

17-Symmetry and its Generalizations

MS-17.01.04 ALGORITHM FOR HIGH DIMENSIONAL POLYTOPE VISUALIZATIONS. By S. S. Im and H. S. Kim*, Dept of Inorganic Materials Engineering, College of Engineering, Chonnam National University, Yongbong-Dong, Buk-Gu, Kwang Ju, 500-757, Korea.

Many articles deal with studies of symmetry in higher dimensions and with applications to incommensurate structures and to quasicrystals. It is very difficult to perceive high-dimensional features. Polytope is the simplest symmetrical shape for representing the space. In this presentation, we develop an algorithm to visualize high-dimensional polytopes with computer graphics in personal computers.

Polytopes are composed of vertices and edges. Vertices are determined by intersections of hyper-planes, and edges are obtained by reducing dimensions. Through use of endless loops in the calculation, the dimension of polytopes is restricted only by available computer memory. Several projections, stereoviews and animations are applied to help our perception of higher dimensional space. In the simplest case, hypercubic, this algorithm requires little computing time for the construction of the hypercube. The interesting relations between the vertices and edges of the hypercube will be discussed. We look forward to discussions about symmetry operations in higher dimensions to improve our understanding.

MS-17.01.05 CRYSTALS ON A WEIQI BOARD: PERIODIC TWO-COLOURINGS OF A NET. J. S. Rutherford, Department of Chemistry, University of Transkei, South Africa.

This work concerns the number of distinct structural derivative lattices (commensurate superlattices) that can be constructed by the periodic arrangement of a number of structural motifs, (represented by colours), on a regular basic lattice. In general the method used consists of four steps:

1. The counting of the derivative lattices by index (Rutherford, Acta Cryst., 1992, A48, 500-508).
2. The identification of the colour lattice groups that may occur for a particular index (Harker, Proc. Natl. Acad. Sci. USA, 1978, 75, 5264-5267), and the partition of the total number of derivative lattices for that index by colour lattice group.
3. The application of Polya's Theorem (Polya, Acta Math., 1937, 68, 145-254) to provide the total number of patterns for each colour lattice group and stoichiometry.
4. The elimination of patterns already counted under a derivative lattice of lower index.

The simplest case of practical importance, that of two colours only on a two-dimensional net, can be usefully modelled using the black and white stones and reticulated board of the game Weiqi (Japanese: Go), and a number of such examples will be illustrated.

MS-17.01.06 THE INDUCED REPRESENTATIONS OF THE POINT GROUPS VIA THE SUBDUCE REPRESENTATIONS OF THEIR SUBGROUPS. By Yves BILLET*, Département de Chimie, Faculté des Sciences, Boite Postale 825, Niamey, Niger.

It is easy to obtain the subduced representations of a point group onto its subgroups. This has been done for all point groups and there exist numerous tables of subduced representations (e.g., Atkins, Child & Phillips, 1970, Tables for Group Theory, Oxford, University Press). As an example, here are the representations subduced from the irreducible representations of the point group $\bar{4}2m$.

$\bar{4}2m$	1	2_c	2_a	m	222	mm2	$\bar{4}$
A_1	A	A	A	A'	A	A_1	A
A_2	A	A	B	A''	B_1	A_2	A
B_1	A	A	A	A''	A	A_2	B
B_2	A	A	B	A'	B_1	A_1	B
E	2A	2B	A+B	A'+A''	B_3+B_2	B_2+B_1	E

Consider an irreducible representation $\pi^\circ(G)$ of a group G and an irreducible representation $\rho^\circ(H)$ of a subgroup H. According to the Frobenius reciprocity theorem, the number of times $\pi^\circ(G)$ is contained in the induced representation $\rho^\circ(H)\uparrow G$ into G is equal to the number of times $\rho^\circ(H)$ is contained in the subduced representation $\pi^\circ(G)\downarrow H$ onto H. For instance let us determine the representation of $\bar{4}2m$ induced by the representation $A+3B$ of the subgroup 2_c . From the previous table we see that $A(2_c)$ appears once in $A_1(\bar{4}2m)\downarrow 2_c$, once in $A_2(\bar{4}2m)\downarrow 2_c$, once in $B_1(\bar{4}2m)\downarrow 2_c$ and once in $B_2(\bar{4}2m)\downarrow 2_c$. Therefore $A_1(\bar{4}2m)$, $A_2(\bar{4}2m)$, $B_1(\bar{4}2m)$ and $B_2(\bar{4}2m)$ appear once in $A(2_c)\uparrow \bar{4}2m$. In the same way $E(\bar{4}2m)$ appears twice in $B(2_c)\uparrow \bar{4}2m$ seeing that $B(2_c)$ appears twice in $E(\bar{4}2m)\downarrow 2_c$. Thus one has $(A+3B)(2_c)\uparrow \bar{4}2m = A_1+A_2+B_1+B_2+6E$, owing to the additivity property of representations. Starting from any representation (in reduced form) of the subgroup H, this process enables to construct easily the connected induced representation (in reduced form) of the group G. In practice, it is sufficient to have at one's disposal tables of the representations of the point groups induced by the irreducible representations of their subgroups. As an example, here are given these tables in the case of the point groups $\bar{4}2m$, 32 and 23.

$$\begin{aligned}
 A(1)\uparrow \bar{4}2m &= A_1+A_2+B_1+B_2+2E, & A(2_c)\uparrow \bar{4}2m &= A_1+A_2+B_1+B_2, \\
 B(2_c)\uparrow \bar{4}2m &= 2E, & A(2_a)\uparrow \bar{4}2m &= A_1+B_1+E, \\
 B(2_a)\uparrow \bar{4}2m &= A_2+B_2+E, & A'(m)\uparrow \bar{4}2m &= A_1+B_2+E, \\
 A''(m)\uparrow \bar{4}2m &= A_2+B_1+E, & A(222)\uparrow \bar{4}2m &= A_1+B_1, \\
 B_3(222)\uparrow \bar{4}2m &= E, & B_1(222)\uparrow \bar{4}2m &= A_2+B_2, \\
 B_2(222)\uparrow \bar{4}2m &= E, & A_1(mm2)\uparrow \bar{4}2m &= A_1+B_2, \\
 B_2(mm2)\uparrow \bar{4}2m &= E, & A_2(mm2)\uparrow \bar{4}2m &= A_2+B_1, \\
 B_1(mm2)\uparrow \bar{4}2m &= E, & A(\bar{4})\uparrow \bar{4}2m &= A_1+A_2, \\
 B(\bar{4})\uparrow \bar{4}2m &= B_1+B_2, & 1/2E(\bar{4})\uparrow \bar{4}2m &= E.^\dagger \\
 A(1)\uparrow 32 &= A_1+A_2+2E, & A(2)\uparrow 32 &= A_1+E, & B(2)\uparrow 32 &= A_2+E, \\
 A(3)\uparrow 32 &= A_1+A_2, & 1/2E(3)\uparrow 32 &= E.^\dagger \\
 A(1)\uparrow 23 &= A+E+3T, & A(2)\uparrow 23 &= A+E+T, & B(2)\uparrow 23 &= 2T, \\
 A(222)\uparrow 23 &= A+E, & B_3(222)\uparrow 23 &= T, & B_1(222)\uparrow 23 &= T, \\
 B_2(222)\uparrow 23 &= T, & A(3)\uparrow 23 &= A+T, & 1/2E(3)\uparrow 23 &= 1/2E+T.^\dagger
 \end{aligned}$$

+ E($\bar{4}$), E(3) are 2-dimensional reducible representations consisting of 2 complex-conjugate 1-dimensional irreducible representations.