Solution to Exercise 2.

(ii) Common subgroups:

Input of the program COMMONSUBS:

```
Please, enter the sequential number of the space group 1 as given in International Tables for Crystallography, Vol. A or choose it:
Please, enter the sequential number of the space group 2 as given in International Tables for Crystallography, Vol. A or choose it:
Ratio between k-indices $k_2/k_1$
HINT: The ratio between $k_2/k_1$ is equal to $Z_2/Z_1$, being $Z_1$, $Z_2$ the number of formula units per primitive unit cells.
Maximum k-index
NOTE: the program uses the default choice for the group setting.
```

Output of the program:

<table>
<thead>
<tr>
<th>Common Subgroup H</th>
<th>Branch G₁ &gt; H</th>
<th>Branch G₂ &gt; H</th>
<th>More info.</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>HM Symbol</td>
<td>$P_H$</td>
<td>ITA</td>
</tr>
<tr>
<td>1</td>
<td>$P_3_1$</td>
<td>3</td>
<td>144</td>
</tr>
<tr>
<td>2</td>
<td>$C2$</td>
<td>2</td>
<td>005</td>
</tr>
<tr>
<td>3</td>
<td>$P1$</td>
<td>1</td>
<td>001</td>
</tr>
</tbody>
</table>

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

Input for the program CELLSUB:

```
Please, enter the sequential number of group as given in International Tables for Crystallography, Vol. A:
Enter the k-index:
Optional: Only subgroups with the chosen k-index
```

Example with output of the CELLSUB program:

(iii 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:

Result of the program:

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

Class 1

<table>
<thead>
<tr>
<th>Check</th>
<th>Chain [indices]</th>
<th>Chain with HM symbols</th>
<th>Transformation</th>
<th>Identical</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td>152 144 [2]</td>
<td>$P3_121 &gt; P3_1$</td>
<td>$\begin{bmatrix} 1 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{bmatrix}$</td>
<td>-</td>
</tr>
</tbody>
</table>

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

Input of the program:

![Image](image1)

Output of the program:

```
<table>
<thead>
<tr>
<th>N</th>
<th>Subgroup</th>
<th>HM Symbol</th>
<th>Index</th>
<th>Setting</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>C2</td>
<td>3</td>
<td>setting...</td>
</tr>
<tr>
<td>2</td>
<td>144</td>
<td>$P3_1$</td>
<td>2</td>
<td>setting...</td>
</tr>
<tr>
<td>3</td>
<td>151</td>
<td>$P3_112$</td>
<td>3</td>
<td>setting...</td>
</tr>
<tr>
<td>4</td>
<td>152</td>
<td>$P3_121$</td>
<td>4</td>
<td>setting...</td>
</tr>
<tr>
<td>5</td>
<td>154</td>
<td>$P3_221$</td>
<td>2</td>
<td>setting...</td>
</tr>
</tbody>
</table>
```

(iv b) Subgroups of type $P3_1(144)$ of space group $F43m(216)$ with index 24

**Zincblende branch: 216 > 144 with index 24**

Input for the program:

![Image](image2)
Result of the program:

**Classification of the subgroups of type \( P3_1(144) \) of group \( F-43m(216) \) with index 24**

### Class 1

<table>
<thead>
<tr>
<th>Check</th>
<th>Chain [indices]</th>
<th>Chain with HM symbols</th>
<th>Transformation</th>
<th>Identical</th>
</tr>
</thead>
</table>
| 1     | 216 160 146 144 [4 2 3] | \( F-43m > R3m > R3 > P3_1 \) | \[
\begin{bmatrix}
0 & -1 \\
1/2 & 0 \\
1/2 & -1/2 \\
0 & 1/2 \\
1/2 & 1/2 \\
\end{bmatrix}
\] | \[
\begin{bmatrix}
1/6 \\
1/6 \\
0 \\
1/6 \\
0 \\
0 \\
\end{bmatrix}
\] | to group 1 |
| 2     | 216 160 146 144 [4 2 3] | \( F-43m > R3m > R3 > P3_1 \) | \[
\begin{bmatrix}
0 & -1 \\
-1/2 & 0 \\
1/2 & -1 \\
0 & 1/2 \\
0 & 1/2 \\
1/2 & 1/2 \\
\end{bmatrix}
\] | \[
\begin{bmatrix}
0 \\
1/6 \\
0 \\
1/6 \\
1/6 \\
-1/6 \\
\end{bmatrix}
\] | to group 2 |
| 3     | 216 160 146 144 [4 2 3] | \( F-43m > R3m > R3 > P3_1 \) | \[
\begin{bmatrix}
0 & -1 \\
1/2 & 0 \\
1/2 & -1 \\
0 & 1/2 \\
-1/2 & -1/2 \\
1/2 & 1/2 \\
\end{bmatrix}
\] | \[
\begin{bmatrix}
1/6 \\
1/6 \\
0 \\
1/6 \\
-1/6 \\
0 \\
\end{bmatrix}
\] | to group 3 |
| 4     | 216 160 146 144 [4 2 3] | \( F-43m > R3m > R3 > P3_1 \) | \[
\begin{bmatrix}
0 & -1 \\
-1/2 & 0 \\
1/2 & -1 \\
0 & 1/2 \\
-1/2 & -1/2 \\
1/2 & 1/2 \\
\end{bmatrix}
\] | \[
\begin{bmatrix}
1/6 \\
1/6 \\
0 \\
1/6 \\
-1/6 \\
0 \\
\end{bmatrix}
\] | to group 4 |

Show graph
(v) Wyckoff-position splitting schemes

**Cinnebar branch: 152 > 144 a,b,c**

Input of the program:

![Image of program input](image)

Result of the program:

**Result from splitting**

<table>
<thead>
<tr>
<th>No</th>
<th>Wyckoff position(s)</th>
<th>Group</th>
<th>Subgroup</th>
<th>More...</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3b</td>
<td>3a</td>
<td>3a</td>
<td>Relations</td>
</tr>
<tr>
<td>2</td>
<td>3a</td>
<td>3a</td>
<td>3a</td>
<td>Relations</td>
</tr>
</tbody>
</table>

**Splitting of Wyckoff position 3b**

<table>
<thead>
<tr>
<th>Representative</th>
<th>Subgroup Wyckoff position</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
<td>group basis</td>
</tr>
<tr>
<td>1</td>
<td>(x, 0, 5/6)</td>
</tr>
<tr>
<td>2</td>
<td>(0, x, 1/6)</td>
</tr>
<tr>
<td>3</td>
<td>(-x, -x, 1/2)</td>
</tr>
</tbody>
</table>
Zincblende branch: 216 > 144

Transformation matrix: \( \frac{1}{2}a + \frac{1}{2}b + \frac{1}{6}, \frac{1}{2}b + \frac{1}{2}c, -a - b + c + \frac{1}{6} \)

Input of the program:

Output of the program:

**Result from splitting**

<table>
<thead>
<tr>
<th>No</th>
<th>Group</th>
<th>Wyckoff position(s)</th>
<th>More...</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4c</td>
<td>3a</td>
<td>Relations</td>
</tr>
<tr>
<td>2</td>
<td>4a</td>
<td>3a</td>
<td>Relations</td>
</tr>
</tbody>
</table>

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 of the input file:

formulae ZnBlende(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 Å 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**

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

<table>
<thead>
<tr>
<th></th>
<th>alpha</th>
<th>beta</th>
<th>gamma</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a )</td>
<td>6.483</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>( b )</td>
<td>6.483</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>( c )</td>
<td>6.483</td>
<td></td>
<td>90</td>
</tr>
</tbody>
</table>

**Cell Parameters**

<table>
<thead>
<tr>
<th></th>
<th>alpha</th>
<th>beta</th>
<th>gamma</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a )</td>
<td>6.483</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>( b )</td>
<td>6.483</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>( c )</td>
<td>6.483</td>
<td></td>
<td>90</td>
</tr>
</tbody>
</table>

**Atoms**

<table>
<thead>
<tr>
<th>ATOM</th>
<th>WP</th>
<th>Orbit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cd1</td>
<td>4a</td>
<td>(0,0,0); (0.1/2,0); (0.1/2,0,0); (0.1/2,0,0)</td>
</tr>
<tr>
<td>Te1</td>
<td>4c</td>
<td>(1/4,0,1/4); (3/4,3/4,1/4); (3/4,1/4,3/4); (1/4,3/4,3/4)</td>
</tr>
</tbody>
</table>

**Structure 2**

**Space Group**

\( P3_21 (152) \) with \( Z=3 \) (formula units per conventional unit cell)

<table>
<thead>
<tr>
<th></th>
<th>alpha</th>
<th>beta</th>
<th>gamma</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a )</td>
<td>4.338</td>
<td>90</td>
<td>120</td>
</tr>
<tr>
<td>( b )</td>
<td>4.338</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>( c )</td>
<td>10.273</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Cell Parameters**

<table>
<thead>
<tr>
<th></th>
<th>alpha</th>
<th>beta</th>
<th>gamma</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a )</td>
<td>4.338</td>
<td>90</td>
<td>120</td>
</tr>
<tr>
<td>( b )</td>
<td>4.338</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>( c )</td>
<td>10.273</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Atoms**

<table>
<thead>
<tr>
<th>ATOM</th>
<th>WP</th>
<th>Orbit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cd1</td>
<td>3a</td>
<td>(0.612,0,0,0,0,0); (0.0,612,0,0,0,0,0,0); (0.388,0.388,0,0,0)</td>
</tr>
<tr>
<td>Te1</td>
<td>3b</td>
<td>(0.556,0.556,0.556); (0.0,556,0.556,0.556,0.556); (0.444,0.444,0.444,0.444,0.444)</td>
</tr>
</tbody>
</table>

Common Subgroups
Common subgroups block:

**Common subgroups of space groups F-43m (216) and P3₁21 (152)**

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

Space group \(G_2\): P3₁21 (152) with \(Z_2 = 3\)

Maximum cell multiplication (for both branches): 4

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

<table>
<thead>
<tr>
<th>N</th>
<th>#</th>
<th>LEVEL</th>
<th>HM Symbol</th>
<th>(P_H)</th>
<th>(Z_H)</th>
<th>ITA</th>
<th>(i_1)</th>
<th>(i_2)</th>
<th>(i_3)</th>
<th>(i_4)</th>
<th>(i_5)</th>
<th>(i_6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>(3,1)</td>
<td>(P3)</td>
<td>3</td>
<td>12</td>
<td>144</td>
<td>24</td>
<td>8</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>(4,1)</td>
<td>C2</td>
<td>2</td>
<td>12</td>
<td>005</td>
<td>36</td>
<td>12</td>
<td>3</td>
<td>3</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>(4,2)</td>
<td>(P1)</td>
<td>1</td>
<td>12</td>
<td>001</td>
<td>72</td>
<td>24</td>
<td>3</td>
<td>6</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

Transition path block:

**Common Subgroups**

Number of Subgroups of \(G_1\): 81
Number of Subgroups of \(G_2\): 20
Max. cell multiplication: 333333

COMMON SUBGROUPS OF SPACE GROUPS F-43m (216) AND P3₁21 (152)

<table>
<thead>
<tr>
<th>N</th>
<th>LEVEL</th>
<th>#</th>
<th>HM</th>
<th>Point</th>
<th>ITA</th>
<th>(Z_H)</th>
<th>(i_1)</th>
<th>(i_2)</th>
<th>(i_3)</th>
<th>(i_4)</th>
<th>(i_5)</th>
<th>(i_6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(3,1)</td>
<td>#</td>
<td>(P3)</td>
<td>3</td>
<td>144</td>
<td>12</td>
<td>24</td>
<td>8</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>(4,1)</td>
<td>#</td>
<td>C2</td>
<td>2</td>
<td>005</td>
<td>12</td>
<td>36</td>
<td>12</td>
<td>3</td>
<td>3</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>(4,2)</td>
<td>#</td>
<td>(P1)</td>
<td>1</td>
<td>001</td>
<td>12</td>
<td>72</td>
<td>24</td>
<td>3</td>
<td>6</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

# Number of common subgroups: 3

**Report**

**Transition Paths**

<table>
<thead>
<tr>
<th>#</th>
<th>H</th>
<th>(Z_H)</th>
<th>index 1</th>
<th>index 2</th>
<th>(P_1)</th>
<th>(P_2)</th>
<th>WP Splitting</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>144 ((P3))</td>
<td>12</td>
<td>24 (3)</td>
<td>2 (1)</td>
<td>-1/2a+1/2b+1/6, -1/2b+1/2c, a+b+c+1/6</td>
<td>a, b, c</td>
<td>4c ((G1) : 3\alpha)</td>
</tr>
</tbody>
</table>

4a \((G1) : 3\alpha\)
3a \((G2) : 3\alpha\)
3b \((G2) : 3\alpha\)