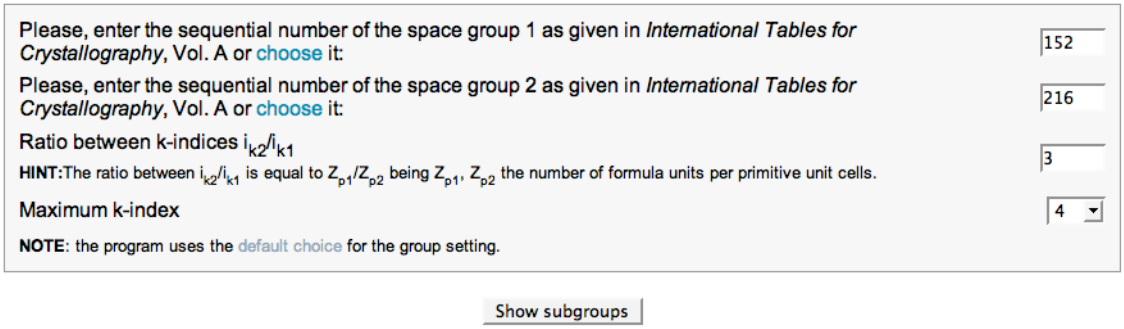
Bilbao Crystallographic Server II. Computer tools in phase-transition problems

Solution to Exercise 2.

(ii) Common subgroups:

Input of the program COMMONSUBS:

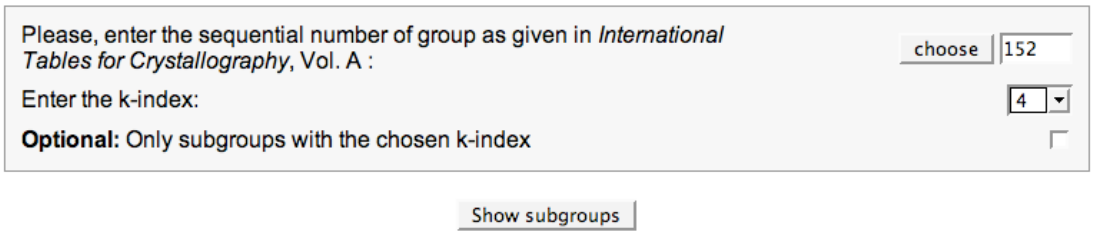


Output of the program:

Common Subgroup H				Branch G_1 > H			Branch G_2 > H			More info.
N	HM Symbol	P_H	ITA	i_1	it_1	ik_1	i_2	it_2	ik_2	show
1	$P3_1$	3	144	2	2	1	24	8	3	show..
2	$C2$	2	005	3	3	1	36	12	3	show..
3	$P1$	1	001	6	6	1	72	24	3	show..

(iii) Subgroups with a given cell-multiplication index, i_k:

Input for the program CELLSUB:



Example with output of the CELLSUB program:

t-subgroups of space group $P3_121$ (152)

N	HM Symbol	ITA	index	t-index	k-index	More info
1	$P3_1$	144	2	2	1	show...
2	$C2$	005	3	3	1	show...
3	$P1$	001	6	6	1	show...

(iv a) Subgroups $P3_1(144)$ of the space group $P3_121(152)$ with index 2

Cinnebar branch: 152 > 144 with index 2

Input of the program SUBGROUPGRAPH:

Please, enter the sequential numbers of the group and the subgroup as given in the *International Tables for Crystallography*, Vol. A:	
Enter the supergroup number (G) or choose it:	152
Enter the subgroup number (H) or choose it:	144
Enter the index ([G:H]):	2

Construct the lattice

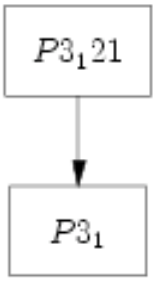
Result of the program:

Classification of the subgroups of type $P3_1(144)$ of group $P3_121(152)$ with index 2

Class 1

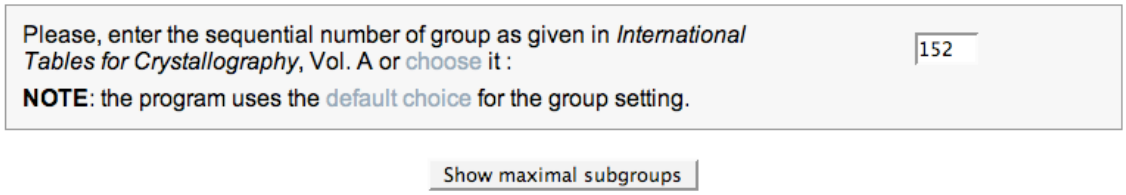
Check		Chain [indices]	Chain with HM symbols	Transformation	Identical
◉	1	152 144 [2]	$P3_121 > P3_1$	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]	--

Show graph



Other possibility is to use **MAXSUB** program because $P3_1$ is a maximal subgroup of $P3_121$:

Input of the program:



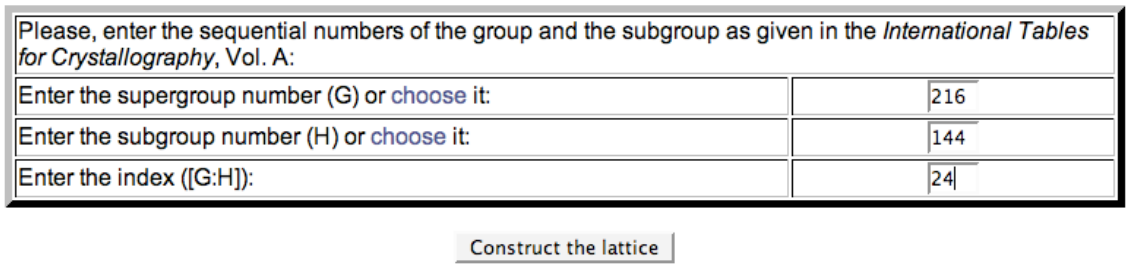
Output of the program:

N	Subgroup	HM Symbol	Index	Setting ...
1	5	$C2$	3	setting...
2	144	$P3_1$	2	setting...
3	151	$P3_112$	3	setting...
4	152	$P3_121$	4	setting...
5	154	$P3_221$	2	setting...

(iv b) Subgroups of type $P3_1$(144) of space group F-43m(216) with index 24

Zincblende branch: 216 > 144 with index 24

Input for the program:



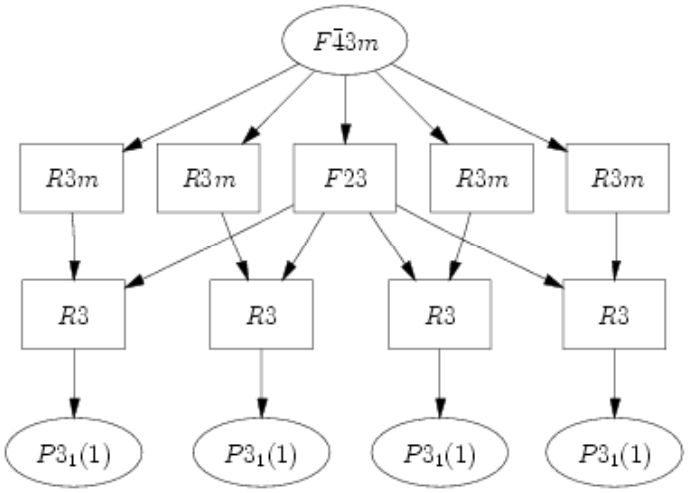
Result of the program:

Classification of the subgroups of type $P3_1(144)$ of group $F\text{-}43m(216)$ with index 24

Class 1

Check		Chain [indices]	Chain with HM symbols	Transformation	Identical
◉	1	216 160 146 144 [4 2 3]	$F\text{-}43m > R3m > R3 > P3_1$	[1/2 0 -1] [1/6] [-1/2 1/2 -1] [0] [0 1/2 1] [1/6]	to group 1
○	2	216 160 146 144 [4 2 3]	$F\text{-}43m > R3m > R3 > P3_1$	[-1/2 0 1] [-1/6] [1/2 -1/2 1] [0] [0 1/2 1] [1/6]	to group 2
○	3	216 160 146 144 [4 2 3]	$F\text{-}43m > R3m > R3 > P3_1$	[1/2 0 -1] [1/6] [1/2 -1/2 1] [0] [0 -1/2 -1] [-1/6]	to group 3
○	4	216 160 146 144 [4 2 3]	$F\text{-}43m > R3m > R3 > P3_1$	[-1/2 0 1] [-1/6] [-1/2 1/2 -1] [0] [0 -1/2 -1] [-1/6]	to group 4

Show graph



(v) Wyckoff-position splitting schemes

Cinnebar branch: 152 > 144 a,b,c

Input of the program:

Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:				
Enter supergroup or choose it	152			
Enter subgroup or choose it	144			
Please, define the transformation relating the group and the subgroup bases. (NOTE: If you don't know the transformation click here for possible workarounds)				
rotational matrix:	1	0	0	
	0	1	0	
	0	0	1	
origin shift:	0	0	0	

Show group-subgroup data.

Result of the program:

Result from splitting

No	Wyckoff position(s)		
	Group	Subgroup	More...
1	3b	3a	Relations
2	3a	3a	Relations

Splitting of Wyckoff position 3b

Representative			Subgroup Wyckoff position	
No	group basis	subgroup basis	name[n]	representative
1	(x, 0, 5/6)	(x, 0, 5/6)	$3a_1$	(x_1, y_1, z_1)
2	(0, x, 1/6)	(0, x, 1/6)		(-y_1, x_1-y_1, z_1+1/3)
3	(-x, -x, 1/2)	(-x, -x, 1/2)		(-x_1+y_1, -x_1, z_1+2/3)

Zincblende branch: 216 > 144

Transformation matrix: 1/2a+1/2b+1/6, 1/2b+1/2c, -a-b+c+1/6

Input of the program:

Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:			
Enter supergroup or choose it	216		
Enter subgroup or choose it	144		
Please, define the transformation relating the group and the subgroup bases. (NOTE: If you don't know the transformation click here for possible workarounds)			
rotational matrix:	1/2	0	-1
	-1/2	1/2	-1
	0	1/2	1
origin shift:	1/6	0	1/6

Show group-subgroup data.

Output of the program:

Result from splitting

No	Wyckoff position(s)		
	Group	Subgroup	More...
1	4c	3a	Relations
2	4a	3a	Relations

The program TRANPATH

The above-discussed sequential steps of the symmetry search for possible transition paths are combined in the program **TRANPATH** (TRANsition PATHs)**.**

The **INPUT** of **TRANPATH** consists of a structure-data file that can be loaded via the web interface of the program:

Transitions Paths

An example for the input file can be found here

Structure Data	/Users/cesar/work/path/bin/input/cdte.inp	Examinar...	Load
Maximum k-index (maximum cell multiplication)	4		

An example of the input file:

```
formulae zinblende(B3) to cinnabar structure types
# Space groups ITA number
sgr1      216
sgr2      152
# Number of formula units per conventional unit cell
z1          4
z2          3
# Cell parameters in \AA and degrees
cell1       6.483 6.483 6.483  90 90 90
cell2       4.338 4.338 10.273 90 90 120
# The atom positions of Structure 1
atoms1
Cd1         4a      0     0     0
Te1         4c      0.25 0.25 0.25
# The atom positions of Structure 2
atoms2
Cd1         3a      0.612     0     0.3333333
Te1         3b      0.556     0     0.8333333
```

The **OUTPUT** of **TRANPATH** consists of several blocks:

Structure data block:

Structure Data

Structure 1

Space Group *F*-43*m* (216) with Z=4 (formula units per conventional unit cell)

Cell parameters

a	6.483	**b**	6.483	**c**	6.483
alpha	90	**beta**	90	**gamma**	90

Atoms

ATOM	WP	Orbit
Cd1	4a	(0,0,0) ; (0,1/2,1/2) ; (1/2,0,1/2) ; (1/2,1/2,0)
Te1	4c	(1/4,1/4,1/4) ; (3/4,3/4,1/4) ; (3/4,1/4,3/4) ; (1/4,3/4,3/4)

Structure 2

Space Group $P3_121$ (152) with Z=3 (formula units per conventional unit cell)

Cell parameters

a	4.338	**b**	4.338	**c**	10.273
alpha	90	**beta**	90	**gamma**	120

Atoms

ATOM	WP	Orbit
Cd1	3a	(0.61200,0,1/3) ; (0,0.61200,2/3) ; (0.38800,0.38800,0)
Te1	3b	(0.5560,0,5/6) ; (0,0.5560,1/6) ; (0.44400,0.44400,1/2)

Common Subgroups

Common subgroups block:

Common subgroups of space groups *F*-43*m* (216) and $P3_121$ (152)

Space group G_1:*F*-43*m* (216) with $Z_1 = 4$

Space group G_2:$P3_121$ (152) with $Z_2 = 3$

Maximum cell multiplication (for both branches): 4

NOTE: The program uses the default choice for the group settings.

Common Subgroup H							Branch G_1 > H			Branch G_2 > H		
N	#	LEVEL	HM Symbol	P_H	Z_H	ITA	i_1	it_1	ik_1	i_2	it_2	ik_2
1	☐	(3,1)	$P3_1$	3	12	144	24	8	3	2	2	1
2	☐	(4,1)	*C*2	2	12	005	36	12	3	3	3	1
3	☐	(4,2)	*P*1	1	12	001	72	24	3	6	6	1

Show Transition Paths

Transition path block:

Common Subgroups

```
Number of Subgroups of G1: 81
Number of Subgroups of G2: 20
Max. cell  multiplication:
ZA/ZB: 0.333333

COMMON SUBGROUPS OF SPACE GROUPS F-43m (216) AND P3_121 (152)

N   LEVEL #  HM            Point    ITA    ZH   i1   it1  ik1  i2   it2  ik2
=============================================================================
1   (3,1) # P3_1           3        144    12   24   8    3    2    2    1
2   (4,1) # C2             2        005    12   36   12   3    3    3    1
3   (4,2) # P1             1        001    12   72   24   3    6    6    1

# Number of common subgroups: 3
```

Report

Transition Paths

#	H	Z_H	index 1	index 2	P_1	P_2	WP Splitting
1	144 ($P3_1$)	12	24 (3)	2 (1)	-1/2a+1/2b-1/6, -1/2b+1/2c, a+b+c+1/6	a, b, c	4c (G1) : 3a 4a (G1) : 3a 3a (G2) : 3a 3b (G2) : 3a