

## Using the machine-readable file

All 38,290 double antisymmetry space groups generated by applying formulae in Table 1 to the standard representative group of each of the 230 crystallographic space group types are listed in “DASGMachineReadable.txt”. Each group is represented as eight lines; the entire file contains a total of 306,320 lines (8\*38,290).

The first line of each set of eight contains three numbers: the serial number of the type (1 to 17,803), the “setting” number to identify groups with the same type (1 to the number of groups in that type), and the number of the category of the group (1 to 12).

The second line contains five numbers: the space group number of **Q** (1 to 230), the space group number of **H** (1 to 230), the space group number of **K** (1 to 230), the space group number of **L** (1 to 230), and the space group number of **R** (1 to 230). **Q**, **H**, and **K**, have the same meaning as previously given in Table 1. **R** is  $\mathbf{H} \cap \mathbf{K}$  and is therefore an index-4 subgroup of **Q**. **L** is an index-2 subgroup of **Q** which is equivalent to  $\mathbf{Q} - (\mathbf{H} + \mathbf{K}) + \mathbf{R}$ . If a number is not applicable to the current category then “0” is given.

The third line contains 80 numbers. These are to be partitioned into five 4-by-4 matrices representing the transformations from **Q**<sub>0</sub>, **H**<sub>0</sub>, **K**<sub>0</sub>, **L**<sub>0</sub>, and **R**<sub>0</sub>, onto **Q**, **H**, **K**, **L**, and **R** respectively, e.g. the third matrix is  $T_H$  such that  $\mathbf{H} = T_H \mathbf{H}_0 T_H^{-1}$ . **Q**<sub>0</sub>, **H**<sub>0</sub>, **K**<sub>0</sub>, **L**<sub>0</sub>, and **R**<sub>0</sub> are standard representative groups as given in first 230 groups of this listing, i.e. the category 1) groups (also these standard representative groups of the conventional space group types in the International Tables for Crystallography). Since **Q**<sub>0</sub> = **Q** for all groups in this listing, the first matrix is always an identity matrix. If a matrix is not applicable to the current category then zeros are given for all elements of the matrix.

The fourth line contains between three and six numbers. These give the color of the translation subgroup generators; 1 means colorless (coupled with 1), 2 means primed (colored with 1'), 3 means starred (colored with 1\*), and 4 means prime-starred (colored with 1'\*). The translation indicated by each position is depends on the lattice type of **Q** as follows:

	1 <sup>st</sup> position	2 <sup>nd</sup> position	3 <sup>rd</sup> position	4 <sup>th</sup> position	5 <sup>th</sup> position	6 <sup>th</sup> position
P	$t_{[100]}$	$t_{[010]}$	$t_{[001]}$			
C	$t_{[100]}$	$t_{[010]}$	$t_{[001]}$	$t_{[\frac{1}{2}\frac{1}{2}0]}$		
A	$t_{[100]}$	$t_{[010]}$	$t_{[001]}$	$t_{[0\frac{1}{2}\frac{1}{2}]}$		
I	$t_{[100]}$	$t_{[010]}$	$t_{[001]}$	$t_{[\frac{1}{2}\frac{1}{2}\frac{1}{2}]}$		
F	$t_{[100]}$	$t_{[010]}$	$t_{[001]}$	$t_{[0\frac{1}{2}\frac{1}{2}]}$	$t_{[\frac{1}{2}0\frac{1}{2}]}$	$t_{[\frac{1}{2}\frac{1}{2}0]}$
R	$t_{[100]}$	$t_{[010]}$	$t_{[001]}$	$t_{[\frac{2}{3}\frac{1}{3}\frac{1}{3}]}$	$t_{[\frac{1}{3}\frac{2}{3}\frac{2}{3}]}$	

The 4<sup>th</sup> through 6<sup>th</sup> positions of the fourth line are always centering translations (those with non-integer values). It is only necessary to use the first three positions generally because the coloring of the centering translations is also given in the fifth through eighth lines.

The fifth line contains a list of numbers whose length is a multiple of 16. This list is to be partitioned into 4-by-4 matrices representing the matrix form of the colorless operations. The sixth, seventh, and eighth lines are to be similarly partitioned and represent the matrix form of primed, starred and prime-starred operations respectively.