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An algorithm has been developed that generates all of the nonequivalent closest-packed stacking sequences of length N. There are $2^N + 2(-1)^N$ different labels for closest-packed stacking sequences of length N using the standard A, B, C notation. These labels are generated using an ordered binary tree. As different labels can describe identical structures, we have derived a generalized symmetry group, $Q \simeq D_N \times S_3$, to sort these into crystallographic equivalence classes. This problem is shown to be a constrained version of the classic three-colored necklace problem.

1. Introduction

The most efficient way to pack equal-sized spheres in space is to place them in closest-packed monolayers and stack the monolayers so that the spheres in one layer are over voids in the layer below (Kepler, 1611; Barlow, 1883*a*,*b*; Hales, 2000). Many crystal structures can be represented as a repeating sequence of distorted closest-packed monolayers of anions, with cations in the interstitial voids between or within the monolayers. The variety of possible crystal structures based on a repeat unit of N monolayers depends upon the number of symmetrically nonequivalent stackings of N monolayers. For example, the pyroxene structure can be considered to consist of distorted closest-packed monolayers of O atoms, with alternating layers of tetrahedrally and octahedrally coordinated cations forming chains between the monolayers (Fig. 1). Different pyroxene structures are based on different stacking sequences. Ideal pyroxene topologies based on perfectly closest-packed sequences have been investigated by many authors (*e.g.* Thompson, 1970; Papike *et al.*, 1973; Law & Whittaker, 1980).

We were only able to find one systematic approach to generating stacking sequences in the literature. This approach to deriving the possible nonequivalent stacking sequences of N monolayers was developed by Zhdanov (1945) and extended by Patterson & Kasper (1959). The technique defines an A layer to be any layer with a sphere at [0,0,z]. Plane group $p3m1$ defines the lattice vectors **a** and **b**, and **c** is defined to be orthogonal to these. If the layer above an A layer has a sphere at [2/3, 1/3, $z + c_0$], where $c_0 = |\mathbf{c}|/N$ is the separation between two monolayers, this next layer is termed a B layer. The only other possibility is that the next layer has a sphere at $[1/3, 2/3, z + c_0]$ and, in this case, is called a C layer. If two adjacent monolayers fall somewhere along the ordered sequence $A \rightarrow B \rightarrow C \rightarrow A$ in the stacking direction, then the change between them is called a positive change and one from $A \rightarrow C \rightarrow B \rightarrow A$ is called a negative change. Stacking sequences can be defined in terms of Zhdanov numbers, wherein the digits represent the numbers of successive layers with positive and negative changes. As an example where N = 9, the Zhdanov number 4221 represents the stacking sequence $A^+B^+C^+A^+B^-A^-C^+A^+B^-$. Partitioning a number N into unique Zhdanov numbers gives a set of nonequivalent stacking sequences.

Patterson & Kasper (1959) revisited and extended Zhdanov's work. They added notation to the Zhdanov numbers in order to indicate symmetry operators. Mirror planes can occur only within a monolayer, and only in sequences with an even number of monolayers in the repeat unit. If the first half of the digits in a Zhdanov number repeat in reverse order to complete the number, then there is a mirror plane. This mirror plane is indicated in modified Zhdanov notation by a vertical bar. As an example where N = 8, |31|13| translates to $\underline{A}^+\mathrm{B}^+C^+\mathrm{A}^-\underline{C}^+A^-C^-B^-$ (underlines indicate the location of the mirror planes). Inversion centers in modified Zhdanov numbers are indicated by parentheses. Parentheses around an odd digit in a modified Zhdanov number indicate an inversion center located in the octahedral void between layers and parentheses around an even digit indicate an inversion center located on a sphere. For example, (4)(1) translates to $A^+B^+(C)^+A^+B^{(-)}$, which Patterson and Kasper rewrite as $(C)^+A^+B^{(-)}A^+B^+$, so that the symmetry center is in the first position.

The intent of the Zhdanov approach is to classify different stacking sequences by symmetry. As defined by Zhdanov, a stacking sequence of length N does not necessarily have a physical repeat unit of N monolayers. For stacking sequences with rhombohedral lattices, the repeat unit, in terms of A's, B's and C's, contains $3N$ monolayers. As an example, for $N = 3$, this approach gives a unique stacking sequence with modified Zhdanov notation (2)(1). This translates into a repeat unit of $(A)^+B^{(-)}A^+(B)^+C^{(-)}B^+(C)^+A^{(-)}C^+$. Furthermore, if p is the total number of positive changes represented by a Zhdanov number, n is the total number of negative changes and $(p - n)/3$ is not an integer, then the Zhdanov number represents a sequence with $3N$ monolayers (Beck, 1967). For instance, the Zhdanov number in the previous example is (2)(1). Since $(p - n)/3 = (2 - 1)/3$ is not an integer, the sequence represented by (2)(1) has nine monolayers. Beck rewrites (2)(1) as $2\underline{1}2\underline{1}2\underline{1}$ so that $N = 9$.

Zhdanov numbers make no distinction between ABC and $ABCABCABCABC$. Both of these have Zhdanov number (1)(0).

A general formula for calculating the number of Zhdanov sequences without generating them was developed by Iglesias (1981). Another general formula for calculating the number of sequences that satisfy the Beck criterion was developed by McLarnan (1981*c*).

Our interest lies in creating theoretical closest-packed analogs to crystal structures. When we refer to the length N of a stacking sequence, we mean the number of monolayers in the repeat unit along a stacking vector that is perpendicular to the planes. Thus, we wish to generate the symmetrically nonequivalent ways of mixing up N letters (A's, B's and C's) such that no two adjacent letters are identical. In addition, we cannot consider ABC and $ABCABCABCABC$ to be equivalent when dealing with real crystal structures. Fig. 1 shows a slice of an ideally cubic closest-packed clinopyroxene. Its repeating unit in the stacking direction **a*** is $ABCABCABCABC$.

Law & Whittaker (1980) generated the possible pyroxene and amphibole stacking sequences for the special cases of N = 4 and 8. They used a technique specific to these structures that takes into account the increased number of nonequivalent sequences due to chains of cations running between the monolayers. In this paper, we derive a general mathematical solution and use this to construct an algorithm that will directly generate the possible stacking sequences for any value of N.

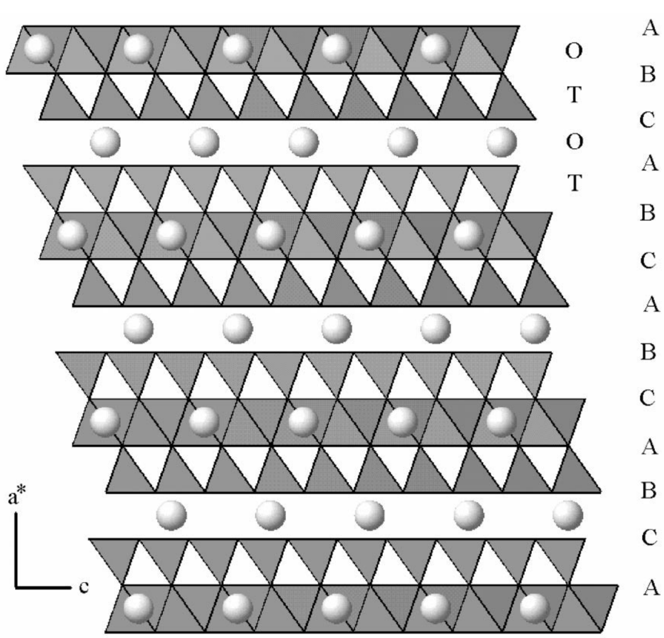

Figure 1
A slice of an ideally cubic closest-packed clinopyroxene showing that the repeat unit in the stacking direction **a*** is 12 monolayers deep.

2. Counting sequences

We first derive a formula for the number of different sequences of N letters (A's, B's and C's) such that no two adjacent letters are identical. Note that many of these sequences will turn out to be equivalent under symmetry operations. Let S_N equal the set of all such sequences. We can determine the number of elements in S_N, $\#S_N$, using the multiplication and addition rules for counting (*cf.* Epp, 1995). There are three choices for the first letter of such a sequence. Each of the next $N - 2$ letters must be different from their predecessors and so each are limited to two possibilities. Therefore, there are $3 \times 2^{N-2}$ partial sequences of length $N - 1$. The last letter of the sequence must be different from both the first and the $(N - 1)$th letter. Let f_A = the fraction of the $3 \times 2^{N-2}$ partial sequences of length $N - 1$ that begin and end with the same letter. For each of these, there are two choices for the Nth letter. There is only one choice for the $3 \times 2^{N-2} \times (1 - f_A)$ remainder of these sequences, since the Nth letter cannot be the same as the first letter or the $(N - 1)$th letter. Counting gives

$$\#S_N = 3 \times 2^{N-2} \times [2f_A + (1 - f_A)]. \quad (1)$$

To derive an expression for f_A, we will use an ordered binary tree of depth N to enumerate our sequences. Fig. 2 illustrates a sequence tree for $N = 4$. The sequences that begin with A are symmetrically equivalent under permutation of the letters to the sequences that begin with B and C, so we will only build trees with A at the root. Owing to this equivalence, f_A = the fraction of the $3 \times 2^{N-2}$ sequences of length $N - 1$ that begin and end with A. Fig. 3 shows two partial branches from an arbitrary sequence tree of depth N, $N > 4$. An examination of the nth row and its two predecessors leads to a formula for the number of A's in row n, a_n. Row $n - 2$ has 2^{n-3} letters, of which m are A's and $(2^{n-3} - m)$ are O's, where O can be either B or C. Each O spawns one A, so row $n - 1$ has 2^{n-2} letters, of which $(2^{n-3} - m)$ are A's, and $(2^{n-3} + m)$ are O's. Row n has 2^{n-1} letters and $(2^{n-3} + m)$ A's. Thus

$$a_n = 2^{n-3} + m = a_{n-1} + 2a_{n-2}.$$

We can now obtain an explicit formula for a_n by using a standard technique for solving a second-order linear homogenous recurrence relation with constant coefficients (*cf.* Epp, 1995). The characteristic equation of our relation for a_n is $t^2 - t - 2 = 0$ with roots 2 and -1. This gives $a_n = C2^n + D(-1)^n$, where C and D are coefficients. Since $a_1 = 1$ and $a_2 = 0$, then

$$a_n = 2^n/6 - 2/3(-1)^n$$

and

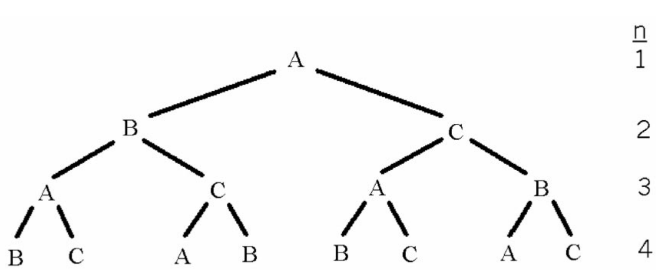

Figure 2
An ordered binary tree representation of all the possible sequences of A's, B's and C's of length $N = 4$ that start with A. Sequences ending in A are not valid closest-packed stacking sequences. Sequences starting with B or C are symmetrically equivalent under the permutation of letters and need not be considered in the quest for representative nonequivalent sequences.

$$f_A = a_{N-1}/2^{N-2}.$$

Making the appropriate substitutions into (1) gives the total number of non-unique stacking sequences

$$\#S_N = 2^N + 2(-1)^N. \quad (2)$$

For example, there are 258 different sequences for $N = 8$.

3. Sorting sequences

Since many of these sequences are equivalent under symmetry operations, we need to partition S_N into symmetrical equivalence classes. From these we can choose representative examples of every nonequivalent sequence of length N. There are three types of symmetry operations under which stacking sequences are equivalent. The first type is permutation of letters, *e.g.* $ABCAB \simeq BCABC$. Note that it is not the physical positions of the letters that are being permuted, but rather which letters are chosen to label the given positions in the sequence. For instance, the permutation (AB) replaces all of the A's with B's and *vice versa*. Such a permutation can result from moving the origin within a monolayer, or rotating the basis vectors **a** and **b** 60° around **c** or a combination of these operations. The details of these permutations are given in the *Appendix*. These permutations form a group of the order 6, isomorphic to the symmetric group S_3. We label this group $P = \{p_i \mid 0 \le i < 6\} = \{1,(AB),(AC),(BC),(ABC),(ACB)\}$.

The second type of symmetry operation reverses the order of the letters in a sequence, *e.g.* $ABCAB \cong BACBA$. The essential feature that distinguishes this symmetry operation from the others is that it reverses the direction of **c** (see *Appendix*), *i.e.* reverses the stacking direction. A double reversal is the identity. We label this operation b. Note that $b^0 = b^2 = e$.

Finally, to illustrate the third type of symmetry operation, let $s \in S_N$. Then s can be written as $L_1L_2...L_N$, where $L_i \in \{A, B, C\}$. Define an operator r such that $r^i(s) = L_{i+1}L_{i+2}...L_NL_1...L_i$. For example, $r^2(ABCAB) = CABAB$, so $ABCAB \simeq CABAB$. Such a rearrangement results from moving the origin along **c**. The operators b and r relate as follows: $r^ib = br^{N-i}$. Thus, they generate a group $R = \{r, b | r^N = b^2 = (rb)^2 = 1\}$ isomorphic to the dihedral group D_N.

Let the group $Q = R \times P = \{q_m = (r^ib^j, p_k) \mid 0 \le i < N, 0 \le j \le 1, 0 \le k \le 5, m = 6i + 6Nj + k\} \simeq D_N \times S_3$ act on S_N so that $q_m(s) = (r^ib^j, p_k)(s) = r^i(b^j(p_k(s)))$. Then $s_2 \simeq s_1$ if and only if $s_2 = q(s_1)$, for some $q \in Q$, is an equivalence relation on S_N, and

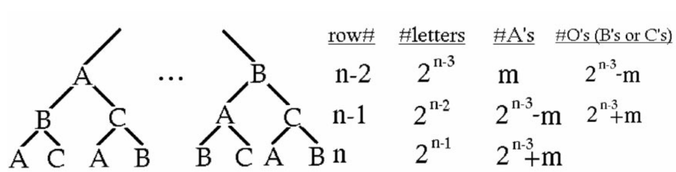

Figure 3
Two branches of an ordered binary sequence tree showing the number of A's in row $n = 2^{n-3} + m = a_{n-1} + 2a_{n-2}$, where a_x is the number of A's in row x.

Table 1
The two nonequivalent sequences for $N = 4$ and their symmetrical equivalents.

ABAB	*ABAC*
ACAC	*ABCB*
BABA	*ACAB*
BCBC	*ACBC*
CACA	*BABC*
CBCB	*BACA*
	BCBA
	BCAC
	CACB
	CABA
	CBCA
	CBAB

Table 2
N and its number of nonequivalent sequences.

1	0
2	1
3	1
4	2
5	1
6	4
7	3
8	8
9	8
10	18
11	21
12	48
13	63
14	133
15	205
16	412
17	685
18	1354
19	2385
20	4644
21	8496
22	16 431
23	30 735
24	59 344

the orbit of s under Q is the set of all sequences that are symmetrically equivalent to s. Q acts on S_N to partition S_N into symmetrical equivalence classes.

4. Algorithm

We designed an algorithm to generate and sort S_N into its symmetrical equivalence classes. First, we build a tree of depth N (Fig. 2) with the letter A at the root, because the trees beginning with B and C are symmetrically equivalent to A under the action of P. Next, the algorithm chooses the sequence held in the leftmost branch of the tree and operates on it with Q. All the resulting sequences, $q_m(s)$, which start with A are marked in the tree as belonging to the same orbit. Sequences that start with B or C are ignored because they are symmetrically equivalent to sequences beginning with A. When this is completed, the algorithm looks for an unmarked sequence and the process begins again. Finally, the tree is traversed and one example from each orbit is output.

5. Results

Table 1 contains two representative nonequivalent sequences for $N = 4$ along with their symmetrical equivalents. Table 2 contains the number of nonequivalent sequences for $N = 1$–24. Table 3 lists those sequences for $N \leq 12$ as determined by our algorithm, including notation using modified Zhdanov numbers (Patterson & Kasper, 1959) and *hc* symbols (*cf.* O'Keeffe & Hyde, 1996).

6. Mathematical context

There is also an analytical procedure that can be followed to generate these sequences. It is based on the solution to a constrained version of the classic necklace problem: How many distinguishable necklaces can be made from N beads, where the beads are chosen from three different colors? The first constraint is that permuted color sequences are considered to be equivalent, *i.e.* blue–red–blue–yellow $\simeq$ red–yellow–red–blue. Note that the colors are permuted, not the beads. The important information is that the first and third beads are the same color, while the second and fourth are different from them and each other. The coloring scheme chosen to communicate this information is not important. The second constraint is that no two adjacent beads can be the same color. This problem is amenable to attack using Pólya theory (*cf.* Grove, 1997). For examples of application of Pólya theory to crystallographic problems, see McLarnan (1978, 1981*a*,*b*,*c*) and Hawthorne (1983).

Any permutation, $\sigma \in$ group G, that acts on a set, S, partitions S. Each element of S in a given partition, p, is cyclically related to every other element in p under the action of σ. A polynomial called the cycle index, Z, of the action of G on S can be created that catalogs the ways each element of G partitions S. For example, examine $Z_{D4,V4} = 1/8({t_1}^4 + 3{t_2}^2 + 2t_4 + 2{t_1}^2t_2)$, the cycle index of the action of the dihedral group D_4 on V_4, the set of vertices of a square (or the beads in a four-beaded necklace). By way of illustration, we dissect the term $2{t_1}^2t_2$. The coefficient 2 indicates that the rest of the term describes how two of the elements of D_4 partition V_4. They both break V_4 into three subsets. The exponent in ${t_1}^2$ indicates two subsets, while the subscript indicates that each contains one vertex. The indeterminate, t_2, represents one subset containing two vertices. These two elements are the 180° rotations about the diagonals of the square. These rotations leave the vertices at the ends of the rotation axis fixed, while taking the other two vertices into each other.

We choose to color the vertices of our square with the letters A, B or C. Substituting $t_1 = A + B + C$, $t_2 = A^2 + B^2 + C^2$, $t_4 = A^4 + B^4 + C^4$ into $Z_{D4,V4}$ gives the pattern inventory $\mathrm{PI}_{D4,V4} = A^4 + B^4 + C^4 + A^3B + A^3C + B^3C + AB^3 + AC^3 + BC^3 + 2A^2B^2 + 2A^2C^2 + 2B^2C^2 + 2A^2BC + 2AB^2C + 2ABC^2$. *Maple* software (Char *et al.*, 1991) was used to construct this pattern inventory. $\mathrm{PI}_{D4,V4}$ tells us how many symmetrically distinguishable necklaces can be made from different combinations of four letters. For instance, the term $2A^2BC$ indicates

Table 3
The unique closest-packed stacking sequences of length $N \leq 12$.

N	*ABC* notation	Zhdanov number	*hc* notation
1	None		
2	*AB*	|(1)|(1)|	*h*
3	*ABC*	(1)(0)	*c*
4	*ABAB*	|(1)|(1)|	*h*
	ABAC	|(2)|(2)|	*hc*
5	*ABABC*	(4)(1)	*hhccc*
6	*ABABAB*	|(1)|(1)|	*h*
	ABABAC	|21|12|	*hhhchc*
	ABACBC	|(3)|(3)|	*hcc*
	ABCABC	(1)(0)	*c*
7	*ABABABC*	(4)1(1)1	*hhhhccc*
	ABABCAC	(3)1(2)1	*hhcchhc*
	ABACABC	(5)(2)	*hchcccc*
8	*ABABABAB*	|(1)|(1)|	*h*
	ABABABAC	|211|112|	*hhhhhchc*
	ABABACAC	|1(2)1|1(2)1|	*hhhc*
	ABABACBC	|31|13|	*hhhcchcc*
	ABABCABC	(7)(1)	*hhcccccc*
	ABABCBAC	(3)2(1)2	*hhchcchc*
	ABACABAC	|(2)|(2)|	*hc*
	ABACBABC	|(4)|(4)|	*hccc*
9	*ABABABABC*	(4)11(1)11	*hhhhhhccc*
	ABABABCAC	312111	*hhhhcchhc*
	ABABACABC	5211	*hhhchcccc*
	ABABCABAC	4221	*hhccchchc*
	ABABCACBC	(2)3(1)3	*hhcchchcc*
	ABABCBCAC	(2)(1)	*hhc*
	ABACBACBC	(6)(3)	*hccccchcc*
	ABCABCABC	(1)(0)	*c*
10	*ABABABABAB*	|(1)|(1)|	*h*
	ABABABABAC	|2111|1112|	*hhhhhhhhchc*
	ABABABACAC	|1211|1121|	*hhhhhchhhc*
	ABABABACBC	|311|113|	*hhhhhcchcc*
	ABABABCABC	(7)1(1)1	*hhhhcccccc*
	ABABABCBAC	(3)21(1)12	*hhhhchcchc*
	ABABACABAC	|221|122|	*hhhchchchc*
	ABABACACBC	321211	*hhhchhchcc*
	ABABACBABC	|41|14|	*hhhccchccc*
	ABABACBCBC	|1(3)1|1(3)1|	*hhhcc*
	ABABCABABC	(4)(1)	*hhccc*
	ABABCABCAC	(6)1(2)1	*hhcccccchhc*
	ABABCABCBC	(5)1(3)1	*hhccccchhcc*
	ABABCACBAC	4312	*hhcchccchc*
	ABABCBABAC	|2(1)2|2(1)2|	*hhchc*
	ABACABACBC	|32|23|	*hchchcchcc*
	ABACABCABC	(8)(2)	*hchcccccccc*
	ABACBACABC	|(5)|(5)|	*hcccc*
11	*ABABABABABC*	(4)111(1)111	*hhhhhhhhccc*
	ABABABABCAC	312111111	*hhhhhhcchhc*
	ABABABACABC	5211111	*hhhhhchcccc*
	ABABABCABAC	422111	*hhhhccchchc*
	ABABABCACAC	(3)111(2)111	*hhhhcchhhhc*
	ABABABCACBC	(2)31(1)13	*hhhhcchchcc*
	ABABABCBCAC	(2)121(1)121	*hhhhchhchhc*
	ABABACABABC	412211	*hhhchchhccc*
	ABABACABCAC	421121	*hhhchccchhc*
	ABABACABCBC	313211	*hhhchcchhcc*
	ABABACACABC	(5)11(2)11	*hhhchhhcccc*
	ABABACBACBC	6311	*hhhccccchcc*
	ABABCABACBC	4331	*hhccchcchcc*
	ABABCABCABC	(10)(1)	*hhccccccccc*
	ABABCABCBAC	5321	*hhccccchcchc*
	ABABCACABAC	(3)12(2)21	*hhcchhchchc*
	ABABCACBCAC	322121	*hhcchchchhc*
	ABABCBACBAC	(6)2(1)2	*hhchccccchc*
	ABACABACABC	(5)2(2)2	*hchchchcccc*
	ABACABCACBC	(4)2(3)2	*hchccchchcc*
	ABACBABCABC	(7)(4)	*hccchcccccc*
12	*ABABABABABAB*	|(1)|(1)|	*h*
	ABABABABABAC	|21111|11112|	*hhhhhhhhhhchc*
	ABABABABACAC	|12111|11121|	*hhhhhhhhchhhc*
	ABABABABACBC	|3111|1113|	*hhhhhhhcchcc*
	ABABABABCABC	(7)11(1)11	*hhhhhhcccccc*
	ABABABABCBAC	(3)211(1)112	*hhhhhhchcchc*
	ABABABACABAC	|2211|1122|	*hhhhhchchchc*
	ABABABACACAC	|11(2)11|11(2)11|	*hhhhhc*
	ABABABACACBC	32121111	*hhhhhchhchcc*
	ABABABACBABC	|411|114|	*hhhhhccchccc*
	ABABABACBCBC	|1311|1131|	*hhhhhcchhhcc*
	ABABABCABABC	(1)14(1)41	*hhhhccchhccc*
	ABABABCABCAC	612111	*hhhhcccccchhc*
	ABABABCABCBC	513111	*hhhhccccchhcc*
	ABABABCACBAC	342111	*hhhhcchccchc*
	ABABABCBABAC	(1)221(1)122	*hhhhchchhchc*
	ABABABCBACAC	32111211	*hhhhchcchhhc*
	ABABACABABAC	|21|12|	*hhhchc*
	ABABACABACAC	(2)211(2)112	*hhhchchchhhc*
	ABABACABACBC	332211	*hhhchchcchcc*
	ABABACABCABC	8211	*hhhchcccccccc*
	ABABACABCBAC	|123|321|	*hhhchccchcchc*
	ABABACACBABC	312114	*hhhchhcchccc*
	ABABACACBCAC	|2121|1212|	*hhhchhchchhc*
	ABABACACBCBC	(3)112(1)211	*hhhchhchhhcc*
	ABABACBABABC	|1(4)1|1(4)1|	*hhhccc*
	ABABACBABCBC	312411	*hhhccchchhcc*
	ABABACBACABC	|51|15|	*hhhcccchcccc*
	ABABACBCACBC	|231|132|	*hhhcchchchcc*
	ABABCABABCAC	413121	*hhccchhcchhc*
	ABABCABACABC	5241	*hhccchchcccc*
	ABABCABACBAC	5412	*hhccchccccchc*
	ABABCABCABAC	7221	*hhccccccchchc*
	ABABCABCACBC	6231	*hhcccccchhcc*
	ABABCABCBCAC	(5)12(1)21	*hhccccchchhc*
	ABABCACABCBC	(3)(1)	*hhcc*
	ABABCACBABAC	|312|213|	*hhcchcchhchc*
	ABABCACBACBC	(5)3(1)3	*hhcchcccchcc*
	ABABCACBCBAC	123123	*hhcchchhcchc*
	ABABCBABCBAC	322212	*hhchchchcchc*
	ABABCBACBCAC	(4)21(2)12	*hhchccchchhc*
	ABACABACABAC	|(2)|(2)|	*hc*
	ABACABACBABC	|42|24|	*hchchccchccc*
	ABACABCBACBC	(4)3(2)3	*hchcchccchcc*
	ABACBACBACBC	(9)(3)	*hcccccccchcc*
	ABACBACBCABC	|(6)|(6)|	*hccccc*
	ABACBCABACBC	|(3)|(3)|	*hcc*
	ABCABCABCABC	(1)(0)	*c*

that there are two distinguishable necklaces made from two *A*'s, one *B* and one *C*.

We now introduce the constraint that permutations of the letters are equivalent. Thus, $A^4 \simeq B^4 \simeq C^4$. Removing terms which are equivalent under this condition results in the modified pattern inventory $\mathrm{MPI}_{Q\,=\,D4\,\times\,S3,V4} = A^4 + A^3B + 2A^2B^2 + 2A^2BC$.

We now apply the final constraint that no two adjacent letters be the same. Any term that has an exponent $e > N/2$ must have adjacent letters, so we need look only at $2A^2B^2 + 2A^2BC$. The two distinguishable necklaces from two *A*'s and two *B*'s are *ABAB* and *AABB*. The two distinguishable necklaces from two *A*'s and one *B* and one *C* are *ABAC* and *AABC*. Therefore, all closest-packed stacking sequences of length $N = 4$ are equivalent to either *ABAB* or *ABAC*. Table 4

Table 4
The number of distinguishable necklaces possible using N beads of three colors, then with the constraint that necklaces whose bead colors are permutations of each other are considered equivalent, and finally such that no two adjacent beads are the same color.

N	1	2	3	4	5	6	7	8	9	10	11	12
Necklaces	3	6	10	21	39	92	198	498	1219	3210	8418	22 913
One constraint	1	2	3	6	9	22	40	100	225	582	1464	3960
Two constraints	0	1	1	2	1	4	3	8	8	18	21	48

shows how adding these constraints reduces the number of possibilities.

The cycle index for the action of $Q \simeq D_N \times S_3$ on S_N also contains useful information, although it is much more difficult to construct than that for D_N on V_N. If we replace t_1 by $1 + x$, t_2 by $1 + x^2$ *etc.*, the coefficient of x is the number of orbits of Q in S_N, which is the number of nonequivalent closest-packed stacking sequences of length N. For $N = 4$, $Z_{Q,S} = 1/48(t_1^{18} + 5t_2^9 + 2t_3^6 + 4t_6^3 + 12t_1^2t_2^8 + 3t_1^4t_2^7 + t_1^6t_2^6 + 2t_1^{12}t_2^3 + 2t_2^3t_4^3 + 2t_3^2t_6^2 + 4t_3^4t_6 + 4t_6t_{12} + 6t_1^2t_2^2t_4^3)$. Making the described replacement gives a coefficient of 2 in the x term.

7. Summary

A given position in a closest-packed stacking sequence label can have one of three values: A, B or C. The action of the group $Q \simeq D_N \times S_3$ on a given sequence explicitly described with A's, B's and C's generates all equivalent sequences. This action is effected through certain types of simple rearrangements of the letters of the sequence. Each rearrangement represents a change of basis. An ordered binary tree can be used to generate all possible stacking sequences of length N and Q can be used to sort them out.

APPENDIX *A*

A1. Permutations

Define α to be a rotation of 60° around **c**. Then $\alpha(A) = A$, $\alpha(B) = C$, $\alpha(C) = B$. Define t_1 to be a translation of the origin to [2/3,1/3,z]. Then $t_1(A) = C$, $t_1(B) = A$, $t_1(C) = B$ and $\alpha t_1(A) = B$, $\alpha t_1(B) = A$, $\alpha t_1(C) = C$. Define t_2 to be a translation of the origin to [1/3,2/3,z]. Then $t_2(A) = B$, $t_2(B) = C$, $t_2(C) = A$ and $\alpha t_2(A) = C$, $\alpha t_2(B) = B$, $\alpha t_2(C) = A$. Thus, $P = \{e, \alpha, t_1, t_2, \alpha t_1, \alpha t_2\}$.

A2. Reversals

An exact reversal of the order of letters in a sequence, s, is accomplished by the operation $r_1\alpha^{[100]}2(s)$, where r_1 shifts the origin by the distance c_0 along **c** and $c_0 = |\mathbf{c}|/N$ is the separation between two monolayers, α is defined as above and $^{[100]}2$ is a twofold rotation parallel to **a**.

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