

# Lattices of subgroups of $N$ -dimensional space groups

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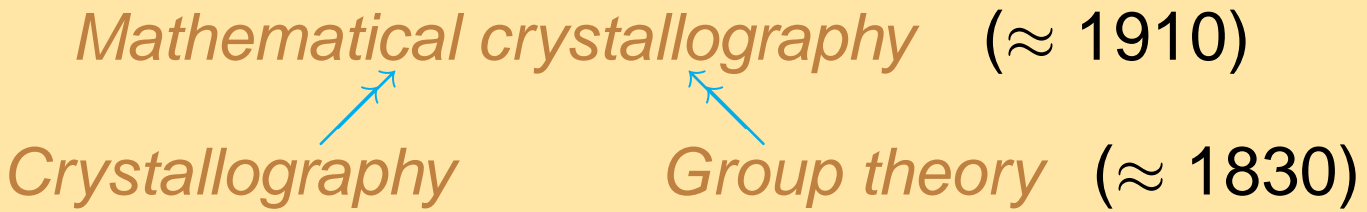
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- Historical remarks
- Formulation of the problem
- Lattice of pairs
- Finite quotient  $\mathcal{L}(\mathcal{G} : \mathcal{H})$
- Illustrative examples
- Summary

# Historical remarks



1890-1 - 230 space groups

Fedorov, Schönflies

1880 - Jordan-Minkowski theorem

Jordan

! finitely many classes of finite integral  $N \times N$  matrix groups

1900 - 18<sup>th</sup> Hilbert problem: ? finite number of space groups (SG) in an  $N$ -dimensional Euclid's space

1912 - YES

Bieberbach

1948 - algorithm to compute  $N$ -dimensional SG

Zassenhaus

1968 - cohomology approach ( $H^1(G, V_n/T_G)$ )

Ascher & Janner

dimension $N$	2	3	4*	5**	6**
arithmetic classes	13	73	710	6 079	85 311
affine classes : SG types	17	219 : 230	4 783 : 4 895	222 018 : -	28 927 922 : -

\* Brown *et al.* (1978)

\*\* Plesken and Schultz (2000)

# Why subgroups of $N$ -dimensional space groups ?

1. “Though this be madness  
yet there is method in’t” (Shakespeare, Hamlet, II.2)

Hermann's theorem on subgroups (C. Hermann, 1929)  
equiclass vs. equitranslational subgroups

2. Isotropy subgroups of a space group  $\mathcal{G} \implies$   
possible low-symmetry phases ( $N = 3$  Hatch and Stokes, 1988)

3. Site-point groups  $\leftrightarrow$  Wyckoff positions in  $N$  dimensions  $\rightarrow$   
structural models of quasicrystals ( $N > 3$  Duneau and Katz, 1985)  
 $N=4$ : dodecagonal ones (Shechtman *et al.*, 1984)

4. Subperiodic groups  $\rightarrow$  superspace description of homologous families of modulated structures ( $N > 3$  Perez-Mato, 1999)  
 $N=4$ :  $\gamma$ -Na<sub>2</sub>CO<sub>3</sub> ... superspace symmetry (de Wolf, 1974)

# Formulation of the problem

Period 1960 - 1990

- revival of C. Herrman's study (Herrman, 1929)

Landau theory of structural phase transitions  $\mathcal{G} \searrow \mathcal{F}$  (Landau, 1937)

prototypic symmetry  $\mathcal{G}$  + order parameter  $\chi \rightarrow$   
symmetry  $\mathcal{F}$  of a distorted phase ... ? ... isotropy subgroup

criteria for low symmetry  $\mathcal{F}$  (Birman and Goldrich, 1968; Ascher, 1977)

1. chain subduction c. }  
2. ker - core c. } ← group-to-subgroup relationships

⇒ numerous tables, mostly not very intelligible ones

most complex - 15.239 isotropy subgroups of 230 space groups

(Hatch and Stokes, 1988)

!!! no information on group-to-subgroup relationships needed  
for checking subgroup chains  $\mathcal{F}_{i_1} \supset \mathcal{F}_{i_2} \supset \dots$  in parent group  $\mathcal{G}$

# $N$ -dimensional space groups

Space group  $\mathcal{G} = (G, T, O, u) \subset \mathcal{E}_N = V_N \wedge O(N)$

$T = \mathcal{G} \cap V_N \dots$  discrete translation group,  $\dim T = N \rightarrow$  finite

Bravais group  $B(T) \subset O(N)$

point group  $G \subseteq B(T) \leftrightarrow T \dots G$ -invariant,  $G \simeq \mathcal{G}/T$

$\implies$  crystallographic pair  $(G, T) \leftrightarrow$  arithmetic class of  $\mathcal{G}$

$$\mathcal{G} = \{e|0\}T + \{g_2|u(g_2)\}T + \dots + \{g_p|u(g_p)\}T, \quad p = |G|$$

$u: G \longrightarrow V_n \dots$  system of non-primitive translations w.r.t. to  $O$

$$g_i u(g_j) - u(g_i g_j) + u(g_i) = 0 \pmod T, \quad g_i, g_j \in G$$

$\dots$  Frobenius congruences

$N$ -dimensional SGs  $\sim$  solutions of Frobenius cng. for all non-equivalent pairs  $(G, T) \longrightarrow$  Zassenhaus algorithm

$\dots$  applied for  $N = 4$  (Brown, Bülow, Neubüser, Wondratschek & Zassenhaus, 1978)

# Subgroups

## Subgroup congruences (Senechal, 1980)

any of infinitely many subgroups  $\mathcal{H}$  of  $\mathcal{G}$  fulfill conditions (i)-(iii)

$$\mathcal{H} = (H, T_H, O, u_H) \subseteq \mathcal{G} = (G, T, O, u) \Leftrightarrow$$

$$(i) H \subseteq G, \quad (ii) T_H \subseteq T$$

$$(iii) u(h) - u_H(h) = 0 \pmod{T_H}, \quad h \in H$$

$(N+1)$  classes of subgroups  $\mathcal{H} = (H, T_H, O, u_H) \subseteq \mathcal{G}$

(1)  $\dim T_H = 0 \sim$  site point groups (Fuksa & Engel, 1994)

(2), ..., (N)  $\dim T_H \in \{1, 2, \dots, N-1\} \sim$  subperiodic groups

$(N+1)$   $\dim T_H = N \sim$  space groups (Fuksa & Engel to appear)

# Lattices of subgroups of space groups

Subgroups of  $\mathcal{G}$  form **lattice**  $\mathcal{L}(\mathcal{G}) = \{\subseteq; \mathcal{F}, \mathcal{H}, \dots\}$  (Birkhoff, 1937)

(i) set-inclusion  $\subseteq$   $\longrightarrow$  partial ordering of subgroups

(ii) binary operations  $\cap$  and  $\cup$ :  $\mathcal{F}, \mathcal{H} \subseteq \mathcal{G}$

$$\mathcal{F} \cap \mathcal{H} \subseteq \mathcal{F}, \mathcal{H} \subseteq \mathcal{F} \cup \mathcal{H}$$

**greatest common subgroup**

**least common supergroup**

**sublattice**  $\mathcal{S} \subset \mathcal{L}(\mathcal{G})$  - subset of  $\mathcal{L}(\mathcal{G})$  closed under both operations

**quotient**  $\mathcal{L}(\mathcal{G} : \mathcal{F})$  - sublattice containing all  $\mathcal{H}, \mathcal{F} \subseteq \mathcal{H} \subseteq \mathcal{G}$

infinite lattice  $\mathcal{L}(\mathcal{G}) \rightarrow (N + 1)^{\text{st}}$  **class** ... closed under  $\cap$  and  $\cup \Rightarrow$

**lattice**  $\mathcal{L}_{\text{fi}}(\mathcal{G})$  of all subgroups of finite index ... **still infinite**  $\longrightarrow$

*Problem:*

**For a given space group  $\mathcal{H}$ , contained in  $\mathcal{G}$ ,  
determine finite quotient  $\mathcal{L}_{\text{fi}}(\mathcal{G} : \mathcal{H}) = \mathcal{L}(\mathcal{G} : \mathcal{H})$**

# Lattice $\mathcal{L}(G, T)$ of pairs

$P(G', T')$  - set of all pairs  $(G', T')$

...  $T'$  - discrete  $N$ -dimensional subgroup of  $V_N$

...  $G' \subseteq B(T') \longleftrightarrow T'$  -  $G'$ -invariant

partial ordering  $\leq$  on  $P(G', T')$

$$(H_1, T_1) \leq (H_2, T_2) \Leftrightarrow H_1 \subseteq H_2, T_1 \subseteq T_2$$

... *minimal element*  $(C_1, 0)$

lattice  $\mathcal{L}(G, T) = \{(G', T'); (G', T') \leq (G, T)\}$

binary operations  $\wedge$  and  $\vee$ :

$$(H_1, T_1) \wedge (H_2, T_2) = (H_1 \cap H_2, T_1 \cap T_2)$$

$$(H_1, T_1) \vee (H_2, T_2) = (H_1 \cup H_2, \overline{(T_1 \cup T_2)}^{H_1 \cup H_2})$$

$\overline{(T_1 \cup T_2)}^{H_1 \cup H_2}$  -  $(H_1 \cup H_2)$ -closure of  $T_1 \cup T_2$

$\sim$  the smallest  $(H_1 \cup H_2)$ -invariant supergroup of  $T_1 \cup T_2$



# Finite quotient $\mathcal{L}(\mathcal{G} : \mathcal{H})$

$$\mathcal{H} = (H, T_H, O, u_H) \subseteq \mathcal{G} = (G, T, O, u)$$

*8-step algorithm:*

1)  $\mathcal{L}(G)$ ,  $G$  - **finite**

2)  $F' ? F' \supseteq H \rightarrow \mathcal{L}(G : H)$

3)  $\mathcal{L}(T : T_H) \simeq \mathcal{L}(T/T_H)$ , factor group  $T/T_H$  - **finite Abelian**

4)  $T' ? B(T') \supseteq H$

5) *basic quotient*  $\mathcal{L}((G, H) : (T, T_H))$

6)  $(F, T_F) \in \mathcal{L}((G, H) : (T, T_H)) \dots$  solutions of coupled Frobenius and subgroup cng  $\Rightarrow$  subgroups  $\mathcal{F}_i \sim (F, T_F)$  of  $\mathcal{G}$

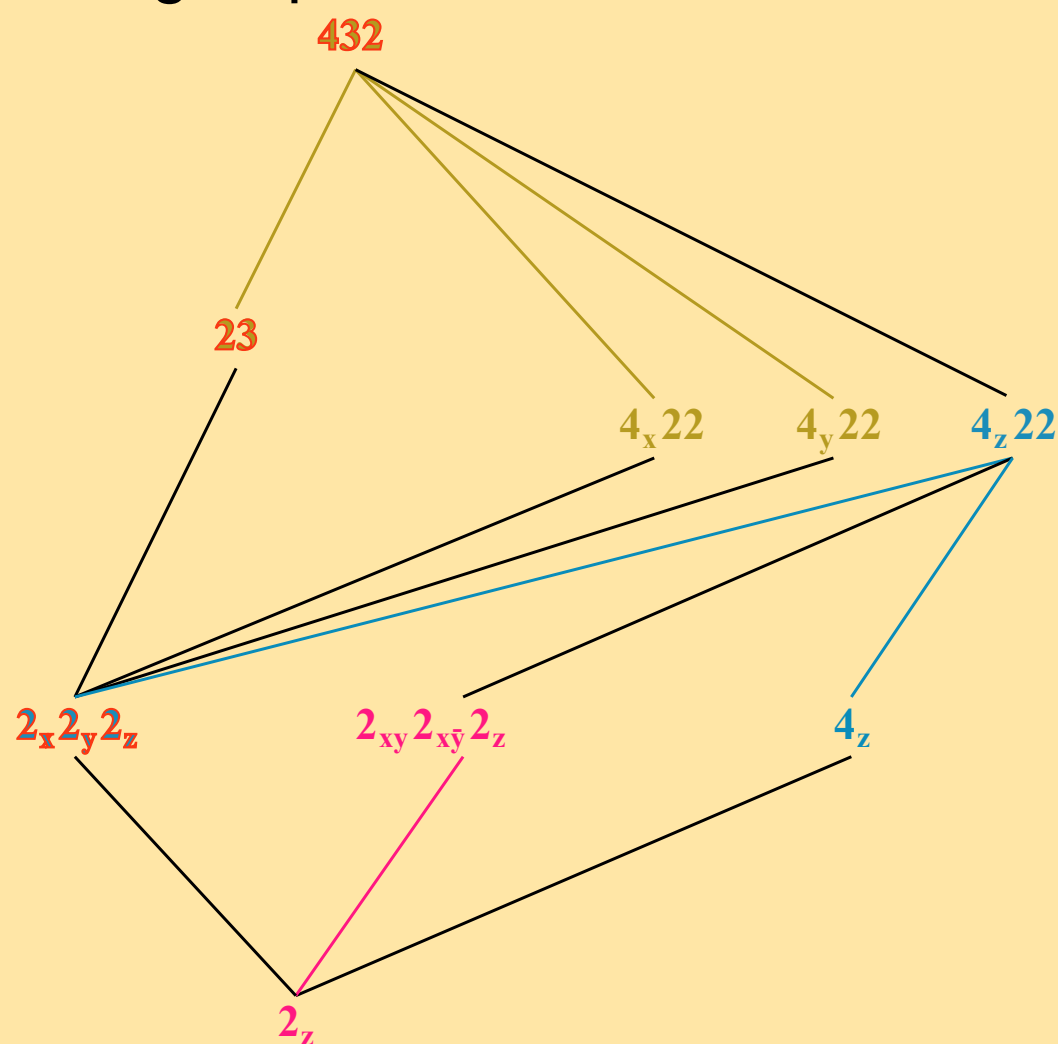
7)  $\mathcal{F}' ? \mathcal{F}' \supseteq \mathcal{H} \rightarrow$  **all SG**  $\mathcal{K}$ ,  $\mathcal{H} \subseteq \mathcal{K} \subseteq \mathcal{G}$

8) **!  $\mathcal{F} \subset \mathcal{K}$  !** - check subgroup cng for any  $\mathcal{F}, \mathcal{K} \supset \mathcal{H} \rightarrow \mathcal{L}(\mathcal{G} : \mathcal{H})$

# Illustrative examples

A.  $\mathcal{G} = 207.P432$ ,  $\mathcal{H} = 5.A112$ ,  $A(\mathbf{a} + \mathbf{b}, 4\mathbf{b}, 4\mathbf{c})$

(1) Point groups:



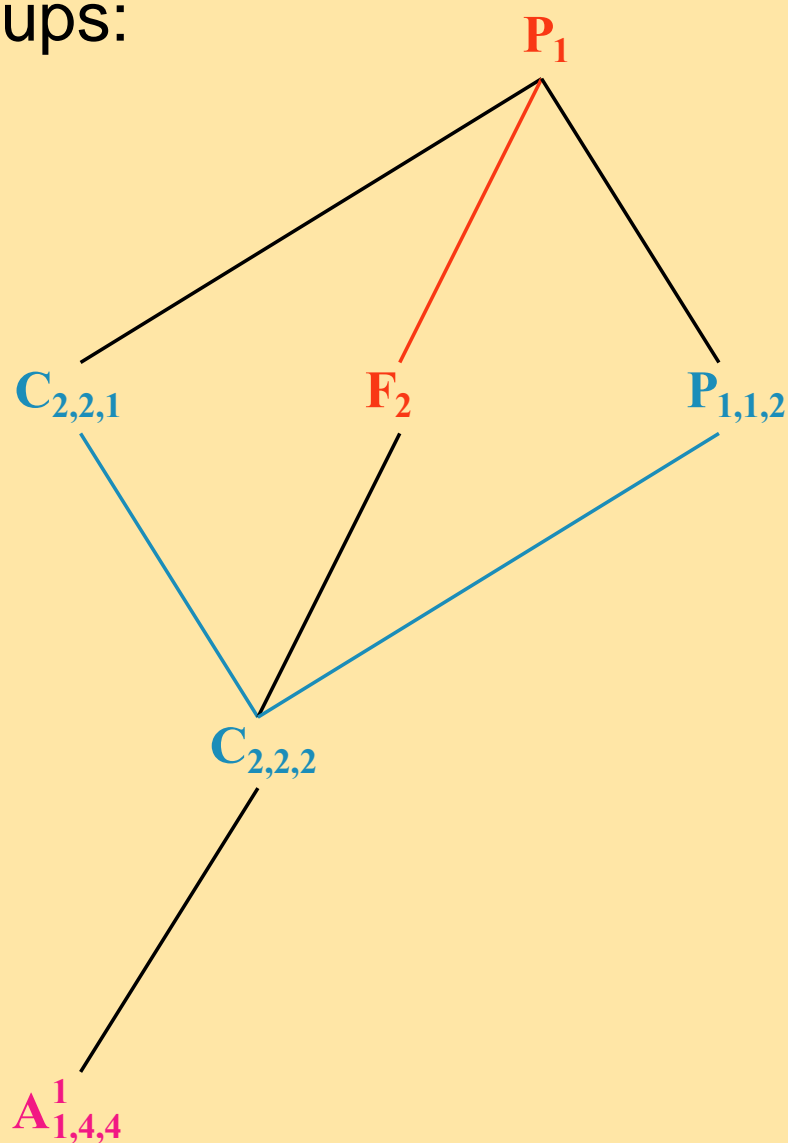
an upward line:  
links a group to  
minimal supergroup

a downward line:  
links a group to  
maximal subgroup

maximal chain —  
several consecutive  
lines

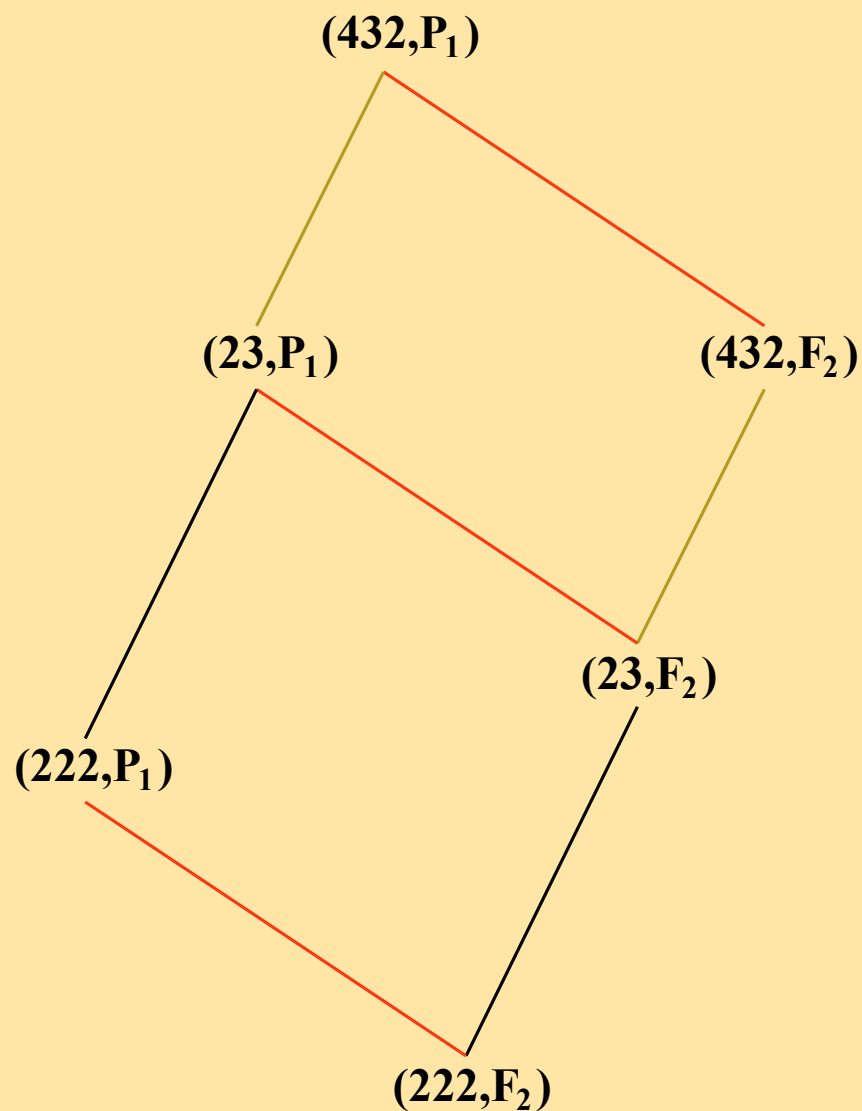
The quotient  $\mathcal{L}(432; 2_z)$ : sublattices  $\mathcal{L}(4_z22; 2_z)$  and  $\mathcal{L}(2_{xy}2_{x\bar{y}}2_z; 2_z)$ .

(2) Translation groups:



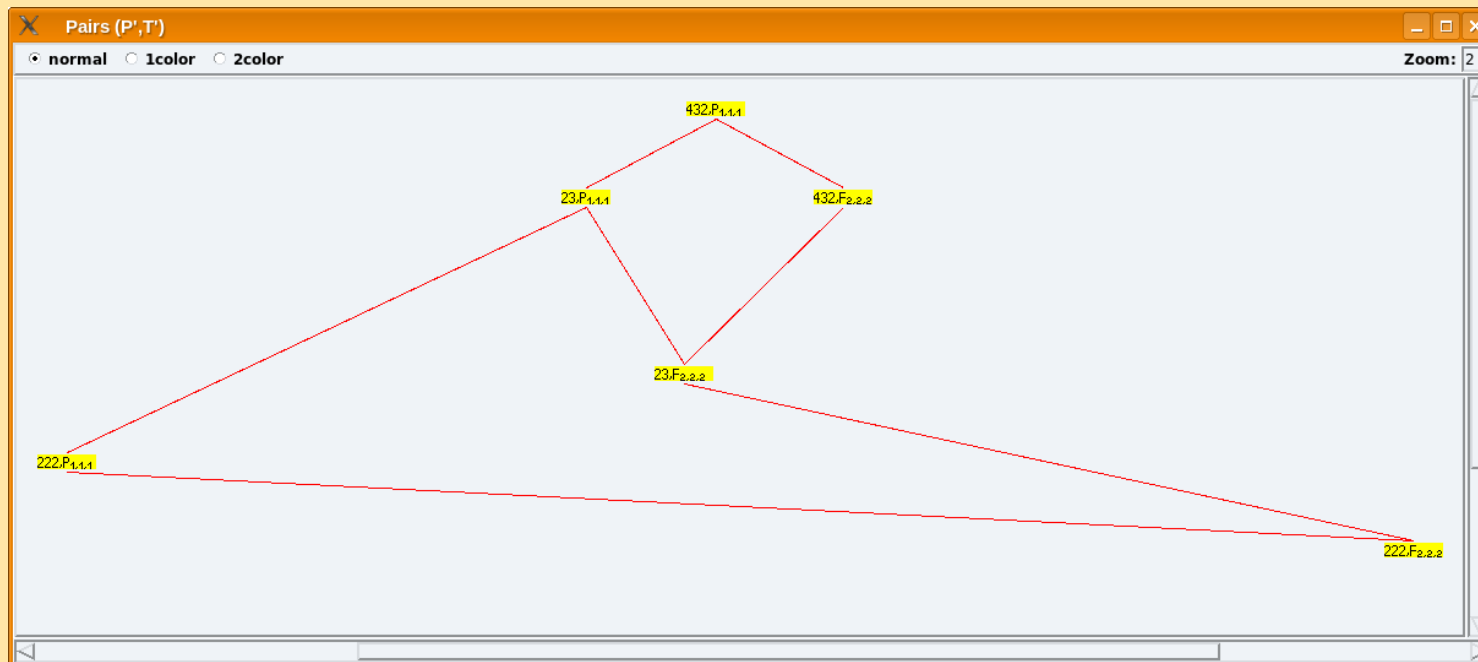
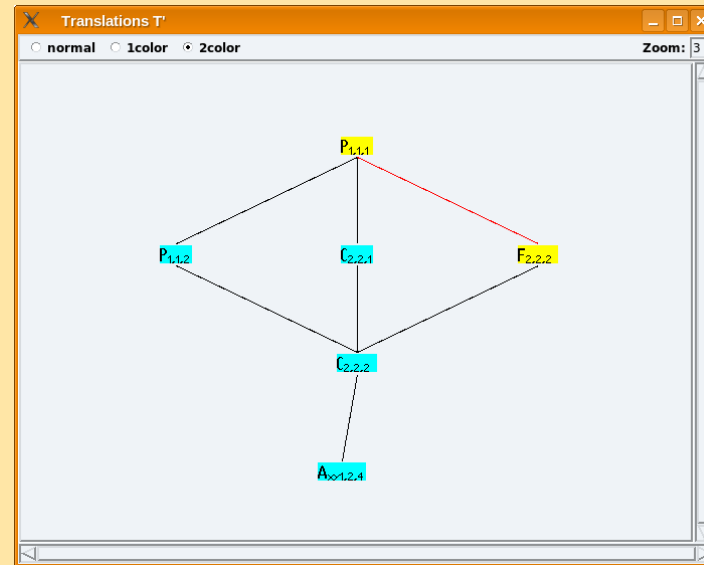
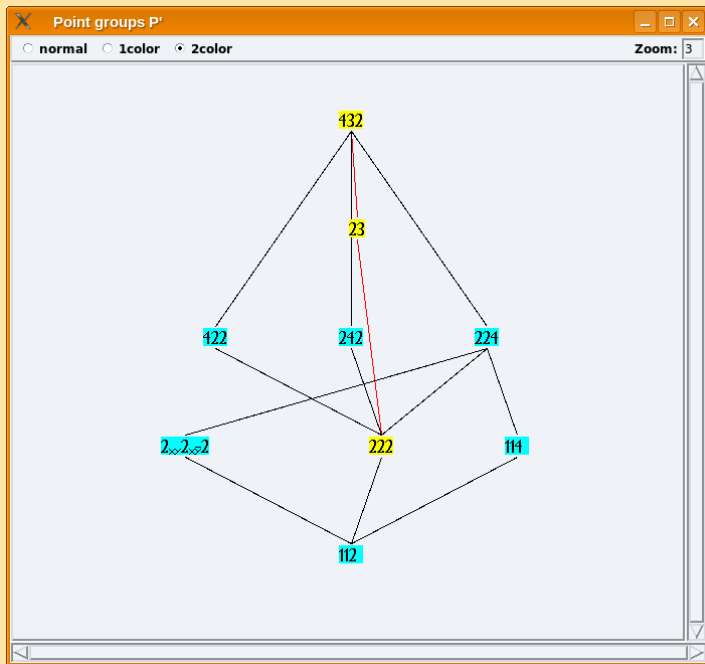
The quotient  $\mathcal{L}^{2z}(P_1; A_{1,4,4}^1)$ : sublattices  $\mathcal{L}(P_1; C_{2,2,2})$  and  $\mathcal{L}(P_1; F_2)$ .

(3) Pairs associated with normal subgroups:

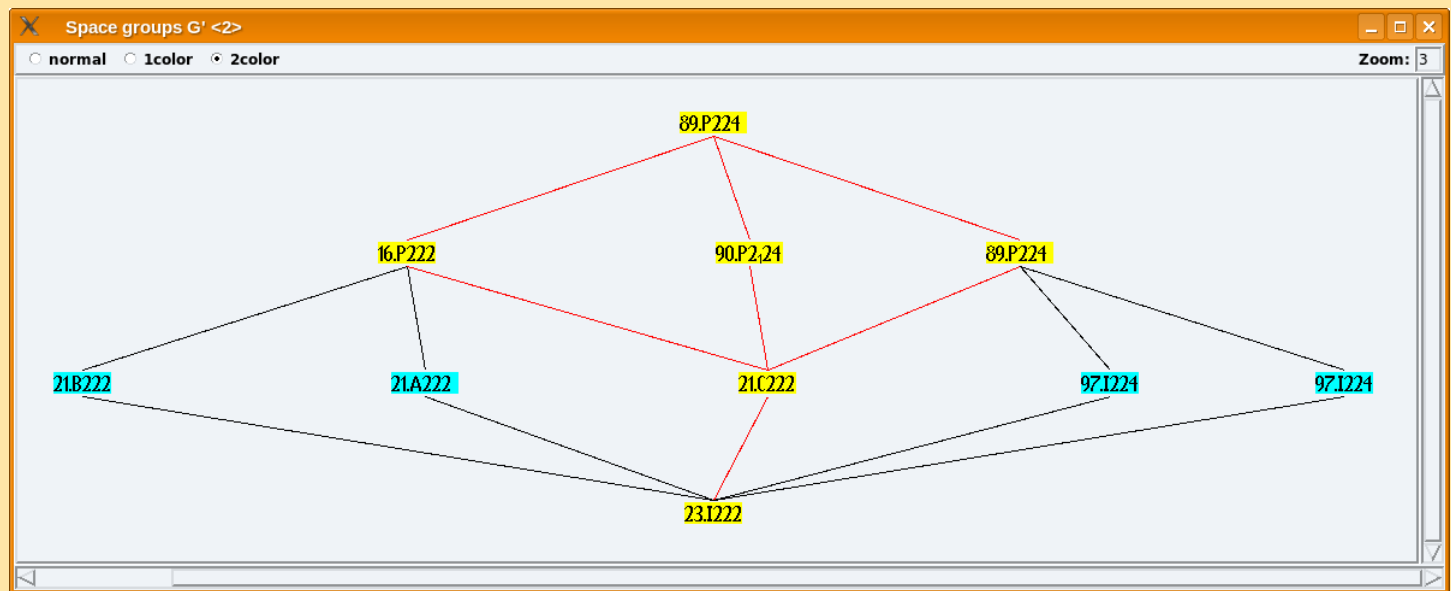
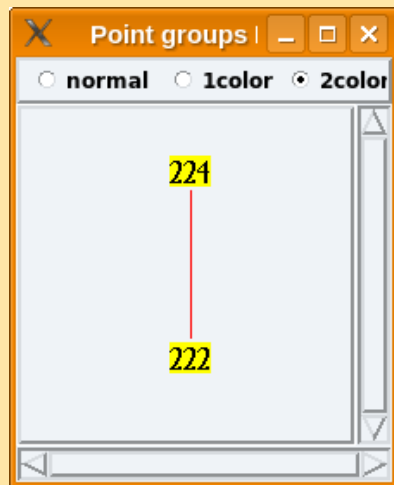
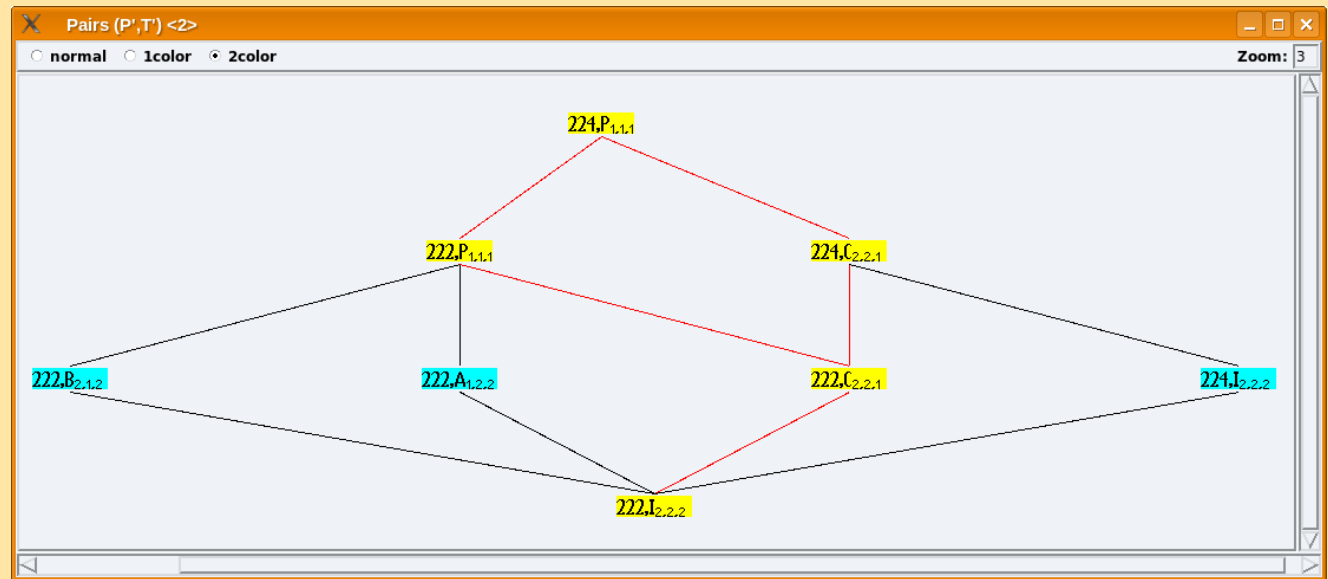
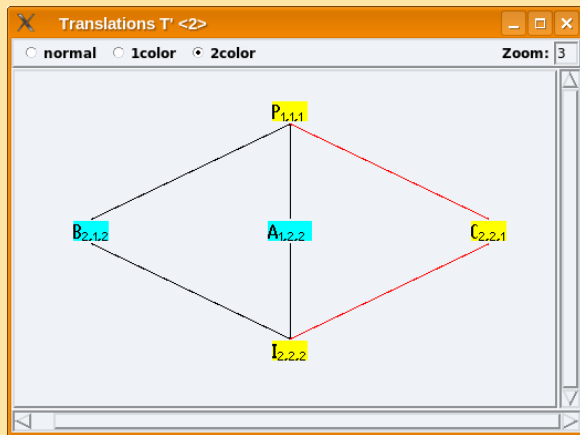


The quotient  $\mathcal{L}^I(432, P_1; 222, F_2) = \mathcal{L}^N(432; 222) \times \mathcal{L}(P_1; F_2)$ .

# Visualization in the program:



B.  $\mathcal{G} = 89.P224$ ,  $\mathcal{H} = 23.I222$ ,  $I(2a, 2b, 2c)$



C.  $\mathcal{G} = 150.P321$ ,  $\mathcal{H} = 1.P1$ ,  $C_{3,3,1} \sim a + 2b, -2a - b, c$

Interactive input:

The image shows five interactive windows from a software application:

- Space Group:** A dialog box with radio buttons for "primitive basis of transl. group" (selected) and "conventional basis of transl. group". It has a "number of generators" field set to 2 and buttons for "Generators", "Save", and "Close".
- Lattice of subgroups:** A dialog box with tabs for "Message", "SPACEGROUP", "SUBGROUP", and "Run". It contains fields for "dimension" (3), "space group symbol" (P321), "output file" (p321\_p1.c331), and "subgroup symbol" (P1-C\_3,3,1). Buttons include "OK" and "Clear".
- Subgroup:** A dialog box with radio buttons for "primitive basis of supergroup lattice" (selected), "primitive basis of subgroup lattice", "conventional basis of supergroup lattice", and "conventional basis of subgroup lattice". It has a "number of generators" field set to 1 and buttons for "Generators", "Save", and "Close".
- 1. generator of the supergroup:** A dialog box with a 3x3 matrix of input fields. The values are:
 

0	-1	0		0
1	-1	0		0
0	0	1		0

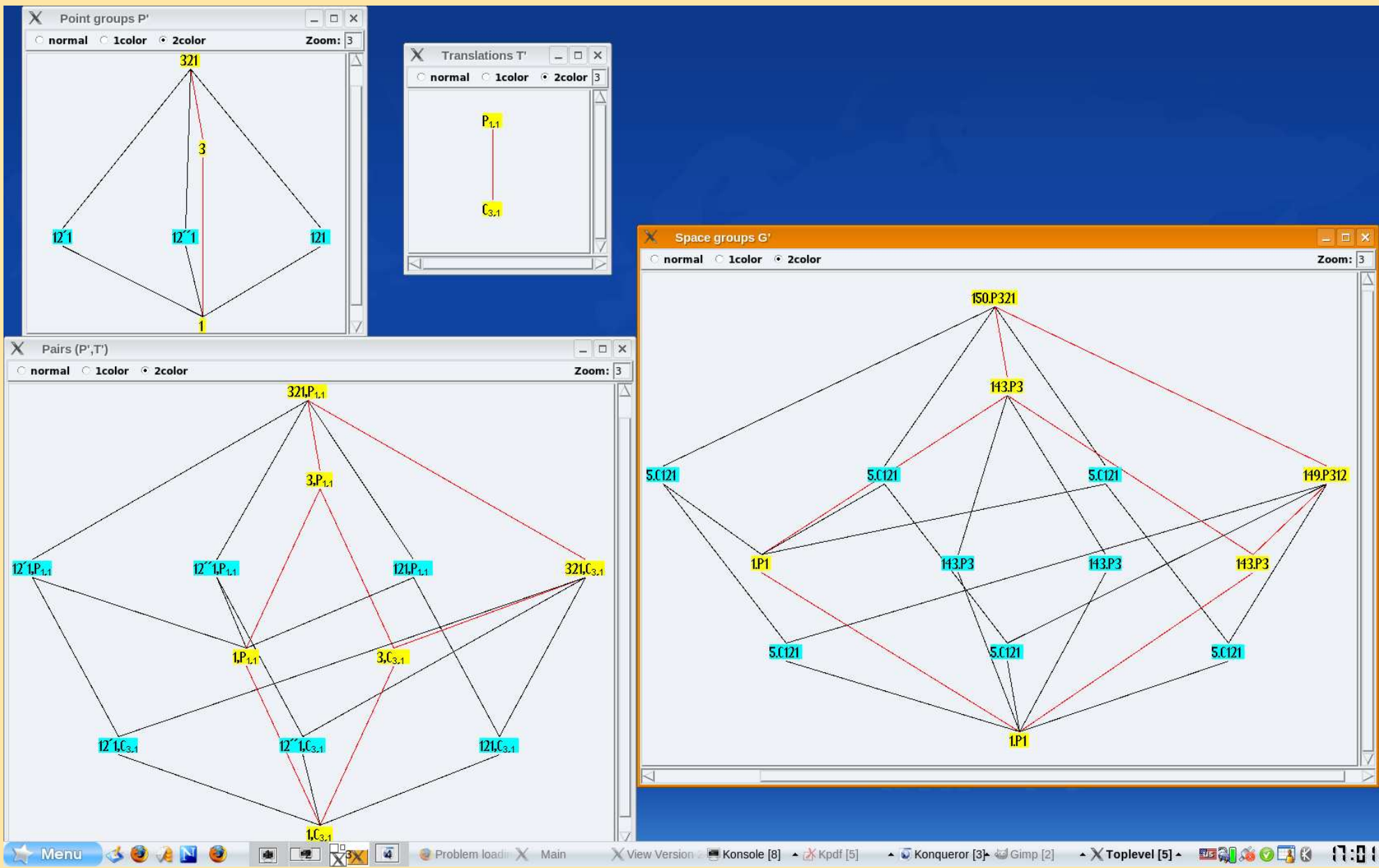
 Buttons include "OK", "Restore", "Clear", and "Close".
- Enter 2.generator of the supergroup:** A dialog box with a 3x3 matrix of input fields. The values are:
 

-1	0	0	0
-1	1	0	0
0	0	-1	0

 Buttons include "OK", "Restore", "Clear", and "Close".

# Program output:

Rem.  $\Gamma (0, 0, 0) - P_{1,1}, \quad K (\frac{1}{3}, \frac{1}{3}, 0) - C_{3,1}$





# Info provided on mouse click:

**Space groups G'**

normal 1color 2color Zoom: 3

**node information**

subgroup No. 8: 143P3  
P: 3 T:  $C_{3v}$   
index 6  
order of point group: 3  
index of sublattice: 3

transformation matrix  
 $\begin{pmatrix} 1 & 2 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

number of generators: 1  
generator No. 1  
order: 3  
determinant: 1  
dimension of support: 1  
 $\begin{pmatrix} 0 & -1 & 0 & 1 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

number of subgroups: 1  
1P1  
number of supergroups: 1  
143P3

**node information**

subgroup No. 10: 143P3  
P: 3 T:  $C_{3v}$   
index 6  
order of point group: 3  
index of sublattice: 3

transformation matrix  
 $\begin{pmatrix} 1 & 2 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

number of generators: 1  
generator No. 1  
order: 3  
determinant: 1  
dimension of support: 1  
 $\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

number of subgroups: 1  
1P1  
number of supergroups: 2  
143P3, 149P312

**node information**

subgroup No. 6: 149P312  
P: 321 T:  $C_{3v}$   
index 3  
order of point group: 6  
index of sublattice: 3

transformation matrix  
 $\begin{pmatrix} 1 & 2 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

number of generators: 2  
generator No. 1  
order: 3  
determinant: 1  
dimension of support: 1  
 $\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

generator No. 2  
order: 2  
determinant: 1  
dimension of support: 1  
 $\begin{pmatrix} -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$

number of subgroups: 4  
143P3, 5C121, 5C121, 5C121

number of supergroups: 1  
150P321

**node information**

subgroup No. 9: 143P3  
P: 3 T:  $C_{3v}$   
index 6  
order of point group: 3  
index of sublattice: 3

transformation matrix  
 $\begin{pmatrix} 1 & 2 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

number of generators: 1  
generator No. 1  
order: 3  
determinant: 1  
dimension of support: 1  
 $\begin{pmatrix} 0 & -1 & 0 & 2 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

number of subgroups: 1  
1P1  
number of supergroups: 1  
143P3

**node information**

sublattice No. 2:  $C_{3v}$   
index 3  
index of sublattice: 3

transformation matrix  
 $\begin{pmatrix} 1 & 2 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

number of supergroups: 1  
 $P_{3v}$

**Point groups P'**

normal 1color 2color zoom 2

subgroup No. 4:  $121$   
index 3  
order of point group: 2

number of generators: 1  
generator No. 1  
order: 2  
determinant: 1  
dimension of support: 1  
 $\begin{pmatrix} 1 & -1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

number of subgroups: 1  
1  
number of supergroups: 1  
321

**node information**

subgroup No. 3:  $121$   
index 3  
order of point group: 2

number of generators: 1  
generator No. 1  
order: 2  
determinant: 1  
dimension of support: 1  
 $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

number of subgroups: 1  
1  
number of supergroups: 1  
321

# Isotropy subgroups of 150. $P321$

Hatch & Stokes (1988)

$$\Gamma (0,0,0) - P_{1,1}, \quad A (0,0,\frac{1}{2}) - P_{1,2}, \quad K (\frac{1}{3},\frac{1}{3},0) - C_{3,1}, \quad H (\frac{1}{3},\frac{1}{3},\frac{1}{2}) - C_{3,2}$$

correct relationships  
yourself  
http://www.crystallography.net

150  $D_3^2$   $P321$

$\Gamma_1$	$A1a$	1	0	150	$D_3^2$	$P321$	nf	$P1$	1	(1, 0, 0), (0, 1, 0), (0, 0, 1)	(0, 0, 0)
$\Gamma_2$	$A2a$	0	0	143	$C_3^1$	$P3$	pfc	$P1^{**}$	1	(1, 0, 0), (0, 1, 0), (0, 0, 1)	(0, 0, 0)
$\Gamma_3$	$B6a$	1	1	5	$C_2^3$	$C2$	pfc,pfs	$P1$	1	(2, 1, 0), (0, $\bar{1}$ , 0), (0, 0, $\bar{1}$ )	(0, 0, 0)
					$C_1^1$	$P1$	pfc,pfs	$C1$	1	(1, 0, 0), (0, 1, 0), (0, 0, 1)	(0, 0, 0)
$A_1$	$A2a$	0	0	150	$D_3^2$	$P321$	nf	$P1^{**}$	2	(1, 0, 0), (0, 1, 0), (0, 0, 2)	(0, 0, 0)
$A_2$	$A2a$	0	0	150	$D_3^2$	$P321$	nf	$P1^{**}$	2	(1, 0, 0), (0, 1, 0), (0, 0, 2)	(0, 0, $\frac{1}{2}$ )
$A_3$	$B12a$	0	1	5	$C_2^3$	$C2$	ifc,ifs	$P1$	2	(1, 2, 0), (1, 0, 0), (0, 0, $\bar{2}$ )	(0, 0, 0)
					$C_2^3$	$C2$	ifc,ifs	$P2$	2	(1, 2, 0), (1, 0, 0), (0, 0, $\bar{2}$ )	(0, 0, $\frac{1}{2}$ )
					$C_1^1$	$P1$	ifc,ifs	$C1$	2	(1, 0, 0), (0, 1, 0), (0, 0, 2)	(0, 0, 0)
$H_1H_1$	$B6b$	0	0	149	$D_3^1$	$P312$	nf	$C1^{**}$	6	(2, 1, 0), ( $\bar{1}$ , 1, 0), (0, 0, 2)	(0, 0, 0)
$H_2H_2$	$B6b$	0	0	149	$D_3^1$	$P312$	nf	$C1^{**}$	6	(2, 1, 0), ( $\bar{1}$ , 1, 0), (0, 0, 2)	(0, 0, $\frac{1}{2}$ )
$H_3H_3$	$D36b$	0	2	143	$C_3^1$	$P3$	ifc	$C1$	6	(2, 1, 0), ( $\bar{1}$ , 1, 0), (0, 0, 2)	( $\frac{1}{3}$ , $\frac{2}{3}$ , 0)
					$C_2^3$	$C2$	ifc,ifs	$C11$	6	(1, 2, 0), (3, 0, 0), (0, 0, $\bar{2}$ )	(0, 0, 0)
					$C_2^3$	$C2$	ifc,ifs	$C15$	6	(1, 2, 0), (3, 0, 0), (0, 0, $\bar{2}$ )	(0, 0, $\frac{1}{2}$ )
					$C_1^1$	$P1$	ifc,ifs	$4D1$	6	(1, $\bar{1}$ , 0), (1, 2, 0), (0, 0, 2)	(0, 0, 0)
$K_1K_1$	$B3a$	2	0	149	$D_3^1$	$P312$	nf	$C1$	3	(2, 1, 0), ( $\bar{1}$ , 1, 0), (0, 0, 1)	(0, 0, 0)
$K_2K_2$	$B6b$	0	0	143	$C_3^1$	$P3$	ifc	$C1^{**}$	3	(2, 1, 0), ( $\bar{1}$ , 1, 0), (0, 0, 1)	(0, 0, 0)
$K_3K_3$	$D18a$	2	2	143	$C_3^1$	$P3$	ifc	$C1$	3	(2, 1, 0), ( $\bar{1}$ , 1, 0), (0, 0, 1)	( $\frac{1}{3}$ , $\frac{2}{3}$ , 0)
					$C_2^3$	$C2$	ifc,ifs	$C11$	3	(1, 2, 0), (3, 0, 0), (0, 0, $\bar{1}$ )	(0, 0, 0)
					$C_1^1$	$P1$	ifc,ifs	$4D1$	3	(1, $\bar{1}$ , 0), (1, 2, 0), (0, 0, 1)	(0, 0, 0)

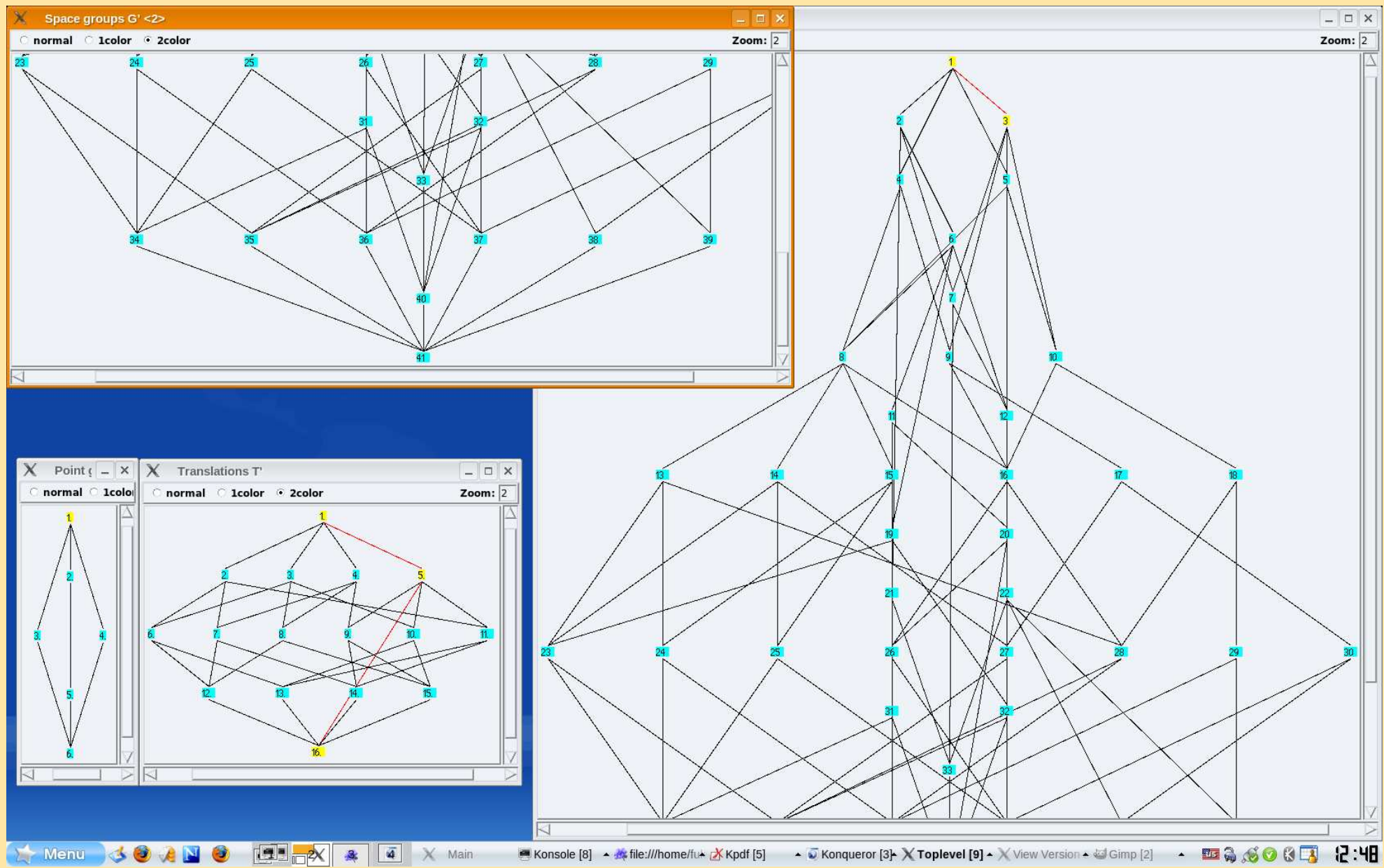
D.  $\dim=4$ :  $\mathcal{G} = P1022$ ,  $\mathcal{H} = P5$ ,  $P_5 \sim 5a, 5b, 5c, 5d$

The screenshot displays a software interface for analyzing space group subgroups. The main window, titled "Space groups G'", shows a Hasse diagram of subgroups for space group  $G' = P1022$ . The subgroups are numbered from 1 to 73. An inset window, titled "Space groups G' <=>", provides a zoomed-in view of a specific part of the diagram, showing subgroups 56 through 73. Several smaller windows provide detailed information for selected subgroups:

- node informations** (sublattice No. 3):
  - sublattice No. 3: 3
  - index 25
  - index of sublattice: 25
  - transformation matrix:
 
$$\begin{pmatrix} 1 & 0 & 2 & 2 \\ 0 & 1 & 3 & 1 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 5 \end{pmatrix}$$
  - number of subgroups: 1
  - 4.
  - number of supergroups: 1
  - 2.
- node information** (subgroup No. 22):
  - subgroup No. 22: 22
  - P: 5 T: 2
  - index 20
  - order of point group: 5
  - index of sublattice: 5
  - transformation matrix:
 
$$\begin{pmatrix} 1 & 0 & 0 & 4 \\ 0 & 1 & 0 & 4 \\ 0 & 0 & 1 & 4 \\ 0 & 0 & 0 & 5 \end{pmatrix}$$
  - number of generators: 1
  - generator No. 1
  - order: 5
  - determinant: 1
  - dimension of support: 0
  - $$\begin{pmatrix} 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \end{pmatrix}$$
  - number of subgroups: 1
  - 39
  - number of supergroups: 12
  - 5, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21
- Point groups P'**:
  - number of subgroups: 1
  - 39
  - number of supergroups: 12
  - 5, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21

The bottom of the screenshot shows a taskbar with various application icons and a system clock displaying 12:06.

E.  $\dim=4$ :  $\mathcal{G} = P5432$ ,  $\mathcal{H} = P4$ ,  $P_5 \sim 5a, 5b, 5c, 5d$



# Summary

(1) For SG  $\mathcal{H} = (H, T_H, O, u_H) \subset \mathcal{G} = (G, T, O, u)$  the software determines 4 quotients:  $\mathcal{L}(\mathcal{G} : \mathcal{H})$ ,  $\mathcal{L}(G : H)$ ,  $\mathcal{L}(T : T_H)$  and  $\mathcal{L}((G, T) : (H, T_H))$ , giving all subgroup chains.

(2) The quotient  $\mathcal{L}(\mathcal{G} : \mathcal{H})$  will include all low-symmetry groups  $\mathcal{F}_j$  of the problem whenever  $\mathcal{H}$  is a maximal  $G$ -invariant translational subgroup of any of them.

(3) The software displays:

(i) the quotient  $\mathcal{L}(\mathcal{H}_1 \cup \mathcal{H}_2 : \mathcal{H}_1 \cap \mathcal{H}_2)$  for any two subgroups  $\mathcal{H}_1$  and  $\mathcal{H}_2$  of  $\mathcal{G}$ .

(ii) the smallest sublattice  $\mathcal{S}_{H', T'}$  of  $\mathcal{L}(\mathcal{G} : \mathcal{H})$  containing all subgroups with same point group  $H'$  and same translational group  $T'$ .

(4) Analogous information is displayed for the normal subgroups.

# Future plans

Possible enhancements, extensions, ...

- more sophisticated procedures for effective calculations in higher dimensions
- identification of possible low-symmetry groups within the quotient  $\mathcal{L}(\mathcal{G} : \mathcal{H})$
- C-program to compute subperiodic subgroups of  $N$ -dimensional SG that would make the collection of C-programs for determining space group subgroups complete