group Generators
Tetragonal						
R_{23}	$\cancel{4}$	75	$P4$	$P\bar{4}$	$\cancel{4}$	ab
R_{24}	$\cancel{4}_1$	76	$P4_1$	$P\bar{4}_1$	$\cancel{4}_1$	$abT_c^{\frac{1}{4}}$
R_{25}	$\cancel{4}_2$	77	$P4_2$	$P\bar{4}_2$	$\cancel{4}_2$	$abT_c^{\frac{1}{2}}$
R_{26}	$\cancel{4}_3$	78	$P4_3$	$P\bar{4}_3$	$\cancel{4}_3$	$abT_c^{\frac{3}{4}}$
R_{27}	$\cancel{4}$	81	$P\bar{4}$	$P4\bar{2}$	$\cancel{4}\bar{2}$	abc
R_{28}	$\cancel{4}/m$	83	$P4/m$	$P\bar{4}2$	$\cancel{4}2$	ab, c
R_{29}	$\cancel{4}_2/m$	84	$P4_2/m$	$P\bar{4}_22$	$\cancel{4}_22$	$abT_c^{\frac{1}{2}}, c$
R_{30}	$\cancel{4}22$	89	$P422$	$P\bar{4}\bar{2}\bar{2}$	$\cancel{4}\bar{2}\bar{2}$	ab, bc
R_{31}	$\cancel{4}_122$	91	$P4_122$	$P\bar{4}_1\bar{2}\bar{2}$	$\cancel{4}_1\bar{2}\bar{2}$	$abT_c^{\frac{1}{4}}, bc$
R_{32}	$\cancel{4}_222$	93	$P4_222$	$P\bar{4}_2\bar{2}\bar{2}$	$\cancel{4}_2\bar{2}\bar{2}$	$abT_c^{\frac{1}{2}}, bc$
R_{33}	$\cancel{4}_322$	95	$P4_322$	$P\bar{4}_3\bar{2}\bar{2}$	$\cancel{4}_3\bar{2}\bar{2}$	$abT_c^{\frac{3}{4}}, bc$
R_{34}	$\cancel{4}mm$	99	$P4mm$	$P4$	$\cancel{4}$	a, b
R_{35}	$\cancel{4}_2cm$	101	$P4_2cm$	$P4$	$\cancel{4}_c$	$aT_c^{\frac{1}{2}}, b$
R_{36}	$\cancel{4}cc$	103	$P4cc$	P_c4_c	$\cancel{4}_c4_c$	$aT_c^{\frac{1}{2}}, bT_c^{\frac{1}{2}}$
R_{37}	$\cancel{4}m2$	115	$P\bar{4}m2$	$P4\bar{2}$	$\cancel{4}\bar{2}$	a, bc
R_{38}	$\cancel{4}c2$	116	$P\bar{4}c2$	$P_c4\bar{2}$	$\cancel{4}_c\bar{4}\bar{2}$	$aT_c^{\frac{1}{2}}, bc$
R_{39}	$\cancel{4}/mmm$	123	$P4/mmm$	$P42$	$\cancel{4}2$	a, b, c
R_{40}	$\cancel{4}/mcc$	124	$P4/mcc$	P_c4_c2	$\cancel{4}_c4_c2$	$aT_c^{\frac{1}{2}}, bT_c^{\frac{1}{2}}, c$
R_{41}	$\cancel{4}_2/mmc$	131	$P4_2/mmc$	$P4_c2$	$\cancel{4}_c2$	$a, bT_c^{\frac{1}{2}}, c$

Table of rod groups

Trigonal rod groups. T_c is omitted.

Rod Group #	Intern. Notat.	3D Space Group #	Intern. 3D SGN	Geom. 3D SGN	Geom. Notat.	Rod Group Generators
Trigonal						
R_{42}	$\cancel{P}3$	143	$P3$	$P\bar{3}$	$\cancel{P}\bar{3}$	ab
R_{43}	$\cancel{P}3_1$	144	$P3_1$	$P\bar{3}_1$	$\cancel{P}\bar{3}_1$	$abT_c^{\frac{1}{3}}$
R_{44}	$\cancel{P}3_2$	145	$P3_2$	$P\bar{3}_2$	$\cancel{P}\bar{3}_2$	$abT_c^{\frac{2}{3}}$
R_{45}	$\cancel{P}\bar{3}$	147	$P\bar{3}$	$P6\bar{2}$	$\cancel{P}6\bar{2}$	abc
R_{46}	$\cancel{P}312$	149	$P312$	$P\bar{3}\bar{2}$	$\cancel{P}\bar{3}\bar{2}$	ab, bc
R_{47}	$\cancel{P}3_112$	151	$P3_112$	$P\bar{3}_1\bar{2}$	$\cancel{P}\bar{3}_1\bar{2}$	$abT_c^{\frac{1}{3}}, bc$
R_{48}	$\cancel{P}3_212$	153	$P3_212$	$P\bar{3}_2\bar{2}$	$\cancel{P}\bar{3}_2\bar{2}$	$abT_c^{\frac{2}{3}}, bc$
R_{49}	$\cancel{P}3m1$	156	$P3m1$	$P3$	$\cancel{P}3$	a, b
R_{50}	$\cancel{P}3c1$	158	$P3c1$	P_c3_c	\cancel{P}_c3_c	$aT_c^{\frac{1}{2}}, bT_c^{\frac{1}{2}}$
R_{51}	$\cancel{P}\bar{3}1m$	162	$P\bar{3}1m$	$P\bar{2}6$	$\cancel{P}6\bar{2}$	a, bc
R_{52}	$\cancel{P}\bar{3}1c$	163	$P\bar{3}1c$	$P\bar{2}_c6$	$\cancel{P}_c6\bar{2}$	$aT_c^{\frac{1}{2}}, bc$



Table of rod groups

Hexagonal rod groups. T_c is omitted.

Rod Group #	Intern. Notat.	3D Space Group #	Intern. 3D SGN	Geom. 3D SGN	Geom. Notat.	Rod Group Generators
R_{53}	$\cancel{P6}$	168	$P6$	$\bar{P6}$	$\cancel{P6}$	ab
R_{54}	$\cancel{P6}_1$	169	$P6_1$	$\bar{P6}_1$	$\cancel{P6}_1$	$abT_c^{\frac{1}{6}}$
R_{55}	$\cancel{P6}_2$	171	$P6_2$	$\bar{P6}_2$	$\cancel{P6}_2$	$abT_c^{\frac{1}{3}}$
R_{56}	$\cancel{P6}_3$	173	$P6_3$	$\bar{P6}_3$	$\cancel{P6}_3$	$abT_c^{\frac{1}{2}}$
R_{57}	$\cancel{P6}_4$	172	$P6_4$	$\bar{P6}_4$	$\cancel{P6}_4$	$abT_c^{\frac{2}{3}}$
R_{58}	$\cancel{P6}_5$	170	$P6_5$	$\bar{P6}_5$	$\cancel{P6}_5$	$abT_c^{\frac{5}{6}}$
R_{59}	$\cancel{P6}$	174	$\bar{P6}$	$P3_2$	$\cancel{P3}_2$	ab, c
R_{60}	$\cancel{P6/m}$	175	$P6/m$	$\bar{P6}_2$	$\cancel{P6}_2$	ab, c
R_{61}	$\cancel{P6}_3/m$	176	$P6_3/m$	$\bar{P6}_3_2$	$\cancel{P6}_3_2$	$abT_c^{\frac{1}{2}}$
R_{62}	$\cancel{P6}_2$	177	$P6_2$	$\bar{P6}_2$	$\cancel{P6}_2$	ab, bc
R_{63}	$\cancel{P6}_1 2$	178	$P6_1 2$	$\bar{P6}_1 \bar{2}$	$\cancel{P6}_1 \bar{2}$	$abT_c^{\frac{1}{6}}, bc$
R_{64}	$\cancel{P6}_2 2$	180	$P6_2 2$	$\bar{P6}_2 \bar{2}$	$\cancel{P6}_2 \bar{2}$	$abT_c^{\frac{1}{3}}, bc$
R_{65}	$\cancel{P6}_3 2$	182	$P6_3 2$	$\bar{P6}_3 \bar{2}$	$\cancel{P6}_3 \bar{2}$	$abT_c^{\frac{1}{2}}, bc$
R_{66}	$\cancel{P6}_4 2$	181	$P6_4 2$	$\bar{P6}_4 \bar{2}$	$\cancel{P6}_4 \bar{2}$	$abT_c^{\frac{2}{3}}, bc$
R_{67}	$\cancel{P6}_5 2$	179	$P6_5 2$	$\bar{P6}_5 \bar{2}$	$\cancel{P6}_5 \bar{2}$	$abT_c^{\frac{5}{6}}, bc$
R_{68}	$\cancel{P6} mm$	183	$P6 mm$	$P6$	$\cancel{P6}$	a, b
R_{69}	$\cancel{P6} cc$	184	$P6 cc$	$P_6 6_c$	$\cancel{P_6} 6_c$	$aT_c^{\frac{1}{2}}, bT_c^{\frac{1}{2}}$
R_{70}	$\cancel{P6}_3 cm$	185	$P6_3 cm$	$P_6 6$	$\cancel{P_6} 6$	$aT_c^{\frac{1}{2}}, b$
R_{71}	$\cancel{P6} m 2$	187	$P6 m 2$	$P3_2$	$\cancel{P3}_2$	a, b, c
R_{72}	$\cancel{P6} c 2$	188	$\bar{P6} c 2$	$P_6 3_2 c$	$\cancel{P_6} 3_2 c$	$aT_c^{\frac{1}{2}}, bT_c^{\frac{1}{2}}, c$
R_{73}	$\cancel{P6} / m m m$	191	$P6 / m m m$	$P6_2$	$\cancel{P6}_2$	a, b, c
R_{74}	$\cancel{P6} / m c c$	192	$P6 / m c c$	$P_6 6_2 c$	$\cancel{P_6} 6_2 c$	$aT_c^{\frac{1}{2}}, bT_c^{\frac{1}{2}}, c$
R_{75}	$\cancel{P6}_3 / m c m$	193	$P6_3 / m c m$	$P_6 6_2$	$\cancel{P_6} 6_2$	$aT_c^{\frac{1}{2}}, b, c$

Layer Groups

Generating vectors a, b, c of triclinic, monoclinic inclined, monoclinic orthogonal, orthorhombic, tetragonal, trigonal, hexagonal and hexagonally centered (Bravais symbol: H or h) cells for 3D layer (and rod) groups. Two **translation directions** a, b .

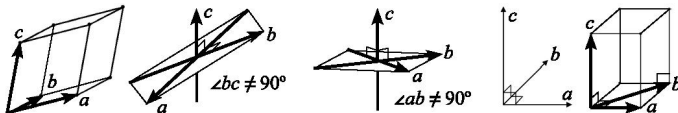


Fig. 3 From left to right: Triclinic, monoclinic inclined, monoclinic orthogonal, orthorhombic, and tetragonal cell vectors a, b, c for rod and layer groups.

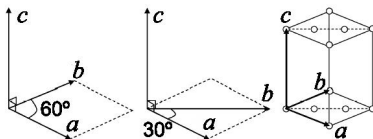


Fig. 4 Generating vectors a, b, c of trigonal (left), hexagonal (center) and hexagonally centered (right, Bravais symbol: H or h) cells for 3D rod and layer groups.

Tables of Crystallography (IUCr)

Depiction of layer group No. 80 in Int. Tables of Cryst. Vol. E. [7]

International Tables for Crystallography (2006). Vol. E, Layer group 80, pp. 388–389.

$p6/mmm$

$6/mmm$

Hexagonal/Hexagonal

No. 80

$p6/mmm$

Patterson symmetry $p6/mmm$

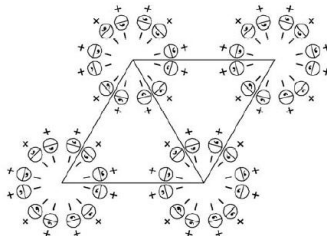
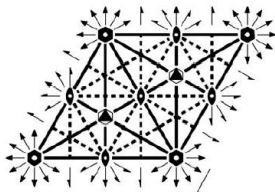




Table of layer groups

Triclinic/oblique and monoclinic/oblique and monoclinic/rectangular layer groups. T_a, T_b are omitted.

Layer Group #	Intern. Notat.	3D Space Group #	Intern. 3D SGN	Geom. 3D SGN	Geom. Notat.	Layer Group Generators
Triclinic/oblique						
L_1	$p1$	1	$P1$	$P\bar{1}$	$p\bar{1}$	
L_2	$p\bar{1}$	2	$P\bar{1}$	$P2\bar{2}$	$p2\bar{2}$	$a \wedge b \wedge c$
Monoclinic/oblique						
L_3	$p112$	3	$P2$	$P2^2$	$p2^2$	$a \wedge b$
L_4	$p11m$	6	Pm	$P1$	$p..1$	c
L_5	$p11a$	7	Pc	P_a1	$p..a1$	$cT_a^{\frac{1}{2}}$
L_6	$p112/m$	10	$P2/m$	$P2\bar{2}$	$p2\bar{2}$	$a \wedge b, c$
L_7	$p112/a$	13	$P2/c$	$P_a2\bar{2}$	$p2\bar{2}_a$	$a \wedge b, cT_a^{\frac{1}{2}}$
Monoclinic/rectangular						
L_8	$p211$	3	$P2$	$P2^2$	$p..2$	$b \wedge c$
L_9	$p2_111$	4	$P2_1$	$P2\bar{2}_1$	$p..2_1$	$(b \wedge c)T_a^{\frac{1}{2}}$
L_{10}	$c211$	5	$C2$	$A\bar{2}$	$c..2$	$b \wedge c, T_{a+b}^{1/2}$
L_{11}	$pm11$	6	Pm	$P1$	$p1$	a
L_{12}	$pb11$	7	Pc	P_a1	p_b1	$aT_b^{\frac{1}{2}}$
L_{13}	$cm11$	8	Cm	$A1$	$c1$	$a, T_{a+b}^{1/2}$
L_{14}	$p2/m11$	10	$P2/m$	$P2\bar{2}$	$p2\bar{2}$	$a, b \wedge c$
L_{15}	$p2_1/m11$	11	$P2_1/m$	$P2\bar{2}_1$	$p2\bar{2}_1$	$a, (b \wedge c)T_a^{\frac{1}{2}}$
L_{16}	$p2/b11$	13	$P2/c$	$P_a2\bar{2}$	$p_b2\bar{2}$	$aT_b^{\frac{1}{2}}, b \wedge c$
L_{17}	$p2_1/b11$	14	$P2_1/c$	$P_a2\bar{2}_1$	$p_b2\bar{2}_1$	$aT_b^{\frac{1}{2}}, (b \wedge c)T_a^{\frac{1}{2}}$
L_{18}	$c2/m11$	12	$C2/m$	$A\bar{2}$	$c2\bar{2}$	$a, b \wedge c, T_{a+b}^{1/2}$



Table of layer groups

Orthorhombic/rectangular layer groups. T_a, T_b are omitted.

Layer Group #	Intern. Notat.	3D Space Group #	Intern. 3D SGN	Geom. 3D SGN	Geom. Notat.	Layer Group Generators
L_{19}	$p222$	16	$P222$	$P2_1^3$	$p2_1^3$	ab, bc
L_{20}	$p2_122$	17	$P222_1$	$P2_1^2$	$p2_1^2$	$ab, bcT_a^{\frac{1}{2}}$
L_{21}	$p2_12_12$	18	$P2_12_12$	$P2_1^2$	$p2_1^2$	$bcT_a^{\frac{1}{2}}, acT_b^{\frac{1}{2}}$
L_{22}	$c222$	21	$C222$	$C222$	$c222$	$ab, bc, T_{a+b}^{\frac{1}{2}}$
L_{23}	$pmm2$	25	$Pmm2$	$P2$	$p2$	a, b
L_{24}	$pma2$	28	$Pma2$	$P2_a$	$p2_a$	$a, bT_a^{\frac{1}{2}}$
L_{25}	$pba2$	32	$Pba2$	$P2_b$	$p2_b$	$aT_b^{\frac{1}{2}}, bT_a^{\frac{1}{2}}$
L_{26}	$cnm2$	35	$Cnm2$	$C2$	$c2$	$a, b, T_{a+b}^{\frac{1}{2}}$
L_{27}	$pm2m$	25	$Pmm2$	$P2$	$p..2$	a, c
L_{28}	$pm2_1b$	26	$Pmc2_1$	$P2_c$	$p..b2$	$a, cT_b^{\frac{1}{2}}$
L_{29}	$pb2_1m$	26	$Pmc2_1$	$P2_c$	$pb..2$	$aT_b^{\frac{1}{2}}, c$
L_{30}	$pb2b$	27	$Pcc2$	$Pc2_c$	$pb..b2$	$aT_b^{\frac{1}{2}}, cT_b^{\frac{1}{2}}$
L_{31}	$pm2a$	28	$Pma2$	$P2_a$	$p..a2$	$a, cT_a^{\frac{1}{2}}$
L_{32}	$pm2_1n$	31	$Pmn2_1$	$P2_n$	$p..n2$	$a, cT_{a+b}^{\frac{1}{2}}$
L_{33}	$pb2_1a$	29	$Pca2_1$	$Pc2_a$	$pb..a2$	$aT_b^{\frac{1}{2}}, cT_a^{\frac{1}{2}}$
L_{34}	$pb2n$	30	$Pnc2$	Pn^2c	$pb..n2$	$aT_b^{\frac{1}{2}}, cT_{a+b}^{\frac{1}{2}}$
L_{35}	$cm2m$	35	$Cmm2$	$C2$	$c..2$	$a, c, T_{a+b}^{\frac{1}{2}}$
L_{36}	$cm2e$	39	$Cem2$	$A2$	$c..a2$	$a, cT_a^{\frac{1}{2}}, T_{a+b}^{\frac{1}{2}}$
L_{37}	$pmmm$	47	$Pmmm$	$P22$	$p22$	a, b, c
L_{38}	$pmca$	49	$Pccm$	$Pc2_c2$	$p2_a2_a$	$a, bT_a^{\frac{1}{2}}, cT_a^{\frac{1}{2}}$
L_{39}	$pban$	50	$Pban$	$Pb2_a2_n$	$pb2_a2_n$	$aT_b^{\frac{1}{2}}, bT_a^{\frac{1}{2}}, cT_{a+b}^{\frac{1}{2}}$
L_{40}	$pmam$	51	$Pmma$	$P22_a$	$p2_a2$	$a, bT_a^{\frac{1}{2}}, c$
L_{41}	$pmma$	51	$Pmma$	$P22_a$	$p22_a$	$a, b, cT_a^{\frac{1}{2}}$
L_{42}	$pmna$	53	$Pmna$	$P2_n2_a$	$p2_a2_n$	$a, bT_a^{\frac{1}{2}}, cT_{a+b}^{\frac{1}{2}}$
L_{43}	$pbca$	54	$Pcca$	$Pc2_c2_a$	$pb2_a2_a$	$aT_b^{\frac{1}{2}}, bT_a^{\frac{1}{2}}, cT_a^{\frac{1}{2}}$
L_{44}	$pbam$	55	$Pbam$	$Pb2_a2$	$pb2_a2$	$aT_b^{\frac{1}{2}}, bT_a^{\frac{1}{2}}, c$
L_{45}	$pbma$	57	$Pbcm$	$Pb2_c2$	$pb22_a$	$aT_b^{\frac{1}{2}}, b, cT_a^{\frac{1}{2}}$
L_{46}	$pmnn$	59	$Pmnn$	$P22_n$	$p22_n$	$a, b, cT_{a+b}^{\frac{1}{2}}$
L_{47}	$cnmm$	65	$Cnmm$	$C22$	$c22$	$a, b, c, T_{a+b}^{\frac{1}{2}}$
L_{48}	$cnme$	67	$Cnme$	$C22_a$	$c22_a$	$a, b, cT_a^{\frac{1}{2}}, T_{a+b}^{\frac{1}{2}}$



Table of layer groups

Tetragonal/square layer groups. T_a, T_b are omitted.

Layer Group #	Intern. Notat.	3D Space Group #	Intern. 3D SGN	Geom. 3D SGN	Geom. Notat.	Layer Group Generators
Tetragonal/square						
L_{49}	$p4$	75	$P4$	$P\bar{4}$	$p\bar{4}$	ab
L_{50}	$p\bar{4}$	81	$P\bar{4}$	$P\bar{4}2$	$p\bar{4}2$	abc
L_{51}	$p4/m$	83	$P4/m$	$P\bar{4}2$	$p\bar{4}2$	ab, c
L_{52}	$p4/n$	85	$P4/n$	$P\bar{4}_n2$	$p\bar{4}_n2$	$ab, cT_b^{\frac{1}{2}}$
L_{53}	$p422$	89	$P422$	$P\bar{4}22$	$p\bar{4}22$	ab, bc
L_{54}	$p42_12$	90	$P42_12$	$P\bar{4}2_1\bar{2}$	$p\bar{4}2_1\bar{2}$	$ab, bcT_{2a-b}^{1/2}$
L_{55}	$p4mm$	99	$P4mm$	$P4$	$p4$	a, b
L_{56}	$p4bm$	100	$P4bm$	P_b4	p_b4	$aT_{a-b}^{1/2}, b$
L_{57}	$p\bar{4}2m$	111	$P\bar{4}2m$	$P\bar{2}4$	$p\bar{2}4$	ac, b
L_{58}	$p\bar{4}2_1m$	113	$P\bar{4}2_1m$	$P\bar{2}_14$	$p\bar{2}_14$	$acT_{a-b}^{1/2}, b$
L_{59}	$p\bar{4}m2$	115	$P\bar{4}m2$	$P\bar{4}2$	$p\bar{4}2$	a, bc
L_{60}	$p\bar{4}b2$	117	$P\bar{4}b2$	$P_b4\bar{2}$	$p_b4\bar{2}$	$aT_{a-b}^{1/2}, bc$
L_{61}	$p4/mmm$	123	$P4/mmm$	$P42$	$p42$	a, b, c
L_{62}	$p4/nbm$	125	$P4/nbm$	P_b42_n	p_b42_n	$aT_{a-b}^{1/2}, b, cT_b^{\frac{1}{2}}$
L_{63}	$p4/mbm$	127	$P4/mbm$	P_b42	p_b42	$aT_{a-b}^{1/2}, b, c$
L_{64}	$p4/nmm$	129	$P4/nmm$	$P42_n$	$p42_n$	$a, b, cT_b^{\frac{1}{2}}$



Trigonal/hexagonal and Hexagonal/hexagonal layer groups. T_a, T_b are omitted.

Layer Group #	Intern. Notat.	3D Space Group #	Intern. 3D SGN	Geom. 3D SGN	Geom. Notat.	Layer Group Generators
Trigonal/hexagonal						
L_{65}	$p\bar{3}$	143	$P\bar{3}$	$P\bar{3}$	$p\bar{3}$	ab
L_{66}	$p\bar{3}$	147	$P\bar{3}$	$P\bar{6}\bar{2}$	$p\bar{6}\bar{2}$	abc
L_{67}	$p\bar{3}12$	149	$P\bar{3}12$	$P\bar{3}\bar{2}$	$p\bar{3}\bar{2}$	ab, bc
L_{68}	$p\bar{3}21$	150	$P\bar{3}21$	$H\bar{3}\bar{2}$	$h\bar{3}\bar{2}$	ab, bc
L_{69}	$p\bar{3}m1$	156	$P\bar{3}m1$	$P\bar{3}$	$p\bar{3}$	a, b
L_{70}	$p\bar{3}1m$	157	$P\bar{3}1m$	$H\bar{3}$	$h\bar{3}$	a, b
L_{71}	$p\bar{3}1m$	162	$P\bar{3}1m$	$P\bar{2}\bar{6}$	$p\bar{2}\bar{6}$	ac, b
L_{72}	$p\bar{3}m1$	164	$P\bar{3}m1$	$P\bar{6}\bar{2}$	$p\bar{6}\bar{2}$	a, bc
Hexagonal/hexagonal						
L_{73}	$p\bar{6}$	168	$P\bar{6}$	$P\bar{6}$	$p\bar{6}$	ab
L_{74}	$p\bar{6}$	174	$P\bar{6}$	$P\bar{3}2$	$p\bar{3}2$	ab, c
L_{75}	$p\bar{6}/m$	175	$P\bar{6}/m$	$P\bar{6}\bar{2}$	$p\bar{6}\bar{2}$	ab, c
L_{76}	$p\bar{6}22$	177	$P\bar{6}22$	$P\bar{6}\bar{2}$	$p\bar{6}\bar{2}$	ab, bc
L_{77}	$p\bar{6}mm$	183	$P\bar{6}mm$	$P\bar{6}$	$p\bar{6}$	a, b
L_{78}	$p\bar{6}m2$	187	$P\bar{6}m2$	$P\bar{3}2$	$p\bar{3}2$	a, b, c
L_{79}	$p\bar{6}2m$	189	$P\bar{6}2m$	$H\bar{3}2$	$h\bar{3}2$	a, b, c
L_{80}	$p\bar{6}/mmm$	191	$P\bar{6}/mmm$	$P\bar{6}2$	$p\bar{6}2$	a, b, c



Conclusions

- We have devised a **new Clifford geometric algebra representation** for the 162 subperiodic space groups using versors (Clifford group, Lipschitz elements).
- In the future this may be extended to **magnetic** subperiodic space groups, the sign of the generators may achieve that.
- We expect that the present work forms a suitable foundation for **interactive visualization** software of subperiodic space groups [5].

Future work

Preview of how the rod groups 13: $\overline{2}\overline{2}\overline{2}$ and 14: $\overline{2}_1\overline{2}\overline{2}$, and the layer group 11: $p1$ and might be **visualized** in the future, based on the Space Group Visualizer.

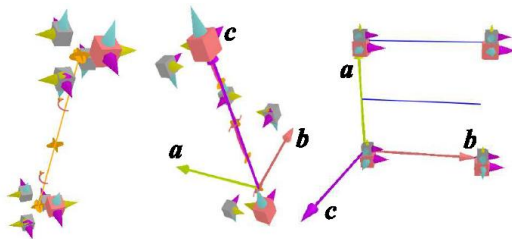


Fig. 5 How a future subperiodic space group viewer software might depict rod groups 13: $\overline{2}\overline{2}\overline{2}$ and 14: $\overline{2}_1\overline{2}\overline{2}$, and the layer group 11: $p1$, based on [5].



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



D. Hestenes, *Point Groups and Space Groups in Geometric Algebra*, in L. Dorst, et al (eds.), AGACSE, Birkhäuser, Boston, 3–34 (2002).



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



D. Hestenes, H. Li, A. Rockwood, New Algebraic Tools for Classical Geometry, in G. Sommer (ed.), *Geometric Computing with Clifford Algebras*, Springer, Berlin, 4–26, (2001).



E. Hitzer, C. Perwass, *The Space Group Visualizer*, Proceedings of ISAMPE, 172–181 (2006). Compare the companion paper: *Interactive 3D Space Group Visualization with CLUCalc based on Geometric Algebra*. Space Group Visualizer, www.spacegroup.info (2005).



D. Ichikawa, E. Hitzer, *Symmetry of orthorhombic materials and interactive 3D visualization in Geometric Algebra*, Proc. of ISAMPE, 302–312 (2007).



V. Kopsky, D. B. Litvin, (eds.), *Int. Tables for Crystallography*, 1st ed., Vol. E, Kluwer, Dordrecht, 2002.



The Holy Bible, New Int. Version Int. Bible Society, Colorado Springs, 1984.

News about Clifford Geometric Algebra

GA-Net

Electronic newsletter:

<http://sinai.mech.fukui-u.ac.jp/GA-Net/index.html>

GA-Net Updates (blog)

Immediate access to latest GA news:

<http://gaupdate.wordpress.com/>

Soli Deo Gloria

J. S. Bach (Leipzig)