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Author
Balasubramanian, K.

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K. Balasubramanian

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Computer Generation of Isomers

K. Balasubramanian

Department of Chemistry
and
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

Abstract

A computer program is developed for the enumeration of the isomers of polysubstituted compounds with b_1 substituents of the type 1, b_2 substituents of the type 2,....,b_n substituents of the type n. The procedure is illustrated with octahedral molecules containing 4 kinds of substituents (such as F, Cl, Br and I) and the isomers of polysubstituted non-rigid pentane with 4 kinds of substituents.

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1. Introduction

Chemical applications of non-numerical computational methods are becoming quite important in recent years. (Randić (1975), Randić (1979), Randić (1980), Masinter et al. (1974a,b), Balasubramanian (1982a,b), Balasubramanian et al. (1980a), Dolhaine (1981)). Several of these papers concern developing algorithms for the generation of discrete combinatorial structures and their applications to chemistry. Recently, Dolhaine (1981) has developed a computer program for the enumeration of isomers of molecules containing 2 kinds of substituents. Balasubramanian (1981d) developed a combinatorial technique for nuclear spin statistics in molecular spectroscopy which was subsequently computerized (Balasubramanian (1982a,b)). In the present paper we develop computer programs and algorithms for the enumeration of isomers of polysubstituted compounds containing several kinds of substituents. The program that we use here is more general than the one given by Dolhaine (1981) in that this program can handle more than 2 substituents by way of multinomial expansions.

The history of isomer enumeration goes back to the last century. Several papers have appeared both in mathematical and chemical literature. (Balaban (1976), Balaban, et al. (1976), Balaban (1975), Balasubramanian (1978, 1979a-c, 1981a-b), Dolhaine (1980), King (1972), Klein and Cowley (1978), Mislow (1976), Nourse (1979), Pólya (1937), Robinson (1970), and Ruch et al. (1970)). The topic has been reviewed by Rouvray (1974, 1975) and in the recent book by Balaban (1976). As pointed out by Dolhaine (1981) recently, even though these methods provide

for generators of isomers, yet, one needs to evaluate several polynomial generators and in general several polynomial products of multinomials. Consequently, an efficient and general computer program is warranted for polysubstituted compounds.

In the present paper we develop algorithms and computer programs which generate isomers of polysubstituted compounds with a minimal input. The required input for this program is just the cycle index and the information concerning the kinds of substituents. The program generates the total generating function wherein the coefficients of the various terms printed out give the number of isomers.

2. Theory

Let G be a group acting on a discrete set D, which is the set of sites in the molecule that can accommodate substituents. Let R be the set of substituents. In general let $|S|$ denote the number of elements in a set S. Consider the set F of maps from D to R. Each element in this set is a map of sites to substituents and consequently, a way in which substituents can be placed on available sites. However, not all maps in F are distinct because one map can be equivalent to another by the action of G which permutes the sites and hence the maps. This action of G on D induces equivalence of maps in F. Two maps f_i and f_j are equivalent if there exists a $g \in G$ such that

$$f_i(d) = f_j(gd), \quad d \in D.$$

Thus maps in F that are equivalent can be grouped together into equivalence classes. A representative in each class is an isomer

and the number of equivalence classes is exactly the number of isomers. In order to book-keep the number of different substituents in a map we introduce the concept of weight of a substituent. Let $w(r)$ be the weight of a substituent r in R. Then with each map $f \in F$, we can associate a weight

$$W(f) = \prod_{d \in D} w(f(d)).$$

For example, if $w_1, w_2, \ldots w_\ell$ are the weights of ℓ substituents in the set R and if a structure contains b_1 substituents of the type 1, b_2 substituents of the type 2,...., b_ℓ substituents of the type ℓ, then the weight of this function would be $w_1^{b_1} w_2^{b_2} \ldots . w_\ell^{b_\ell}$. Pólya (1937) proved a theorem now well-known as Pólya's theorem which gives a generating function for the equivalence classes of maps in F from a group structure known as the cycle index of a group G. With each element $g \in G$ we can associate a cycle representation $x_1^{b_1} x_2^{b_2} \ldots . x_n^{b_n}$ if g has b_1 cycles of length 1, b_2 cycles of length 2,....,b_n cycles of length n. To illustrate, the permutation (12)(345)(67)(89) would have the cycle representation $x_2^3 x_3$ since it has 3 cycles of length 2 and a cycle of length 3. Then one can define a group structure known as the cycle index of a group G, P_G, defined as follows.

$$P_G(x_1, x_2, \ldots) = \frac{1}{|G|} \sum_{g \in G} x_1^{b_1} x_2^{b_2} \ldots . x_n^{b_n} \qquad (1)$$

Pólya (1937) proved that the generating function (G.F.) for isomers is obtained by replacing every x_k by $\sum_{r \in R} (w(r))^k$. In symbols,

$$G.F. = P_G(x_k \rightarrow \sum_{r \in R} (w(r))^k). \qquad (2)$$

3. Algorithms and Programs

As noted by Dolhaine (1981), even though the above theorem is an elegant way to generate isomers, yet, one has to expand several multinomials (in general) and collect the coefficients in various terms. Thus a computer program is warranted for a general polysubstituent compound. Dolhaine's recent program can handle at most 2 substituents. We formulate here an algorithm and computer program, in general, for any number of substituents.

To illustrate, consider an octahedral molecule which contains 6 substitutional sites. The cycle index of the rotational group O of this molecule is shown below.

$$P_O = \frac{1}{24}\,(x_1^6 + 6x_1^2x_4 + 3x_1^2x_2^2 + 6x_2^3 + 8x_3^2) \qquad (3)$$

If the set R has 4 different substituents with the weights a, b, c, and d, then by Pólya's theorem the generating function is given by the following expression.

$$\text{G.F.} = \frac{1}{24}\,[(a+b+c+d)^6 + 6(a+b+c+d)^2(a^4+b^4+c^4+d^4) + 3(a+b+c+d)^2 \times (a^2+b^2+c^3+d^2)^2 + 6(a^2+b^2+c^2+d^2)^3 + 8(a^3+b^3+c^3+d^3)^2]. \qquad (4)$$

The above generating function has several multinomials which have to be expanded, multiplied and added together. The final generating function thus obtained contains 84 unique terms. Thus one can see that the problem addressed here is sufficiently complex that a computer program is warranted for this purpose.

A. Generation of Unique Terms in the Generating Function

With each term $w_1^{b_1} w_2^{b_2} \ldots . w_\ell^{b_\ell}$ we can associate a vector $(b_1, b_2, \ldots, b_\ell)$ such that $\sum_i b_i$ equals the total number of substitutional sites. Let the total number of sites be $|D|$. Then the problem of generating the unique terms in the generating function amounts to generating all vectors $(b_1, b_2, \ldots, b_\ell)$, $b_i \geq 0$ such that $\sum_i b_i = |D|$. This indeed corresponds to the compositions of the integer $|D|$ into $|R|$ parts since $|R| = \ell$ is the number of substituents. This number can be found using the following logic. The procedure shown below is the one given by Nijennuis and Wilf (1975). Suppose we wish to distribute $|D|$ indistinguishable balls into $|R|$ labelled cells such that any cell contains 0, 1, 2,....up to $|D|$ balls, then each such distribution yields a composition. This can be accomplished by constructing the cell boundaries as follows. Consider a cell containing 2 walls with $|D| + |R| - 1$ spaces as shown below.

$$\overset{|}{1}\ \overset{|}{2}\ \cdots\cdots\ \overset{|}{|D|+|R|}\ \overset{|}{|D|+|R|+1}$$

The number of ways of distributing $|D|$ balls in the available $|D| + |R| - 1$ spaces is

$$\binom{|D| + |R| - 1}{|D|}$$

After distributing these balls cell boundaries can be constructed in the rest $|R| - 1$ available spaces. Such an arrangement contains exactly $|R|$ cells among which we have distributed $|D|$ indistinguishable balls. Consequently, we have obtained a composition of $|D|$ into $|R|$ parts. The above procedure has

facilitated not only a method to count the number of compositions but also to construct them. The above procedure, in fact, amounts to finding all $|R|-1$ subsets from a $|D| + |R|-1$ set. There are standard combinatorial algorithms for this purpose, for example, see the algorithm NEXCOM given by Nijenhuis and Wilf (1975). The subroutine which is based on this algorithm generates all the unique terms in the generating function for isomers.

B. Generation of Coefficients (the number of isomers in the Generating Function)

A subroutine called "VEC" expands each multinomial in the generating function (the terms are given by the subroutine NEXCOM). By expand we mean that it generates the coefficient for each unique term in a multinomial. Then it multiplies together several multinomials contained in each term of the cycle index. For example, the second term in the generating function for the isomers of polysubstituted octahedral compounds has two multinomials shown below.

$$(a+b+c+d)^2(a^4+b^4+c^4+d^4).$$

VEC expands each multinomial separately then multiplies them together and returns the total coefficients and terms in this product. The main program multiplies these coefficients with the corresponding coefficient in the cycle index and adds to the previously generated vector and coefficients. In this manner the program scans through all the terms in the cycle index and generates the overall generating function for isomers.

C. Input and Output Descriptions

The present program can actually handle the generalized character cycle indices introduced elsewhere (Balasubramanian (1981d). For the present purpose, however, we need to consider only the cycle index corresponding to the totally symmetric representation. The required input is essentially the coefficients and various terms in the cycle index. Note that to generate isomers, we restrict ourselves to the totally symmetric irreducible representation (which we denote by A1) of the rotational subgroup. The input description is shown in Table 1. We will expound further here on this table with examples. Let us consider the rotational group D_4 acting on 4 corners of a square. The cycle index is shown below.

$$P_G = \frac{1}{8} (x_1^4 + 3x_2^2 + 2x_4 + 2x_1^2x_2) \qquad (5)$$

In particular we will concentrate on cards ensuing the fourth card. The last term $x_1^2x_2$ in the cycle index has 2 components (NPRO = 2), the superfix and suffix of the first component is 2 and 1 (because it is x_1^2), while for the second component it is 1 and 2. Cards 4-9 are shown below for this cycle index.

Card						
4	5					(Number of terms in the cycle index)
5	1	3	2	2		(Coefficients in the same order as shown in (5))
6	1	4	1			(The first term)
7	1	2	2			(The second term)
8	1	1	4			(The third term)
9	2	2	1	1	2	(The fourth term).

An example of a complete input is given in Table 2 for the isomers of polysubstituted octahedral compounds. The cycle index for this case is shown in Eq (3). We consider 4 different substituents. The output corresponding to this input is shown in Table 3. As one can see, Table 3 contains the total number of all isomers, the number of isomers with different types of substituents. The vector in each term of the generating function gives the number of times several different substituents occur. For example, a typical vector $(b_1,b_2,\ldots,b_\ell)$, stands for the isomers of a molecule containing b_1 substituents of the type 1, b_2 substituents of the type 2,....,b_ℓ substituents of the type ℓ. The coefficient of the corresponding vector gives the number of isomers of that kind. For example, the coefficient of the vector (4, 2, 0, 0) is 2 indicating there are 2 isomers for a compound of the type Mx_4Y_2, where M is the atom at the center.

As a second example let us consider a non-rigid unbranched pentane with 4 different substituents. The cycle index is shown below with the rotational group being the generalized wreath product $C_2[C_3,E]$. For details of the cycle index of generalized wreath product, see Balasubramanian (1979a).

$$P(C_2[C_3,E]) = \frac{1}{18}\,[x_1^{12} + 4x_1^9x_3 + 4x_1^6x_3^2 + 3x_2^6 + 6x_2^3x_6]. \qquad (6)$$

The input and the output for this molecule are shown in Tables 4 and 5, respectively.

D. Limitations and Error Messages

Arrays in the present program are dimensioned to sufficiently large numbers that most of the chemically interesting cases can be handled. The present program can handle generating functions of isomers with at most 1000 terms. Nevertheless, the program can be easily modified by a suitable expansion of arrays. The present version is restricted to cycle index which contains terms $x_1^{b_1} x_2^{b_2} \ldots x_n^{b_n}$ with $n \leq 5$. For $n \geq 6$, a message is printed out by the subroutine VEC specifying this limitation. This subroutine contains comment statements giving instructions as to where modifications are necessary.

This program can detect a number of inconsistent input errors. For example, it checks each term $x_1^{b_1} x_2^{b_2} \ldots x_n^{b_n}$ in the cycle index to see if that term satisfies the following condition.

$$\sum_{i=1}^{n} ib_i = |D| = NT.$$

If this condition is not met then the program prints out an error message "Input error for this term check N(I), I exp(I)". The user should check the term just printed out and correct it. The second error message is based on the requirement that the coefficient of any term in the polynomial

$$|G| \; P_G(x_k \rightarrow \sum_{r \in R} (w(r))^k)$$

should be divisible by $|G|$. If not the program prints out an error message "ICO(J) is not divisible by MODG. Input error". The error is either in the set of coefficients in the cycle index or in the terms of the cycle index that could not otherwise be detected by the earlier criterion.

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Table 1. Input for the Program Isomer

Card	Format	Input Variables	Description
1	10A8	Title	Alphanumeric title
2	16I5	NGCI	Number of cycle indices. Always 1 for generating isomers.
		NSUBS	|R|, number of different substituents.
		NT	|D|, total number of substitutional sites
		MODG	|G|, number of elements in the group G.
3	A10	SYM	Label of the irreducible representation. For the generation of Isomers it is always A1.
4	16I5	NCI	Number of terms in the cycle index.
5	16I5	ICOCI(2), I=1, NCI	Coefficients of NCI terms in the cycle index.
For each J=1, NCI feed a card described as Card 6.			
6	16I5	NPRO	Number of distinct components in each term of the cycle index
		N(I,J), I=1, NPRO	The superfixes of each component of a term in the cycle index.
		Iexp(I,J), I=1, NPRO	The suffixes of each component of a term in the cycle index.

Table 2. Input for the Isomers of Octahedral Molecules with Six Different Substituents

Card					
1	Isomers of polysubstituent octahedral molecules				
2	1	4	6	24	
3	A1				
4	5				
5	1	6	3	6	8
6	1	6	1		
7	2	2	1	1	4
8	2	2	2	1	2
9	1	3	2		
10	1	2	3		

Table 3

```
 ISOMERS OF POLYSUBSTITUTED OCTAHEDRAL COMPOUNDS
A1
NPRO,N(I),I=1,NPRO     1     6
 IEXPS     1
NPRO,N(I),I=1,NPRO     2     2     1
 IEXPS     1     4
NPRO,N(I),I=1,NPRO     2     2     2
 IEXPS     1     2
NPRO,N(I),I=1,NPRO     1     3
 IEXPS     2
NPRO,N(I),I=1,NPRO     1     2
 IEXPS     3
     TOTAL NUMBER OF ISOMERS       240
   THE GENERATING FUNCTION FOR ISOMERS
 COEFFICIENT            VECTOR
```

1	6	0	0	0
1	5	1	0	0
2	4	2	0	0
2	3	3	0	0
2	2	4	0	0
1	1	5	0	0
1	0	6	0	0
1	5	0	1	0
2	4	1	1	0
3	3	2	1	0
3	2	3	1	0
2	1	4	1	0
1	0	5	1	0
2	4	0	2	0
3	3	1	2	0
6	2	2	2	0
3	1	3	2	0
2	0	4	2	0
2	3	0	3	0
3	2	1	3	0
3	1	2	3	0
2	0	3	3	0
2	2	0	4	0
2	1	1	4	0
2	0	2	4	0
1	1	0	5	0
1	0	1	5	0
1	0	0	6	0
1	5	0	0	1
2	4	1	0	1
3	3	2	0	1
3	2	3	0	1
2	1	4	0	1
1	0	5	0	1
2	4	0	1	1
5	3	1	1	1
8	2	2	1	1
5	1	3	1	1
2	0	4	1	1
3	3	0	2	1
8	2	1	2	1
8	1	2	2	1
3	0	3	2	1
3	2	0	3	1
5	1	1	3	1
3	0	2	3	1

2	1	0	4	1
2	0	1	4	1
1	0	0	5	1
2	4	0	0	2
3	3	1	0	2
6	2	2	0	2
3	1	3	0	2
2	0	4	0	2
3	3	0	1	2
8	2	1	1	2
8	1	2	1	2
3	0	3	1	2
6	2	0	2	2
8	1	1	2	2
6	0	2	2	2
3	1	0	3	2
3	0	1	3	2
2	0	0	4	2
2	3	0	0	3
3	2	1	0	3
3	1	2	0	3
2	0	3	0	3
3	2	0	1	3
5	1	1	1	3
3	0	2	1	3
3	1	0	2	3
3	0	1	2	3
2	0	0	3	3
2	2	0	0	4
2	1	1	0	4
2	0	2	0	4
2	1	0	1	4
2	0	1	1	4
2	0	0	2	4
1	1	0	0	5
1	0	1	0	5
1	0	0	1	5
1	0	0	0	6

Table 4. Input for the Isomers of Polysubstituted Unbranched Pentane with Four Kinds of Substituents

Card					
1	Isomers of unbranded polysubstituted pentanes				
2	1	4	12	18	
3	A1				
4	5				
5	1	4	4	3	6
6	1	12	1		
7	2	9	1	1	3
8	2	6	2	1	3
9	1	6	2		
10	2	3	1	2	6

Table 5

```
 ISOMERS OF UNBRANCHED POLYSUBSTITUTED PENTANES
A1
NPRO,N(I),I=1,NPRO     1    12
 IEXPS    1
NPRO,N(I),I=1,NPRO     2     9     1
 IEXPS    1     3
NPRO,N(I),I=1,NPRO     2     6     2
 IEXPS    1     3
NPRO,N(I),I=1,NPRO     1     6
 IEXPS    2
NPRO,N(I),I=1,NPRO     2     3     1
 IEXPS    2     6
     TOTAL NUMBER OF ISOMERS  1180416
   THE GENERATING FUNCTION FOR ISOMERS
 COEFFICIENT          VECTOR
```

COEFFICIENT				
1	12	0	0	0
4	11	1	0	0
17	10	2	0	0
36	9	3	0	0
67	8	4	0	0
88	7	5	0	0
102	6	6	0	0
88	5	7	0	0
67	4	8	0	0
36	3	9	0	0
17	2	10	0	0
4	1	11	0	0
1	0	12	0	0
4	11	0	1	0
30	10	1	1	0
106	9	2	1	0
240	8	3	1	0
356	7	4	1	0
504	6	5	1	0
504	5	6	1	0
356	4	7	1	0
240	3	8	1	0
106	2	9	1	0
30	1	10	1	0
4	0	11	1	0
17	10	0	2	0
106	9	1	2	0
360	8	2	2	0
748	7	3	2	0
1147	6	4	2	0
1300	5	5	2	0
1147	4	6	2	0
748	3	7	2	0
360	2	8	2	0
106	1	9	2	0
17	0	10	2	0
36	9	0	3	0
240	8	1	3	0
748	7	2	3	0
1460	6	3	3	0
1956	5	4	3	0
1956	4	5	3	0
1460	3	6	3	0
748	2	7	3	0
240	1	8	3	0
36	0	9	3	0
67	8	0	4	0
356	7	1	4	0
1147	6	2	4	0
1956	5	3	4	0
2400	4	4	4	0
1956	3	5	4	0
1147	2	6	4	0
356	1	7	4	0
67	0	8	4	0
88	7	0	5	0
504	6	1	5	0
1300	5	2	5	0
1956	4	3	5	0
1956	3	4	5	0
1300	2	5	5	0
504	1	6	5	0
88	0	7	5	0
102	6	0	6	0
504	5	1	6	0
1147	4	2	6	0
1460	3	3	6	0
1147	2	4	6	0
504	1	5	6	0
102	0	6	6	0
88	5	0	7	0
356	4	1	7	0
748	3	2	7	0
748	2	3	7	0
356	1	4	7	0
88	0	5	7	0
67	4	0	8	0
240	3	1	8	0
360	2	2	8	0
240	1	3	8	0
67	0	4	8	0
36	3	0	9	0
106	2	1	9	0
106	1	2	9	0
36	0	3	9	0
17	2	0	10	0
30	1	1	10	0
17	0	2	10	0
4	1	0	11	0
4	0	1	11	0
1	0	0	12	0
4	11	0	0	1
30	10	1	0	1
106	9	2	0	1
240	8	3	0	1
356	7	4	0	1
504	6	5	0	1
504	5	6	0	1
356	4	7	0	1
240	3	8	0	1
106	2	9	0	1
30	1	10	0	1
4	0	11	0	1
30	10	0	1	1
212	9	1	1	1
706	8	2	1	1
1456	7	3	1	1
2272	6	4	1	1

Table 5
(continued)

2600	5	5	1	1
2272	4	6	1	1
1496	3	7	1	1
706	2	8	1	1
212	1	9	1	1
30	0	10	1	1
106	9	0	2	1
706	8	1	2	1
2200	7	2	2	1
4296	6	3	2	1
5876	5	4	2	1
5876	4	5	2	1
4296	3	6	2	1
2200	2	7	2	1
706	1	8	2	1
106	0	9	2	1
240	8	0	3	1
1496	7	1	3	1
4296	6	2	3	1
7560	5	3	3	1
9040	4	4	3	1
7560	3	5	3	1
4296	2	6	3	1
1496	1	7	3	1
240	0	8	3	1
396	7	0	4	1
2272	6	1	4	1
5876	5	2	4	1
9040	4	3	4	1
9040	3	4	4	1
5876	2	5	4	1
2272	1	6	4	1
396	0	7	4	1
504	6	0	5	1
2600	5	1	5	1
5876	4	2	5	1
7560	3	3	5	1
5876	2	4	5	1
2600	1	5	5	1
504	0	6	5	1
504	5	0	6	1
2272	4	1	6	1
4296	3	2	6	1
4296	2	3	6	1
2272	1	4	6	1
504	0	5	6	1
396	4	0	7	1
1496	3	1	7	1
2200	2	2	7	1
1496	1	3	7	1
396	0	4	7	1
240	3	0	8	1
706	2	1	8	1
706	1	2	8	1
240	0	3	8	1
106	2	0	9	1
212	1	1	9	1
106	0	2	9	1
30	1	0	10	1
30	0	1	10	1
4	0	0	11	1
17	10	0	0	2

106	9	1	0	2
360	8	2	0	2
748	7	3	0	2
1147	6	4	0	2
1300	5	5	0	2
1147	4	6	0	2
748	3	7	0	2
360	2	8	0	2
106	1	9	0	2
17	0	10	0	2
106	9	0	1	2
706	8	1	1	2
2200	7	2	1	2
4296	6	3	1	2
5876	5	4	1	2
5876	4	5	1	2
4296	3	6	1	2
2200	2	7	1	2
706	1	8	1	2
106	0	9	1	2
360	8	0	2	2
2200	7	1	2	2
6342	6	2	2	2
11128	5	3	2	2
13340	4	4	2	2
11128	3	5	2	2
6342	2	6	2	2
2200	1	7	2	2
360	0	8	2	2
748	7	0	3	2
4296	6	1	3	2
11128	5	2	3	2
17140	4	3	3	2
17140	3	4	3	2
11128	2	5	3	2
4296	1	6	3	2
748	0	7	3	2
1147	6	0	4	2
5876	5	1	4	2
13340	4	2	4	2
17140	3	3	4	2
13340	2	4	4	2
5876	1	5	4	2
1147	0	6	4	2
1300	5	0	5	2
5876	4	1	5	2
11128	3	2	5	2
11128	2	3	5	2
5876	1	4	5	2
1300	0	5	5	2
1147	4	0	6	2
4296	3	1	6	2
6342	2	2	6	2
4296	1	3	6	2
1147	0	4	6	2
748	3	0	7	2
2200	2	1	7	2
2200	1	2	7	2
748	0	3	7	2
360	2	0	8	2
706	1	1	8	2
360	0	2	8	2

Table 5
(continued)

1C6	1	0	9	2
1C6	C	1	9	2
17	0	0	10	2
36	9	0	0	3
240	8	1	0	3
748	7	2	0	3
146C	6	3	0	3
1456	5	4	0	3
1456	4	5	0	3
146C	3	6	0	3
748	2	7	0	3
240	1	8	0	3
3E	C	9	0	3
240	8	0	1	3
1456	7	1	1	3
4256	6	2	1	3
7560	5	3	1	3
904C	4	4	1	3
7560	3	5	1	3
4256	2	6	1	3
1456	1	7	1	3
240	C	8	1	3
748	7	0	2	3
4256	6	1	2	3
11128	5	2	2	3
1714C	4	3	2	3
17140	3	4	2	3
11128	2	5	2	3
4256	1	6	2	3
748	0	7	2	3
146C	6	0	3	3
756C	5	1	3	3
17140	4	2	3	3
22C8C	3	3	3	3
1714C	2	4	3	3
7560	1	5	3	3
146C	C	6	3	3
1956	5	0	4	3
904C	4	1	4	3
1714C	3	2	4	3
17140	2	3	4	3
904C	1	4	4	3
1956	0	5	4	3
1956	4	0	5	3
756C	3	1	5	3
11128	2	2	5	3
7560	1	3	5	3
1456	C	4	5	3
1460	3	0	6	3
4256	2	1	6	3
4256	1	2	6	3
146C	0	3	6	3
74E	2	0	7	3
1456	1	1	7	3
748	0	2	7	3
240	1	0	8	3
240	0	1	8	3
36	0	0	9	3
67	8	0	0	4
35E	7	1	0	4
1147	6	2	0	4
1456	5	3	0	4
2400	4	4	0	4
1456	3	5	0	4
1147	2	6	0	4
396	1	7	0	4
67	C	8	0	4
356	7	0	1	4
2272	6	1	1	4
5E76	5	2	1	4
9040	4	3	1	4
9040	3	4	1	4
5E76	2	5	1	4
2272	1	6	1	4
356	0	7	1	4
1147	6	0	2	4
5876	5	1	2	4
13340	4	2	2	4
17140	3	3	2	4
13340	2	4	2	4
5876	1	5	2	4
1147	0	6	2	4
1456	5	0	3	4
9040	4	1	3	4
17140	3	2	3	4
1714C	2	3	3	4
9040	1	4	3	4
1456	0	5	3	4
2400	4	0	4	4
9040	3	1	4	4
13340	2	2	4	4
904C	1	3	4	4
2400	0	4	4	4
1456	3	0	5	4
5d76	2	1	5	4
5876	1	2	5	4
1956	C	3	5	4
1147	2	0	6	4
2272	1	1	6	4
1147	C	2	6	4
396	1	0	7	4
396	0	1	7	4
67	C	0	8	4
88	7	0	0	5
5C4	6	1	0	5
1300	5	2	0	5
1456	4	3	0	5
1456	3	4	0	5
1300	2	5	0	5
5C4	1	6	0	5
EE	C	7	0	5
5C4	6	0	1	5
2600	5	1	1	5
5876	4	2	1	5
7560	3	3	1	5
5E76	2	4	1	5
2600	1	5	1	5
5C4	C	6	1	5
1300	5	0	2	5
5876	4	1	2	5
11128	3	2	2	5
11128	2	3	2	5
5876	1	4	2	5
1300	C	5	2	5

Table 5
(continued)

1496	4	0	3	5
756C	3	1	3	5
11128	2	2	3	5
756C	1	3	3	5
1956	C	4	3	5
1956	3	0	4	5
5e7e	2	1	4	5
5E1E	1	2	4	5
1496	0	3	4	5
13CC	2	0	5	5
20CC	1	1	5	5
13C0	0	2	5	5
5C4	1	0	6	5
5C4	0	1	6	5
88	C	0	7	5
1C2	6	0	0	6
5C4	5	1	0	6
1147	4	2	0	6
146C	3	3	0	6
1147	2	4	0	6
5C4	1	5	0	6
1C2	C	6	0	6
5C4	5	0	1	6
2272	4	1	1	6
4296	3	2	1	6
4256	2	3	1	6
2272	1	4	1	6
5C4	C	5	1	6
1147	4	0	2	6
4256	3	1	2	6
6342	2	2	2	6
4256	1	3	2	6
1147	C	4	2	6
1460	3	0	3	6
4256	2	1	3	6
4296	1	2	3	6
1460	0	3	3	6
1147	2	0	4	6
2272	1	1	4	6
1147	C	2	4	6
5C4	1	0	5	6
5C4	0	1	5	6
1C2	C	0	6	6
88	5	0	0	7
396	4	1	0	7
748	3	2	0	7
748	2	3	0	7
396	1	4	0	7
88	C	5	0	7
396	4	0	1	7
1496	3	1	1	7
2200	2	2	1	7
1496	1	3	1	7
396	C	4	1	7
748	3	0	2	7
22C0	2	1	2	7
22CC	1	2	2	7
748	0	3	2	7
748	2	0	3	7
1496	1	1	3	7
748	0	2	3	7
396	1	0	4	7

396	C	1	4	7
68	C	0	5	7
67	4	0	0	8
240	3	1	0	8
360	2	2	0	8
240	1	3	0	8
67	0	4	0	8
24C	3	0	1	8
7C6	2	1	1	8
1C6	1	2	1	8
24C	0	3	1	8
360	2	0	2	8
7C6	1	1	2	8
360	0	2	2	8
240	1	0	3	8
24C	0	1	3	8
67	0	0	4	8
36	3	0	0	9
1C6	2	1	0	9
1C6	1	2	0	9
36	0	3	0	9
1C6	2	0	1	9
212	1	1	1	9
1C6	0	2	1	9
1C6	1	0	2	9
1C6	0	1	2	9
36	C	0	3	9
17	2	0	0	10
30	1	1	0	10
17	C	2	0	10
30	1	0	1	10
30	C	1	1	10
17	0	0	2	10
4	1	0	0	11
4	C	1	0	11
4	C	0	1	11
1	0	0	0	12

TECHNICAL INFORMATION DEPARTMENT
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720