

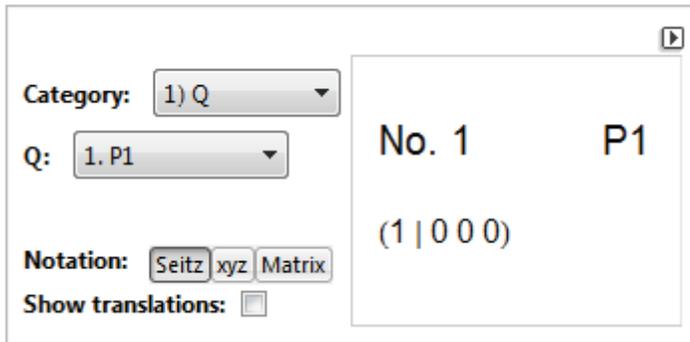
Double antisymmetry space groups CDF tutorial

Either:

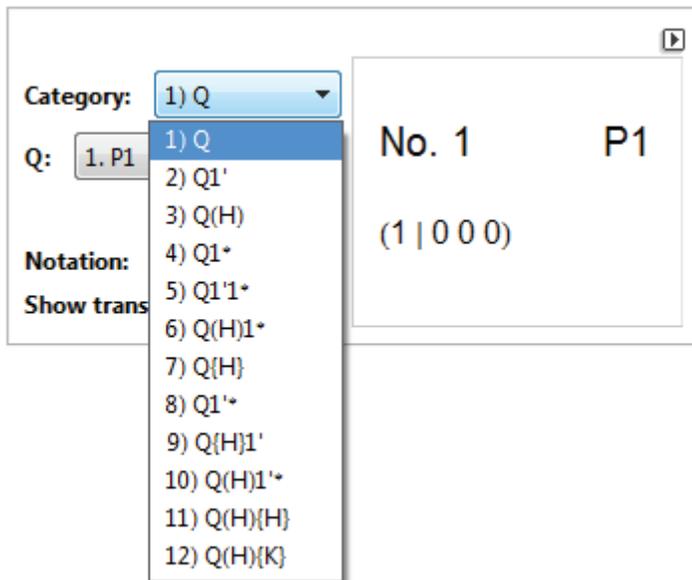
- Download the standalone CDF player from <http://www.wolfram.com/cdf-player/> and load "Double antisymmetry space groups.cdf"
- Or, access the embedded web version at <http://sites.psu.edu/gopalan/research/symmetry/> (requires CDF plugin)

If prompted, click "Enable Dynamics".

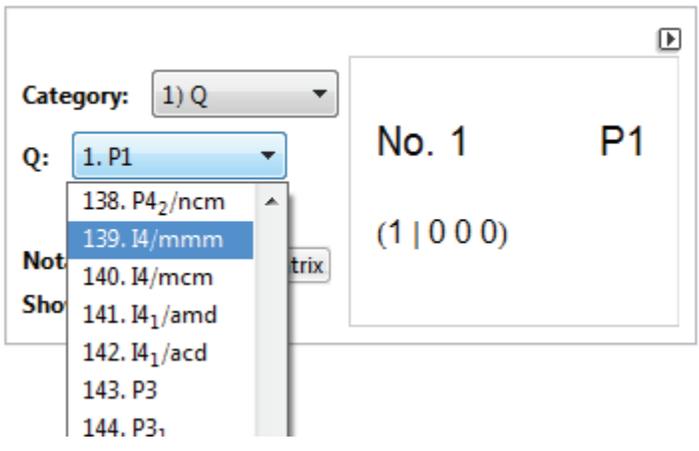
You should now see this on your screen:



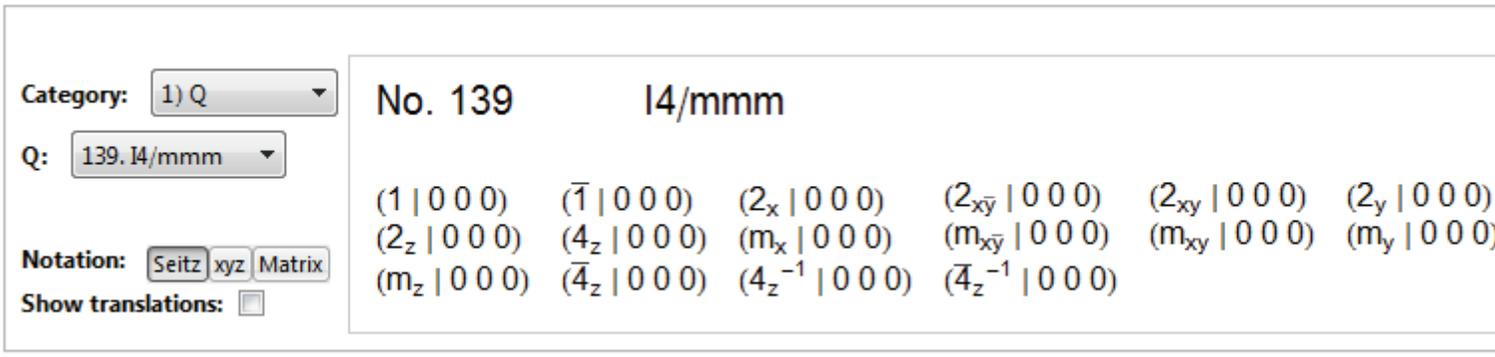
You can access the twelve categories of double antisymmetry space groups using the drop down menu as shown:



The drop down menu labeled "Q:" allows the colorblind parent group to be chosen:



For example:



The symmetry operations displayed under the number and symbol for the group are the symmetry elements of the group (more precisely, they are a set of coset representatives of the coset decomposition of the group with respect to the translational subgroup).

The buttons next to "Notation:" allow the notation used to represent the symmetry operations to be changed:

Category: 1) Q  
 Q: 139. I4/mmm  
 Notation: Seitz xyz Matrix  
 Show translations:

No. 139 I4/mmm

$(-x, -y, -z)$   $(-x, -y, z)$   $(-x, y, -z)$   $(-x, y, z)$   $(x, -y, -z)$   $(x, -y, z)$   
 $(x, y, -z)$   $(x, y, z)$   $(-y, -x, -z)$   $(-y, -x, z)$   $(-y, x, -z)$   $(-y, x, z)$   
 $(y, -x, -z)$   $(y, -x, z)$   $(y, x, -z)$   $(y, x, z)$

Category: 1) Q  
 Q: 139. I4/mmm  
 Notation: Seitz xyz Matrix  
 Show translations:

No. 139 I4/mmm

$\begin{pmatrix} 0 & -1 & 0 & | & 0 \\ -1 & 0 & 0 & | & 0 \\ 0 & 0 & -1 & | & 0 \end{pmatrix}$   $\begin{pmatrix} 0 & -1 & 0 & | & 0 \\ -1 & 0 & 0 & | & 0 \\ 0 & 0 & 1 & | & 0 \end{pmatrix}$   $\begin{pmatrix} 0 & -1 & 0 & | & 0 \\ 1 & 0 & 0 & | & 0 \\ 0 & 0 & -1 & | & 0 \end{pmatrix}$   $\begin{pmatrix} 0 & -1 & 0 & | & 0 \\ 1 & 0 & 0 & | & 0 \\ 0 & 0 & 1 & | & 0 \end{pmatrix}$   $\begin{pmatrix} 0 & 1 & 0 & | & 0 \\ -1 & 0 & 0 & | & 0 \\ 0 & 0 & -1 & | & 0 \end{pmatrix}$   
 $\begin{pmatrix} 0 & 1 & 0 & | & 0 \\ 1 & 0 & 0 & | & 0 \\ 0 & 0 & -1 & | & 0 \end{pmatrix}$   $\begin{pmatrix} 0 & 1 & 0 & | & 0 \\ 1 & 0 & 0 & | & 0 \\ 0 & 0 & 1 & | & 0 \end{pmatrix}$   $\begin{pmatrix} -1 & 0 & 0 & | & 0 \\ 0 & -1 & 0 & | & 0 \\ 0 & 0 & -1 & | & 0 \end{pmatrix}$   $\begin{pmatrix} -1 & 0 & 0 & | & 0 \\ 0 & -1 & 0 & | & 0 \\ 0 & 0 & 1 & | & 0 \end{pmatrix}$   $\begin{pmatrix} -1 & 0 & 0 & | & 0 \\ 0 & 1 & 0 & | & 0 \\ 0 & 0 & -1 & | & 0 \end{pmatrix}$   
 $\begin{pmatrix} 1 & 0 & 0 & | & 0 \\ 0 & -1 & 0 & | & 0 \\ 0 & 0 & -1 & | & 0 \end{pmatrix}$   $\begin{pmatrix} 1 & 0 & 0 & | & 0 \\ 0 & -1 & 0 & | & 0 \\ 0 & 0 & 1 & | & 0 \end{pmatrix}$   $\begin{pmatrix} 1 & 0 & 0 & | & 0 \\ 0 & 1 & 0 & | & 0 \\ 0 & 0 & -1 & | & 0 \end{pmatrix}$   $\begin{pmatrix} 1 & 0 & 0 & | & 0 \\ 0 & 1 & 0 & | & 0 \\ 0 & 0 & 1 & | & 0 \end{pmatrix}$

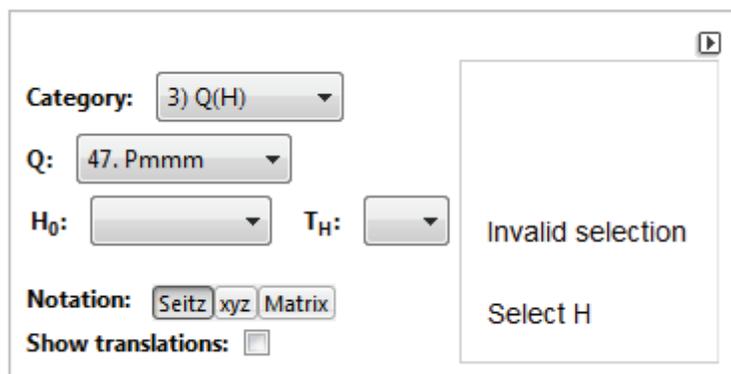
Checking the "Show translations:" box adds a line of 3 to 6 operations (underlined in red in the example below) which generate the translational subgroup (the subgroup which contains every translation of the symmetry group).

Category: 1) Q  
 Q: 139. I4/mmm  
 Notation: Seitz xyz Matrix  
 Show translations:

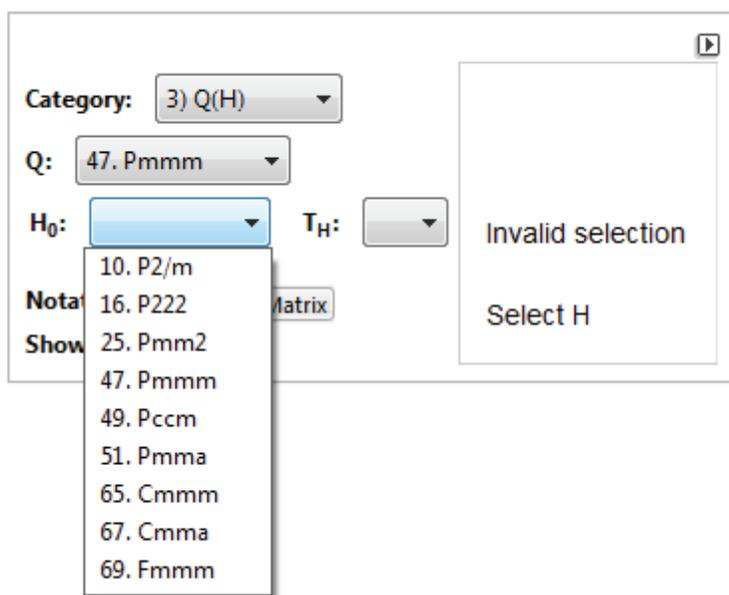
No. 139 I4/mmm

$(1 | 1 0 0)$   $(1 | 0 1 0)$   $(1 | 0 0 1)$   $(1 | 1/2 1/2 1/2)$   
 $(1 | 0 0 0)$   $(\bar{1} | 0 0 0)$   $(2_x | 0 0 0)$   $(2_{x\bar{y}} | 0 0 0)$   $(2_{xy} | 0 0 0)$   $(2_y | 0 0 0)$   
 $(2_z | 0 0 0)$   $(4_z | 0 0 0)$   $(m_x | 0 0 0)$   $(m_{x\bar{y}} | 0 0 0)$   $(m_{xy} | 0 0 0)$   $(m_y | 0 0 0)$   
 $(m_z | 0 0 0)$   $(\bar{4}_z | 0 0 0)$   $(4_z^{-1} | 0 0 0)$   $(\bar{4}_z^{-1} | 0 0 0)$

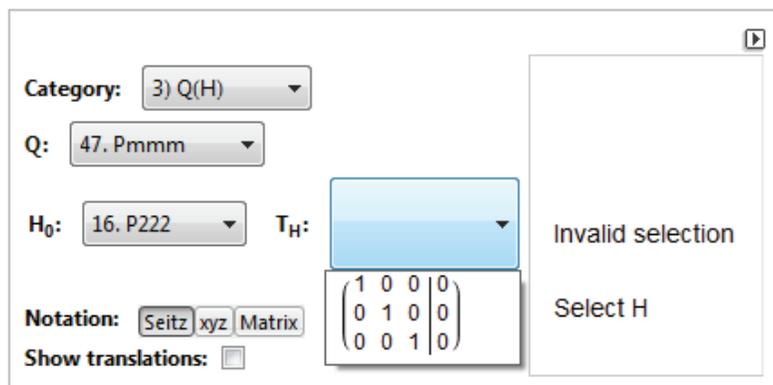
If currently selected category requires H, an index-2 subgroup of the colorblind parent group Q, to be defined, "Invalid selection" will be displayed until the required input is provided. In the example below, H must be selected:



The dropdown menu next to H<sub>0</sub> gives the possible options for the space group type of H (this is restricted by the currently selected Q).



The dropdown menu next to T<sub>H</sub> gives the possible options for transformations for a standard representation of a group of type H<sub>0</sub> an index-2 subgroup of Q (T<sub>H</sub> is restricted to the currently selected H<sub>0</sub> and the currently selected Q).



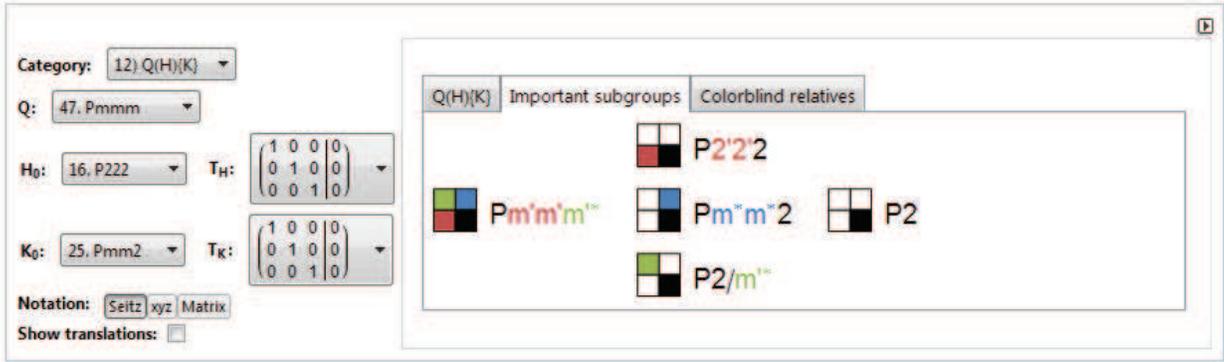
As discussed in the main text, T<sub>H</sub> and H<sub>0</sub> define H.

For category 12)  $Q(H)\{K\}$ , both H and K subgroups must be defined:

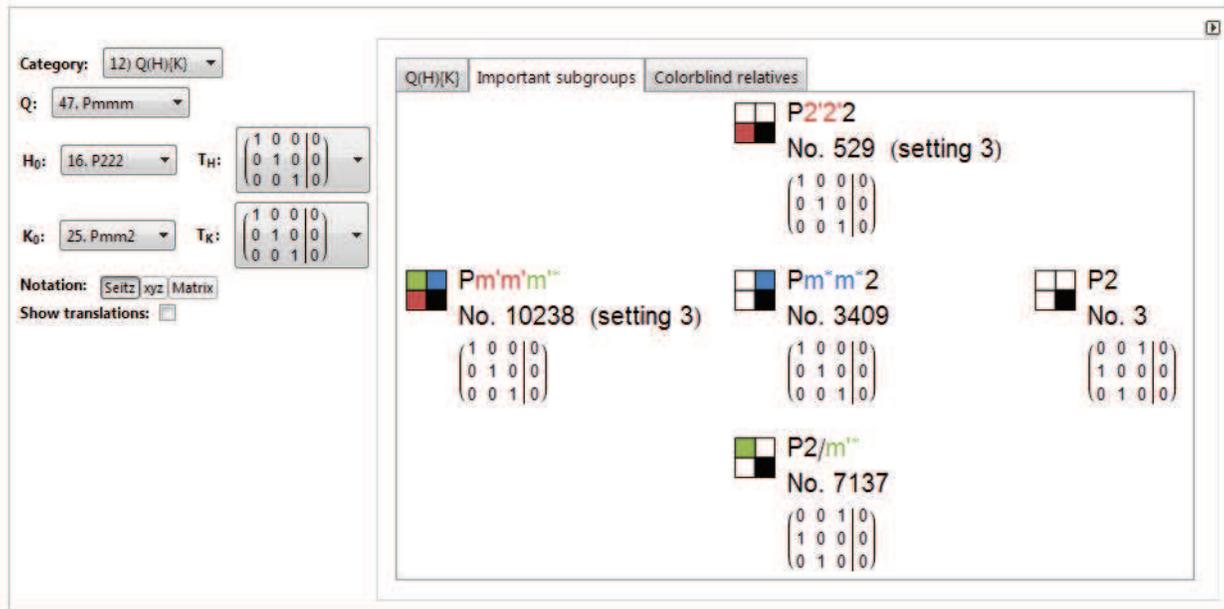
When valid selections have been made to define H and K,  $Q(H)\{K\}$  is displayed:

For category 12)  $Q(H)\{K\}$ , tabs appear in the window labeled: “ $Q(H)\{K\}$ ”, “Important subgroups”, and “Colorblind relatives”.

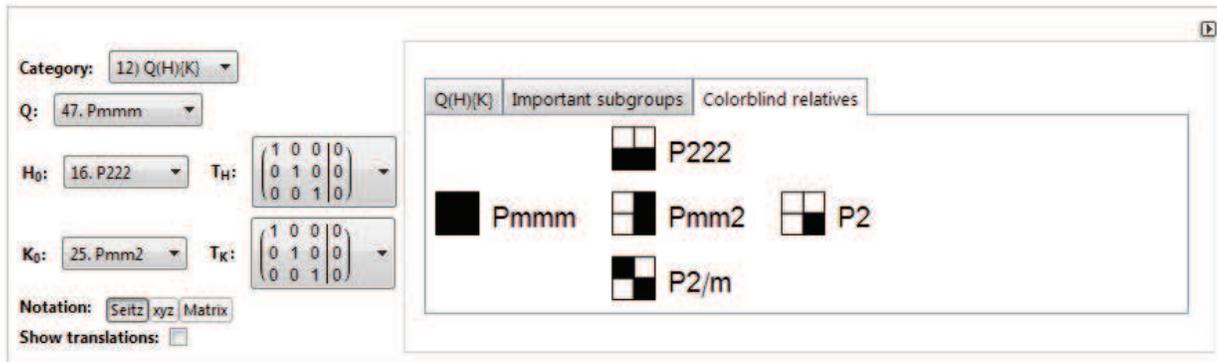
The "Important subgroups" tab shows some subgroups of the currently selected  $Q(H)\{K\}$  group. Note that the colored squares have the same meaning as in Appendix A.



Clicking on the display flips to a more detailed version that gives the numbers and settings of the double antisymmetry space groups and the transformation to the basis of  $Q(H)\{K\}$ .



The "Colorblind relatives" tab shows the colorblind versions of the subgroups given under the "Important subgroups" tab.



Again, clicking the display gives more details:

