Lattices of subgroups of N-dimensional space groups

Jiří Fuksa* *and Peter Engel**

* Institute of Physics, Academy of Sciences of the Czech Republic, Prague
* Laboratory of Crystallography, University Bern, Switzerland

fuksa@fzu.cz

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

Historical remarks

Mathematical crystallography (≈ 1910)

↗ ↖

Crystallography *Group theory* (≈ 1830)

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^{th} 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 $\mathcal{G} \Longrightarrow$ 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)
$N{=}4$: γ-Na_2CO_3 ... *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.

$\} \leftarrow$ group-to-subgroup relationships

$\Rightarrow$ 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 $\mathcal{F}_{i_1} \supset \mathcal{F}_{i_2} \supset \cdots$ in parent group $\mathcal{G}$

N-dimensional space groups

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

$T = \mathcal{G} \cap V_N$ ... discrete *translation group*, dim $T = N$ $\rightarrow$ finite Bravais group $B(T) \subset O(N)$

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

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

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

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

$$g_i u(g_j) - u(g_i g_j) + u(g_i) = 0 \text{ mod } T\,, \quad g_i, g_j \in G$$

... Frobenius congruences

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

... 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) $H \subseteq G$, (ii) $T_H \subseteq T$

(iii) $u(h) - u_H(h) = 0 \bmod T_H,\ h \in H$

$(N+1)$ 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)

$(2), \ldots, (N)$ $\dim T_H \in \{1, 2, \ldots, N-1\} \sim$ 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 $\mathcal{L}(\mathcal{G}) = \{\subseteq; \mathcal{F}, \mathcal{H}, \ldots\}$ (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 $\mathcal{L}(\mathcal{G}) \rightarrow (N+1)^{\mathrm{st}}$ class $\ldots$ closed under $\cap$ and $\cup$ $\Rightarrow$
lattice $\mathcal{L}_{\mathrm{fi}}(\mathcal{G})$ of all subgroups of finite index $\ldots$ still infinite $\longrightarrow$

Problem:

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

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

$P(G',T')$ - set of all pairs (G',T')
$\ldots T'$ - discrete N-dimensional subgroup of V_N
$\ldots G' \subseteq B(T') \longleftrightarrow T'$ - G'-invariant

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

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

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

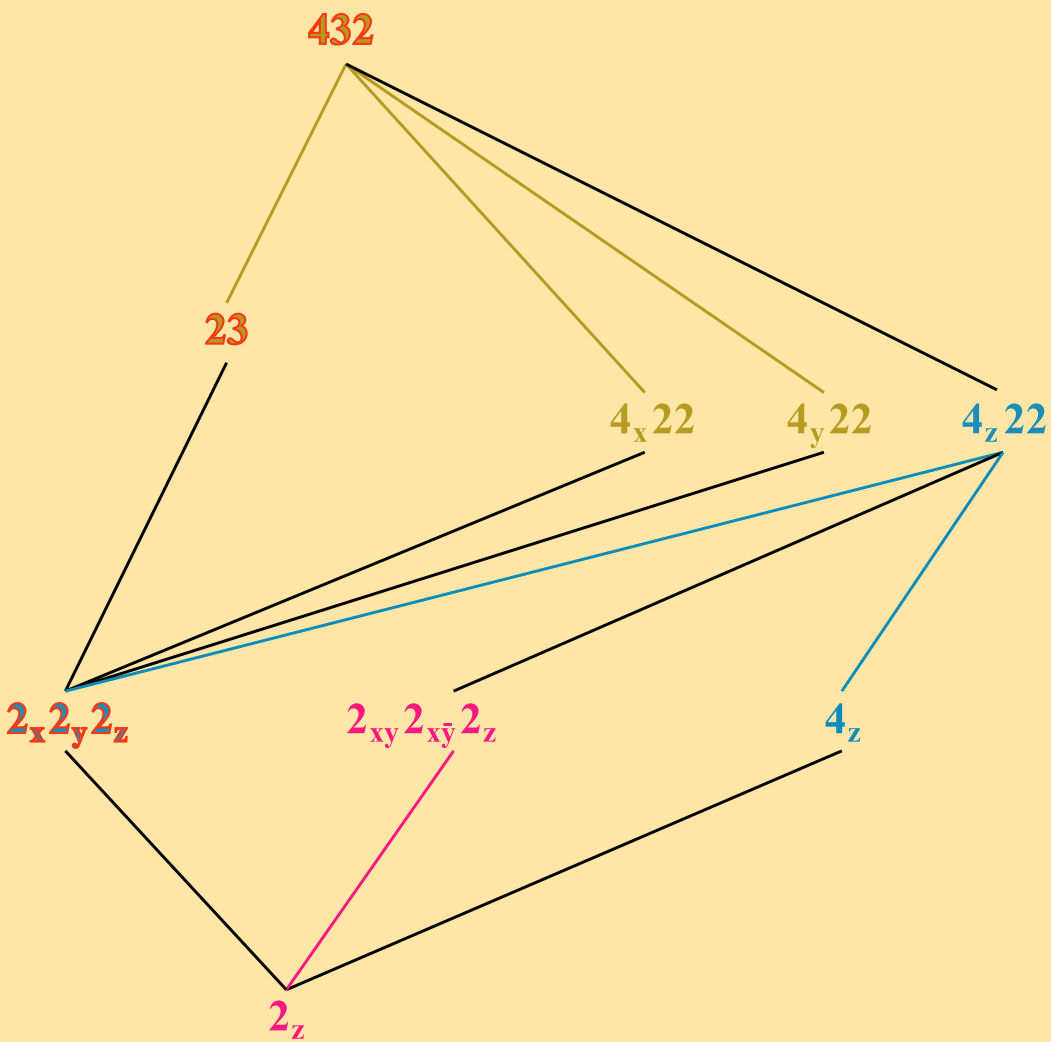
7) $\mathcal{F}'$? $\mathcal{F}' \supseteq \mathcal{H} \rightarrow$ all SG $\mathcal{K}$, $\mathcal{H} \subseteq \mathcal{K} \subseteq \mathcal{G}$

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

(1) Point groups:



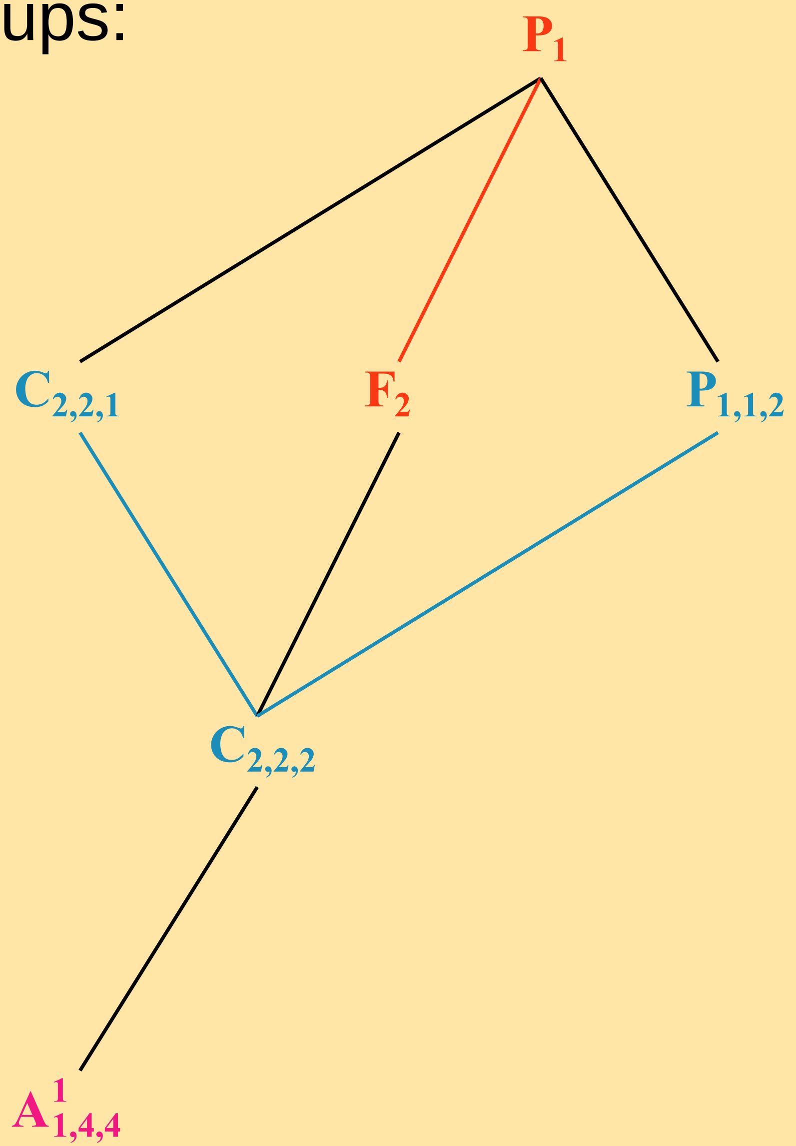
an upward line:
links a group to minimal supergroup

a downward line:
links a group to maximal subgroup

maximal chain –
several consecutive lines

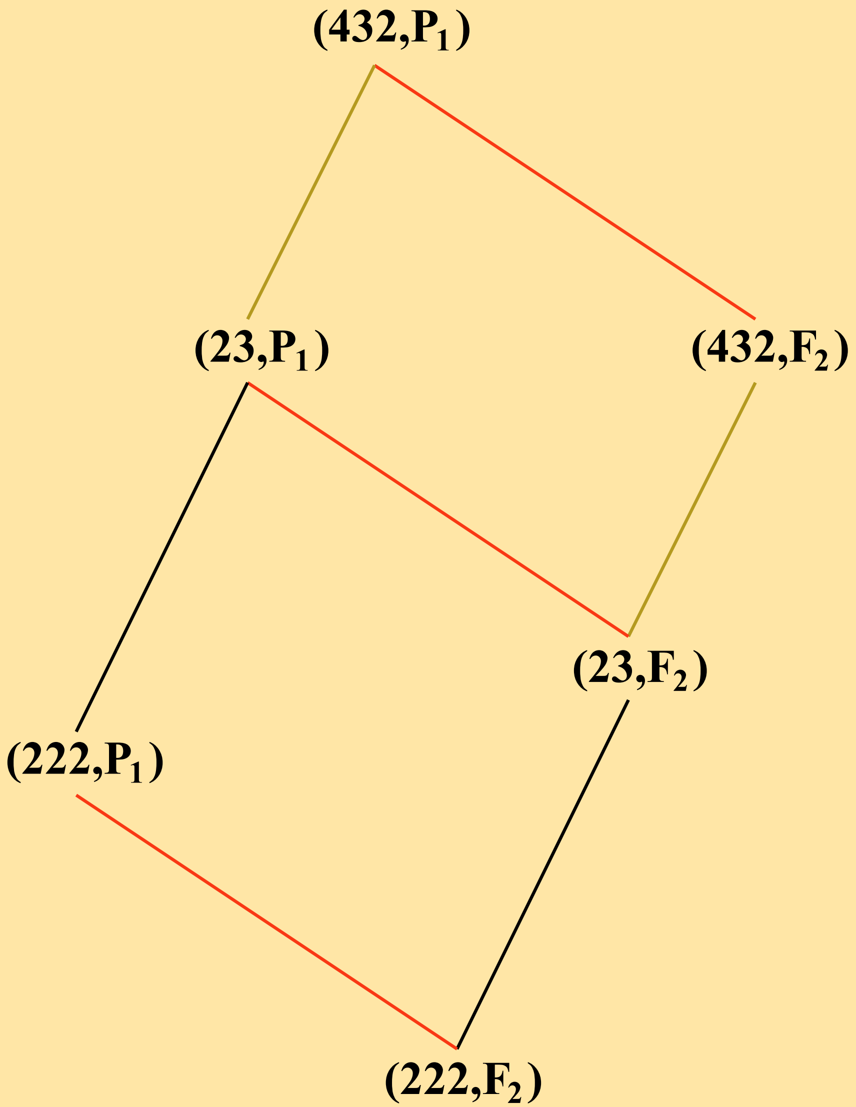
The quotient $\mathcal{L}(432; 2_z)$: sublattices $\mathcal{L}(4_z22; 2_z)$ and $\mathcal{L}(2_{xy}2_{x\bar{y}}2_z; 2_z)$.

(2) Translation groups:



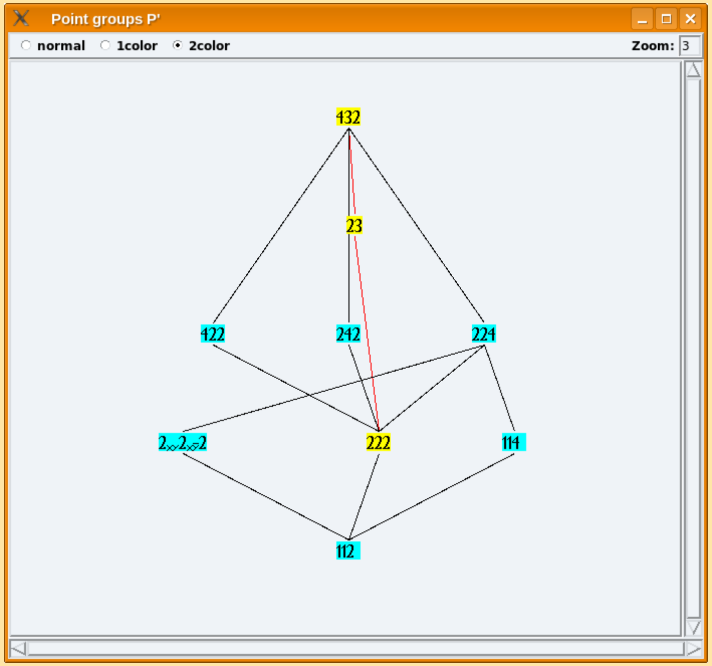
The quotient $\mathcal{L}^{2_z}(P_1; A^1_{1,4,4})$: sublattices $\mathcal{L}(P_1; C_{2,2,2})$ and $\mathcal{L}(P_1; F_2)$.

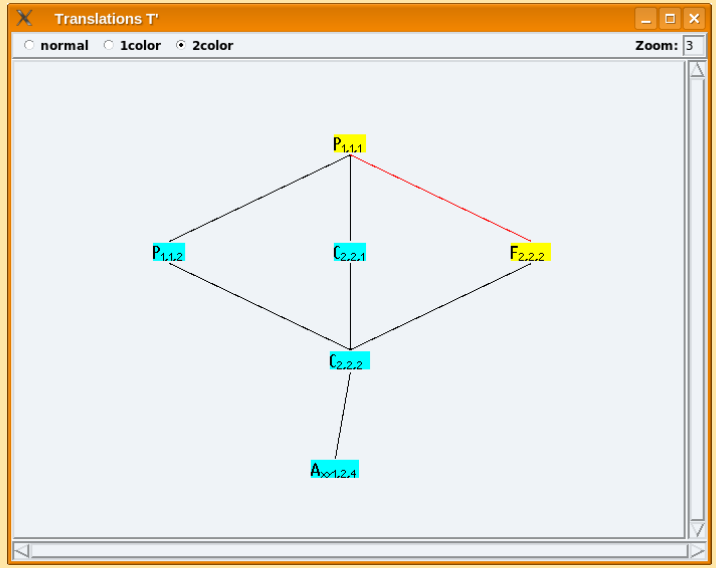
(3) Pairs associated with normal subgroups:

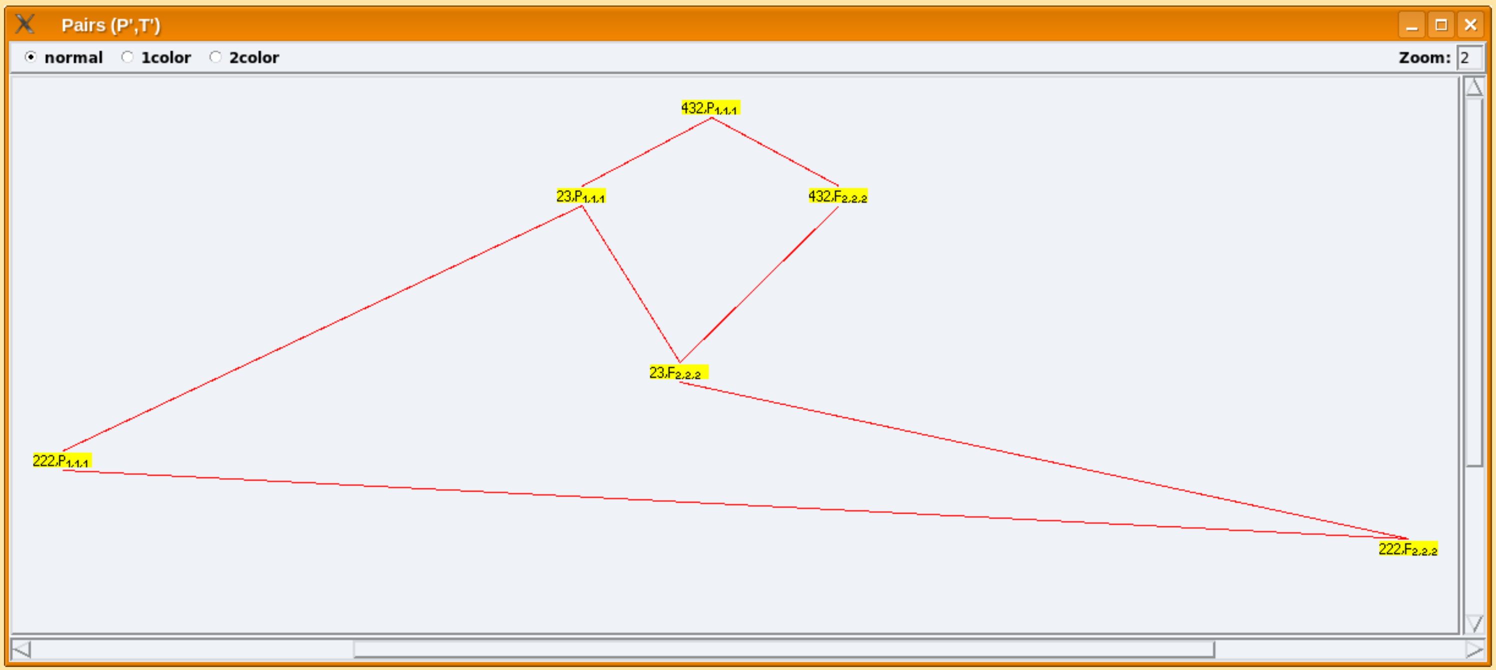


The quotient $\mathcal{L}^I(432, P_1; 222, F_2) = \mathcal{L}^N(432; 222) \times \mathcal{L}(P_1; F_2)$.

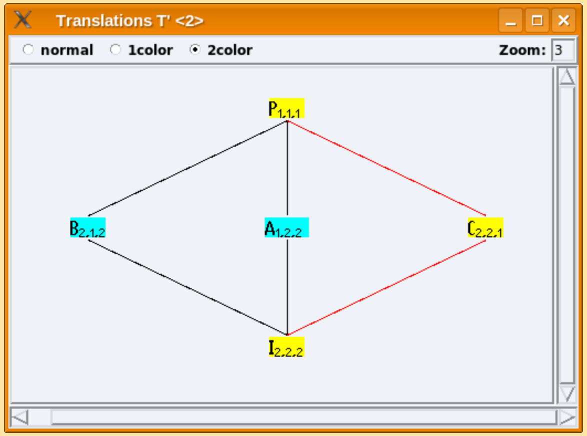
Visualization in the program:

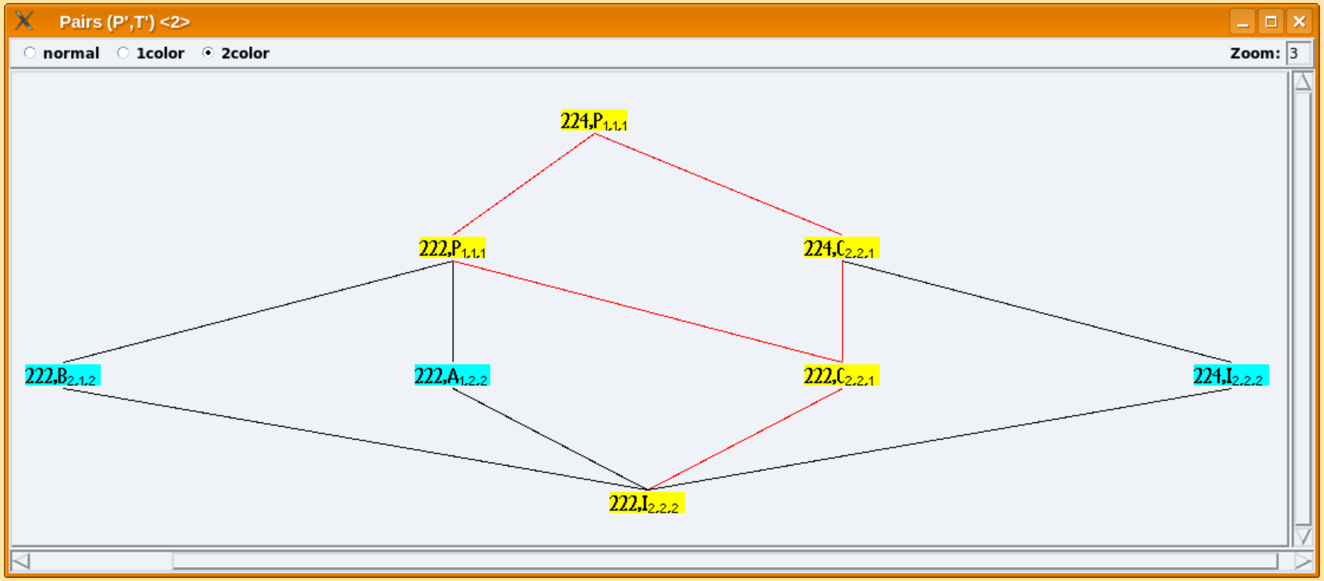


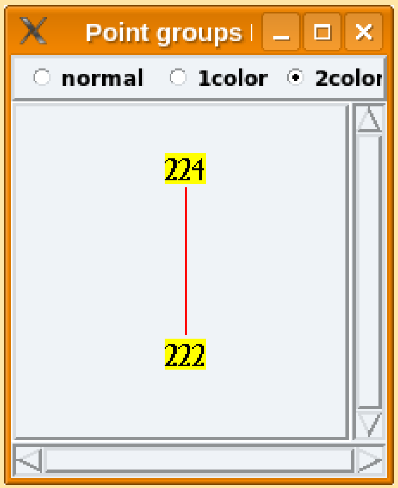


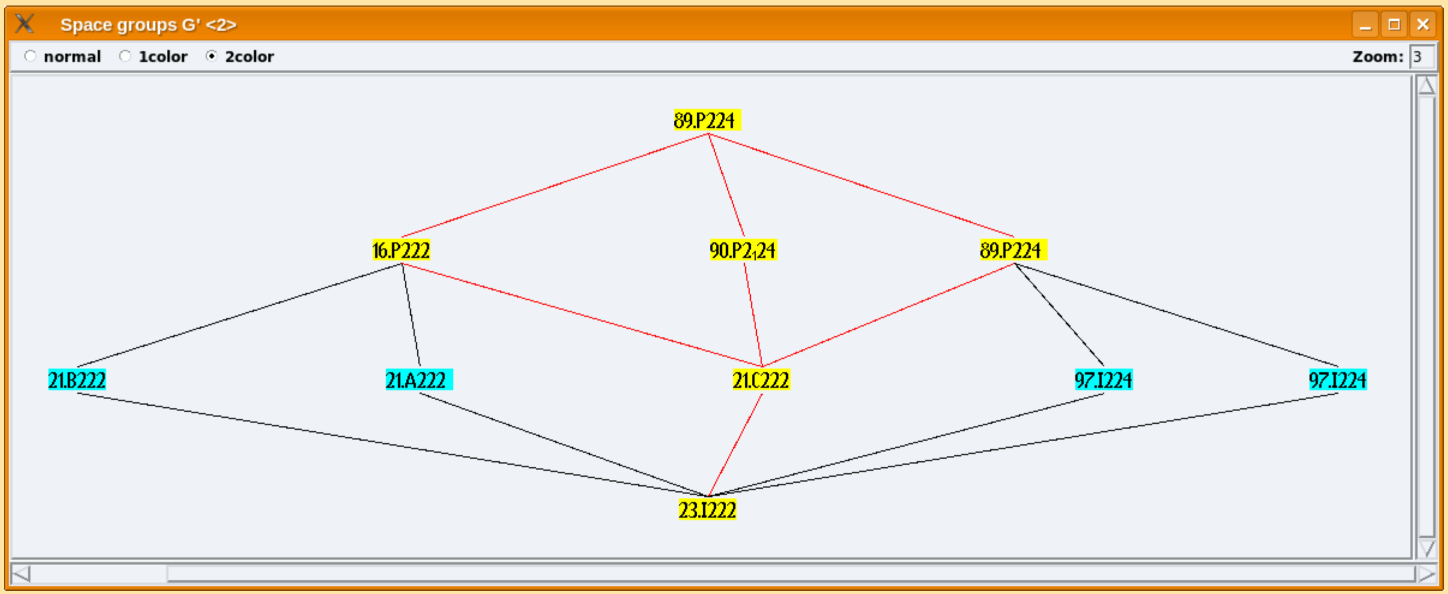


B. $\mathcal{G} = 89.P224$, $\mathcal{H} = 23.I222$, $I(\mathbf{2a}, \mathbf{2b}, \mathbf{2c})$



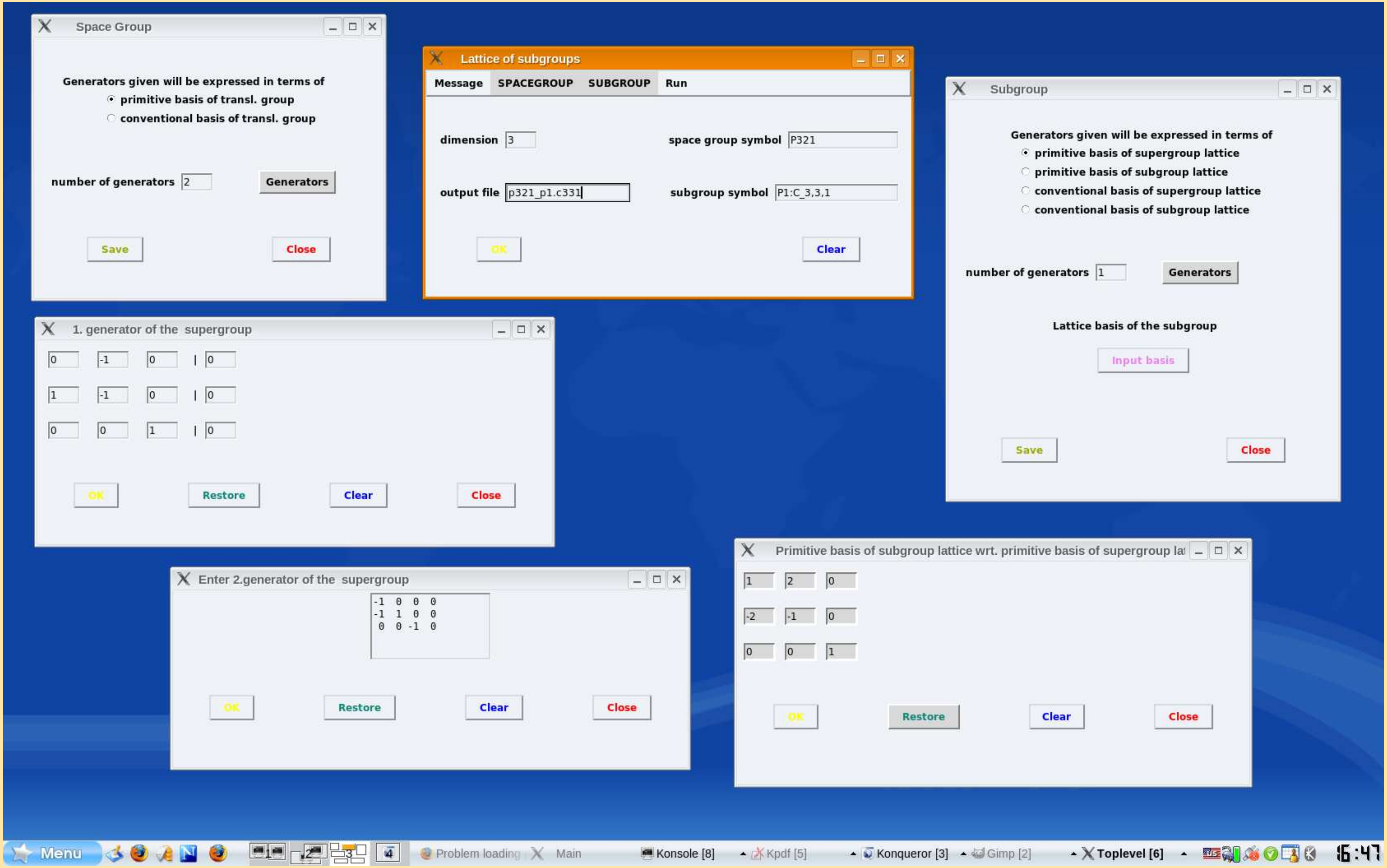






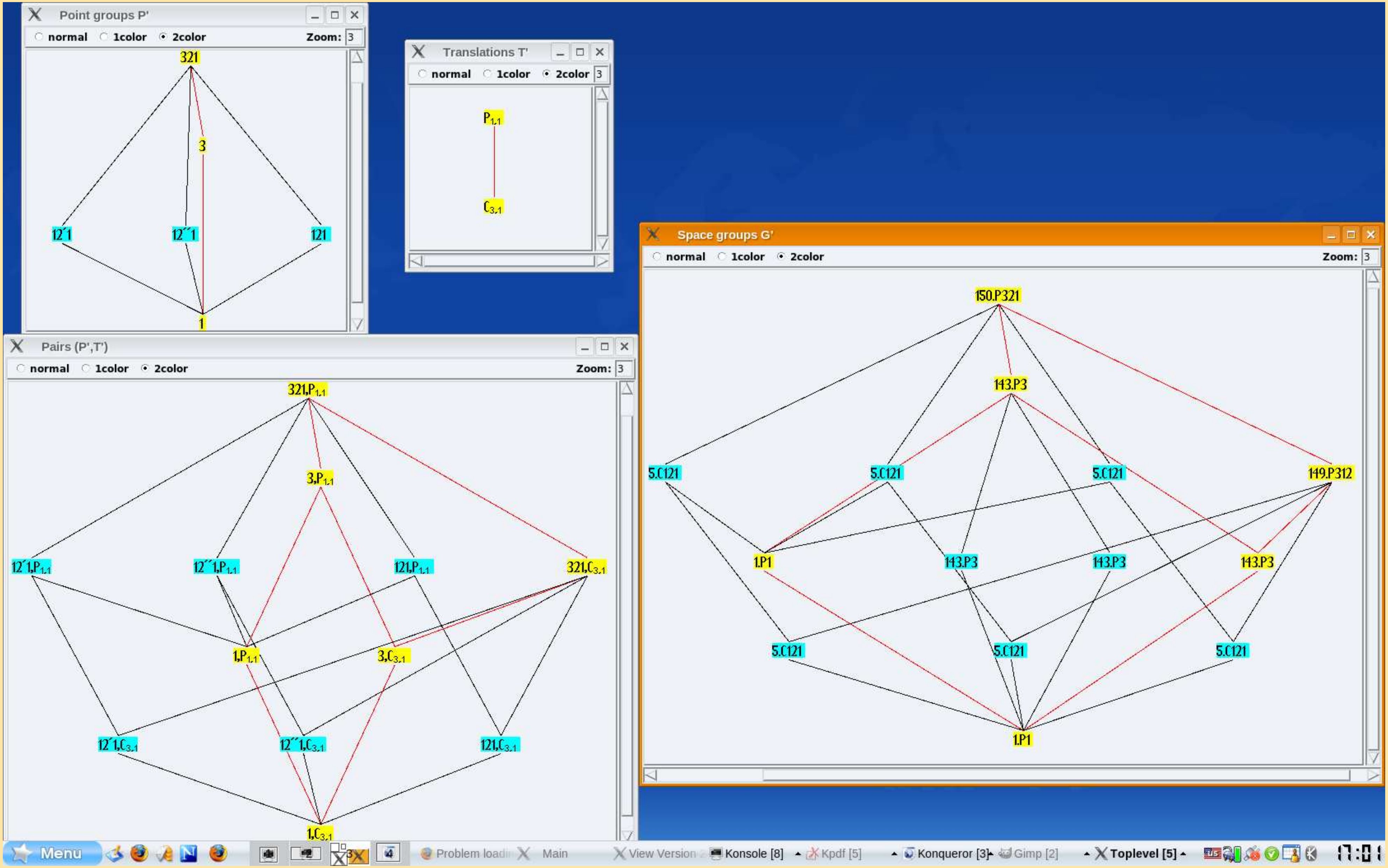
C. $\mathcal{G} = 150.P321$, $\mathcal{H} = 1.P1$, $C_{3,3,1} \sim \boldsymbol{a} + \boldsymbol{2b}, \boldsymbol{-2a} - \boldsymbol{b}, \boldsymbol{c}$

Interactive input:

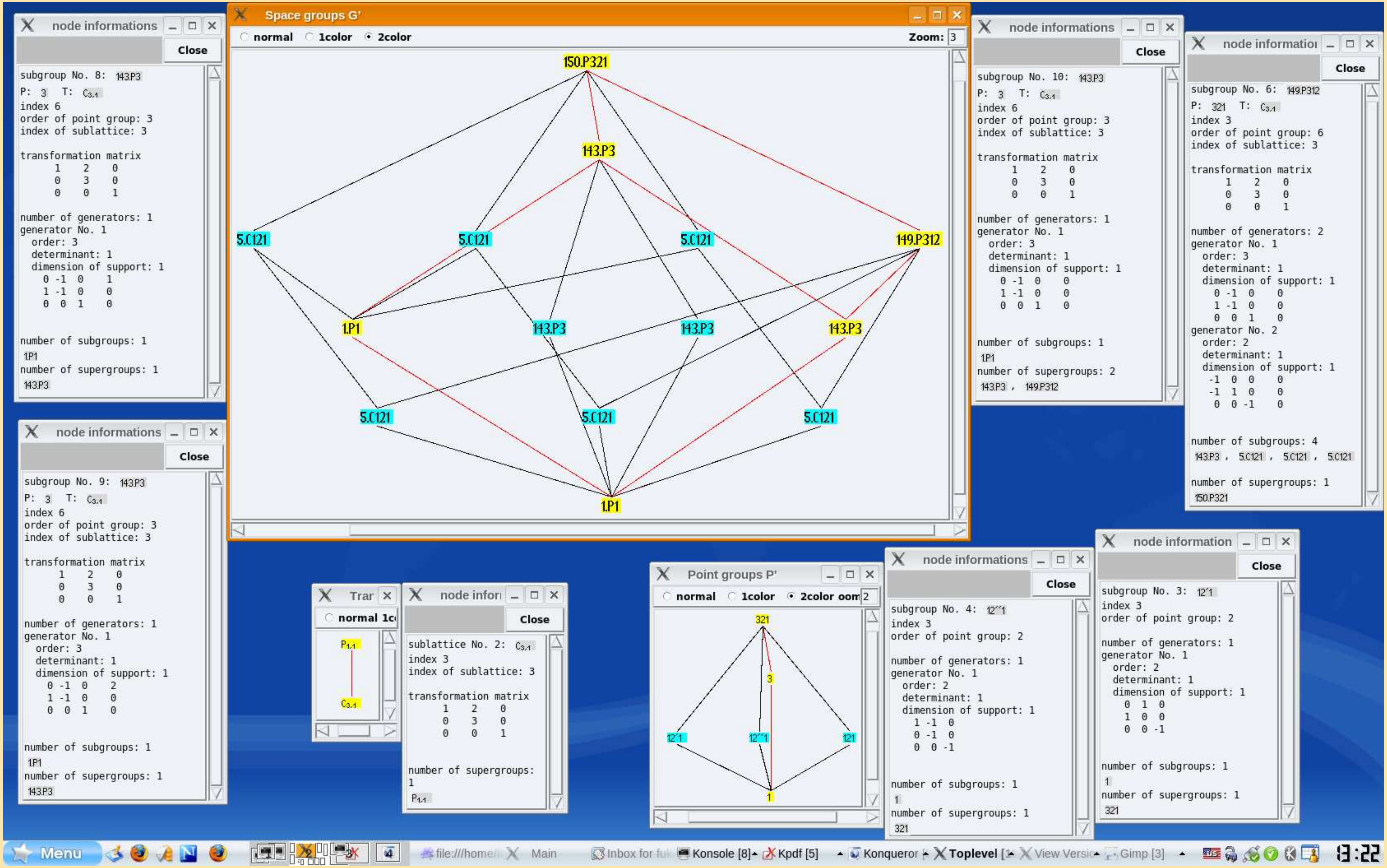


Program output:

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



Info provided on mouse click:



Isotropy subgroups of $150.P321$ Hatch & Stokes (1988)

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

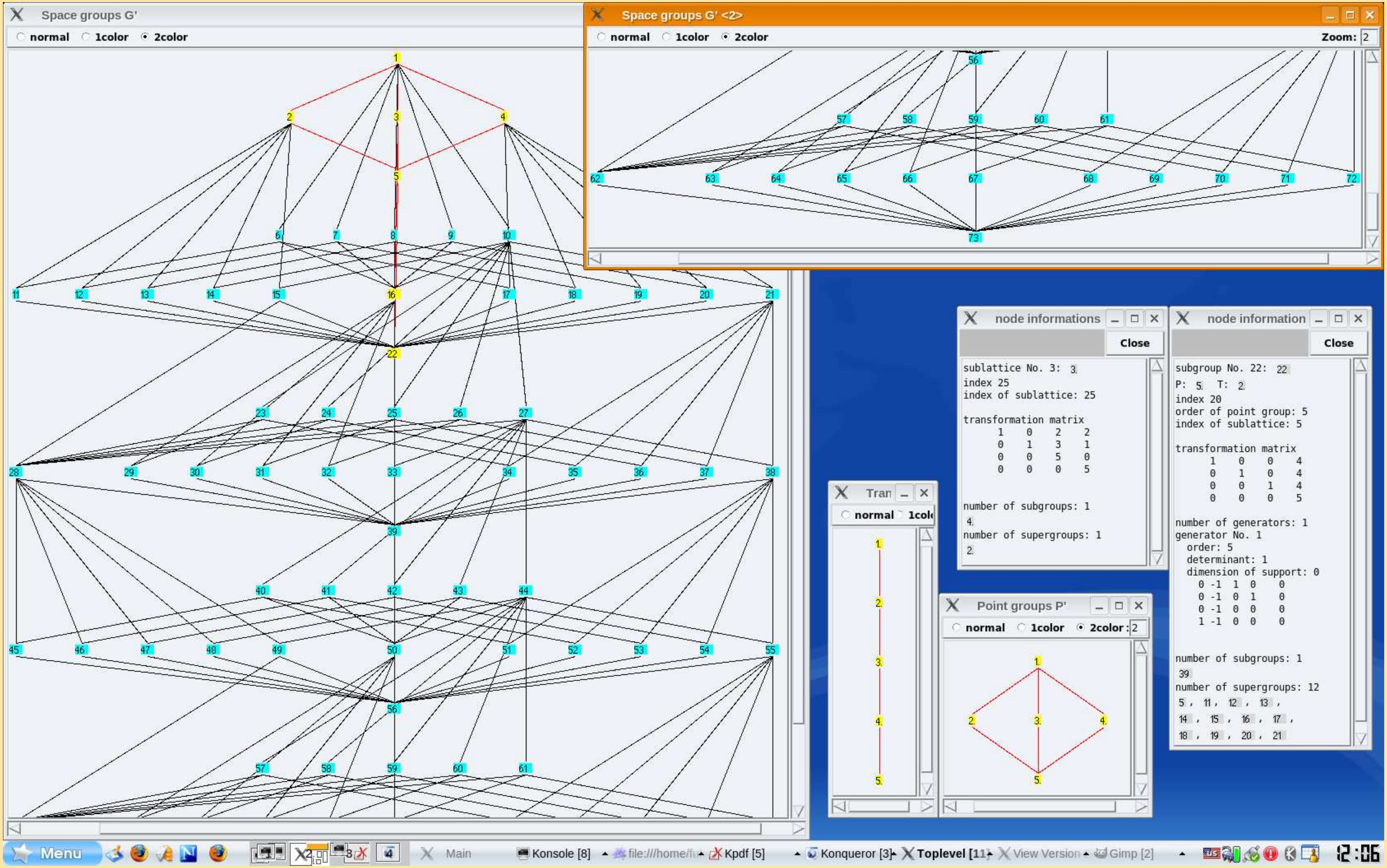
150 D_3^2 $P321$

Γ_1	$A1a$	1	0	150 D_3^2	$P321$	nf	$P1$	1	$(1,0,0),(0,1,0),(0,0,1)$	$(0,0,0)$
Γ_2	$A2a$	0	0	143 C_3^1	$P3$	pfc	$P1^{**}$	1	$(1,0,0),(0,1,0),(0,0,1)$	$(0,0,0)$
Γ_3	$B6a$	1	1	5 C_2^3	$C2$	pfc,pfs	$P1$	1	$(2,1,0),(0,\bar{1},0),(0,0,\bar{1})$	$(0,0,0)$
				1 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	$(1,2,0),(1,0,0),(0,0,\bar{2})$	$(0,0,0)$
				5 C_2^3	$C2$	ifc,ifs	$P2$	2	$(1,2,0),(1,0,0),(0,0,\bar{2})$	$(0,0,\frac{1}{2})$
				1 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	$(2,1,0),(\bar{1},1,0),(0,0,2)$	$(\frac{1}{3},\frac{2}{3},0)$
				5 C_2^3	$C2$	ifc,ifs	$C11$	6	$(1,2,0),(3,0,0),(0,0,\bar{2})$	$(0,0,0)$
				5 C_2^3	$C2$	ifc,ifs	$C15$	6	$(1,2,0),(3,0,0),(0,0,\bar{2})$	$(0,0,\frac{1}{2})$
				1 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	$(2,1,0),(\bar{1},1,0),(0,0,1)$	$(\frac{1}{3},\frac{2}{3},0)$
				5 C_2^3	$C2$	ifc,ifs	$C11$	3	$(1,2,0),(3,0,0),(0,0,\bar{1})$	$(0,0,0)$
				1 C_1^1	$P1$	ifc,ifs	$4D1$	3	$(1,\bar{1},0),(1,2,0),(0,0,1)$	$(0,0,0)$

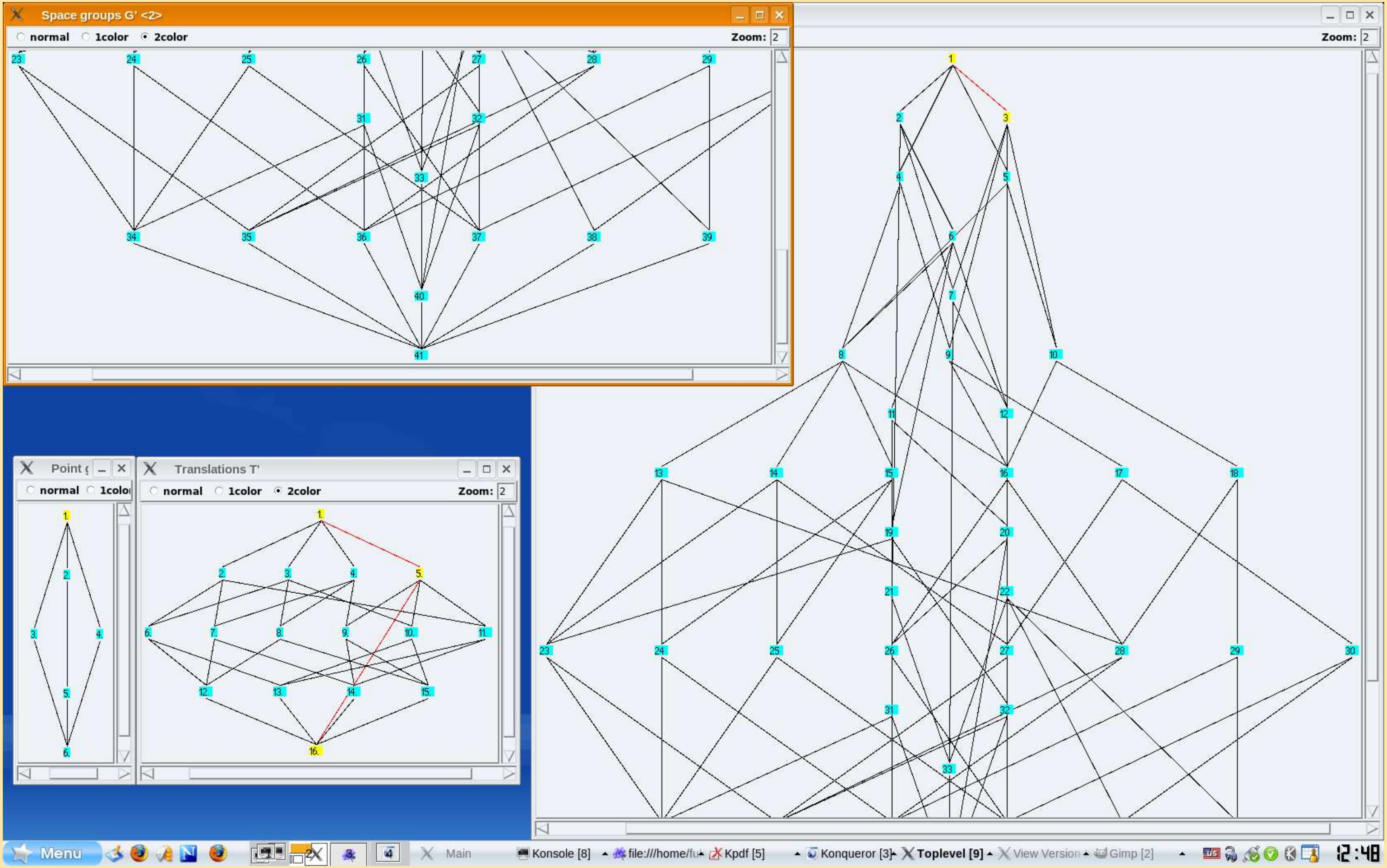
decipher yourself correct

group-subgroup relationships

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



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



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