Applications of Degree Distribution. 1. (a) General Discussion and Computer Generation of Degree Distributions. (b) Maximal Degree Distributions

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The degree distribution equation has the general form $a + 2b + 3c + 4d = 2(n - 1 + r)$, where n is the number of skeletal atoms (usually carbon atoms), r is the number of rings (very liberally defined), and a, b, c, and d denote the numbers of skeletal atoms of degrees 1, 2, 3, and 4, respectively. For a given n and r there are normally numerous $[a,b,c,d]$ solutions, all readily obtainable by a computer program. Each solution represents a valid degree distribution. All isomers that conform to a certain degree distribution can be considered to belong to the same domain. A maximal degree distribution is defined as a degree distribution $[a,b,c,d]$ in which at least one term is maximal for the given n and r. Maximal values follow a predictable pattern for an infinite range of n for the chosen r and are easily calculated for any desired case.

INTRODUCTION

This paper is the first in a series devoted primarily to the enumeration of isomers by a new method utilizing degree distributions. The present paper sets the stage for this method and furthermore deals with subject matters important in their own right.

GENERAL DISCUSSION AND COMPUTER GENERATION OF DEGREE DISTRIBUTIONS

A connected graph consists of vertices and edges such that at least one pathway over the edges exists between any two vertices. If the number of vertices in a connected graph is n and the number of edges is e, the smallest possible value for e is $n - 1$.[1] In such a case the connected graph is a tree; i.e. it is acyclic. Rings cause e values to be larger than $n - 1$. We use the term "rings" in a broad sense, meaning to include not merely "ordinary" rings but also rings resulting from loops or multiple edges.

A loop is a particular kind of edge. It issues from a vertex and connects with the same vertex. The combination of vertex and loop may be considered a one-membered ring. Each such ring causes the value of e to increase by 1.

If two vertices are joined by z edges, where z is greater than 1, the value of e is increased by $z - 1$. We may regard one of the z edges as the "intrinsic" edge and the other $z - 1$ as "auxiliary" edges. The two vertices together with the intrinsic edge and one auxiliary edge can be considered a two-membered ring. In this sense, the two vertices are involved in as many two-membered rings as there are auxiliary edges, i.e. $z - 1$.

If one deletes from a connected graph all loops and all auxiliary edges (i.e. all one- and two-membered rings), one is left with a *simple* connected graph. This is either a tree or else it contains one or more "ordinary" rings, defined as rings that are at least three-membered in terms of vertices. Deletion of any one of the edges within the pathway of such a ring destroys the ring without diminishing n. It follows that each ordinary ring causes the value of e to increase by 1.

Sometimes the pattern of sharing of vertices by ordinary rings is quite complex, so that the number of ordinary rings in a simple graph may not be immediately evident. In actual fact the decision is easy: The number of such rings is identical with the number of edges that must be deleted in order to convert the graph to a tree with the same n.

We can now generalize: The number of edges, e, in a connected graph of n vertices is $n - 1 + r$, where r is the number of rings of *any* kind.

Any vertex of a connected graph has a certain degree. This is defined as the number of half-edges issuing from a vertex. Obviously, a loop is counted as two half-edges for the vertex involved. On the other hand, any edge that connects two vertices, no matter whether it does so alone or as a member of multiple edges, is counted as *one* half-edge for *each* of the vertices involved.

If the sum of the degrees of all the vertices of a connected graph is s, this clearly equals the total number of half-edges, $2e$. Hence, $s = 2e = 2n - 2 + 2r$.

A carbon skeleton represents a connected graph wherein the degree of a vertex (carbon atom) is not allowed to exceed 4. Multiple edges are now multiple bonds between adjacent carbon atoms, and a vertex with a loop is a carbene carbon.

The degree distribution (DD) for a carbon skeleton is expressed as $[a,b,c,d]$, where a, b, c, and d denote, respectively, the number of carbon atoms of degrees 1, 2, 3, and 4.

The degree distribution equation (DD equation) for any carbon skeleton takes the following form:

$$a + 2b + 3c + 4d = s = 2e = 2n - 2 + 2r$$

Since

$$a + b + c + d = n \quad \text{and hence} \quad a = n - b - c - d$$

the DD equation becomes

$$n - b - c - d + 2b + 3c + 4d = 2n - 2 + 2r$$

or more simply

$$b + 2c + 3d = n - 2 + 2r \tag{1}$$

The Fortran computer program shown in Chart I of Appendix A searches for and finds all the possible $[b,c,d]$ combinations that satisfy eq 1 for fixed values assigned to n

and r. As a result all the possible degree distributions $[a,b,c,d]$ are generated for a given n, r assignment.

In Table V of Appendix B degree distributions are listed for 24 such assignments involving the eight n values from 5 to 12 and the three r values from 0 to 2. Degree distributions for other n, r assignments are available from the authors.

We conclude this section by considering a matter of definition. The question arises whether in the characterization of carbon atoms synonymity exists between "primary" and "of degree 1", between "secondary" and "of degree 2", between "tertiary" and "of degree 3", and between "quaternary" and "of degree 4". While synonymity may originally have been intended, it should not be taken for granted. Organic chemists tend to characterize a carbon atom as primary, secondary, tertiary, or quaternary, depending on how many other carbon atoms are directly joined to it, whereas in graph theory characterization of a carbon atom as being of degree x is based on the number of half-bonds surrounding it within the carbon skeleton. The two kinds of characterization are synonymous only if applied to a carbon atom not involved in multiple bonding to some other carbon atom and carrying no loop. Hence these characterizations are freely exchangeable only when one is dealing with carbon skeletons that are *simple* graphs.

DEGREE DISTRIBUTION AND ISOMER DOMAINS

Since all the degree distributions for a given n and r are readily generated, the total number of constitutionally distinct isomers with that n and r may be partitioned among these degree distributions. In other words, all the isomers that conform to a given degree distribution (DD) make up a domain, to be called a DD domain. No isomer can satisfy more than one degree distribution, so that overlap between DD domains (interdomain isomer redundancy) is precluded. Isomers belonging to the same DD domain are also known as valence isomers.[2]

DD domains vary greatly in size, i.e. in the number of isomers they contain. When $r = 0$, their sizes vary from one isomer to very many. When $r > 0$ and n is sufficiently small, graphless (zero-size) DD domains are also encountered.

In forthcoming papers we shall illustrate the enumeration of isomers by a method involving DD domains.

MAXIMAL DEGREE DISTRIBUTIONS

On surveying all the degree distributions generated for a given n and r by the computer program, one observes a range of values for a. The value at the upper end of this range shall be called a_{max} (maximal a). Likewise, one observes a range of values for b with a b_{max}, a range of values for c with a c_{max}, and a range of values for d with a d_{max}. Any degree distribution that contains a maximal value shall be called a *maximal degree distribution*. One may, of course, wish to be more specific. For example, a degree distribution that contains c_{max} is a maximal degree distribution with respect to c.

As indicated above, one way of finding maximal values for a given n and r is to generate all the possible degree distributions and then survey the values for each term. However, a superior strategy is to derive, for a chosen r, maximal degree distributions in which n, or a surrogate of n, appears as a variable. For any specific n, no matter how large this may be, the corresponding maximal values are then easily obtained.

Our deviations of maximal degree distributions invoke *reductio ad absurdum* arguments applied in a highly directional manner. One starts out with the assumption that the term to be maximized equals n, the total number of carbon atoms, and that all the other terms of the degree distribution are consequently zero. In almost every instance this degree distribution has an s that is too high (H) or too low (L). The correct s (C) is, of course, $2(n - 1 + r)$ wherein r is replaced by the chosen value. An incorrect s signifies that the assumed degree distribution is absurd.

Next one judiciously, not randomly, manipulates the degree distribution to obtain the correct s while minimizing the drop from n which the term to be maximized must undergo. The result is an n-variable maximal degree distribution.

In some cases a maximal degree distribution is transformable into another one unaltered with regard to the maximal term but altered with regard to the other three terms. Such a transformation requires that an "equality" with the following characteristics be applicable:

(1) Both sides of the equality involve the same number of carbon atoms, namely, two.

(2) Both sides of the equality represent equal contributions toward s.

Three equalities fit this description.

Equality A. One carbon of degree 1 and one carbon of degree 3 make the same contribution to s as two carbons of degree 2, i.e. $1 \times 1° + 1 \times 3° = 2 \times 2°$. When equality A is applied, the d term remains unchanged.

Equality B. One carbon of degree 2 and one carbon of degree 4 make the same contribution to s as two carbons of degree 3, i.e. $1 \times 2° + 1 \times 4° = 2 \times 3°$. When equality B is applied, the a term remains unchanged.

Equality C. One carbon of degree 1 and one carbon of degree 4 make the same contribution to s as one carbon of degree 2 and one carbon of degree 3, i.e. $1 \times 1° + 1 \times 4° = 1 \times 3° + 1 \times 2°$. When equality C is applied, all four terms change. Hence it cannot be used to convert a maximal degree distribution into one containing the same maximal term. However, all three equalities can be used to interconvert degree distributions in general.

The overall method for deriving n-variable maximal degree distributions will now be illustrated for $r = 0$ (simple trees). It follows that a valid degree distribution must have $s = 2(n - 1 + r) = 2n - 2$.

Each maximal degree distribution will be made salient by the (C) indicating the correctness of s. Maximal terms will be underlined.

$b_{max}(r=0)$

$$[0,n,0,0] \Rightarrow s = 2n \qquad \text{(H)}$$

$$[1,n-1,0,0] \Rightarrow s = 2n - 1 \qquad \text{(H)}$$

$$[2,\underline{n-2},0,0] \Rightarrow s = 2n - 2 \qquad \text{(C)}$$

$c_{max}(r=0)$

$$[0,0,n,0] \Rightarrow s = 3n \qquad \text{(H)}$$

Since this s is much too high, we make a rough assumption that gets s down to the vicinity of the correct value while diminishing c to the least possible extent.

$$[n/2,0,n/2,0] \Rightarrow s = 2n$$

Whether n is even or odd is clearly a matter of importance. Hence we must deal separately with even n's ($n = 2p$) and odd n's ($n = 2p + 1$).

$c_{max}(r=0)$ if $n = 2p$

if $n = 2p$, $s = 2n - 2 = 4p - 2$

$$[p,0,p,0] \Rightarrow s = 4p \qquad \text{(H)}$$

$$[p+1,0,\underline{p-1},0] \Rightarrow s = 4p - 2 \qquad \text{(C)}$$

$c_{max}(r=0)$ if $n = 2p + 1$

if $n = 2p + 1$, $s = 2n - 2 = 4p$

$$[p+1,0,p,0] \Rightarrow s = 4p + 1 \qquad \text{(H)}$$

$$[p+2,0,p-1,0] \Rightarrow s = 4p - 1 \qquad \text{(L)}$$

$$[p+1,1,\underline{p-1},0] \Rightarrow s = 4p \qquad \text{(C)}$$

$d_{max}(r=0)$

$$[0,0,0,n] \Rightarrow s = 4n \qquad \text{(H)}$$

Since this s is much too high, we make a rough assumption that gets s down to the vicinity of the correct value while diminishing d to the least possible extent.

$$[2n/3,0,0,n/3] \Rightarrow s = 2n$$

Whether n is a multiple of 3 ($n = 3m$) or whether its division by 3 leaves a remainder of 1 ($n = 3m + 1$) or a remainder of 2 ($n = 3m + 2$) is obviously a matter of importance. Hence we must deal separately with each of these three types of n.

$d_{max}(r=0)$ if $n = 3m$

if $n = 3m$, $s = 2n - 2 = 6m - 2$

$$[2m,0,0,m] \Rightarrow s = 6m \qquad \text{(H)}$$

$$[2m+1,0,0,m-1] \Rightarrow s = 6m - 3 \qquad \text{(L)}$$

$$[2m,1,0,\underline{m-1}] \Rightarrow s = 6m - 2 \qquad \text{(C)}$$

$d_{max}(r=0)$ if $n = 3m + 1$

if $n = 3m + 1$, $s = 2n - 2 = 6m$

$$[2m+1,0,0,m] \Rightarrow s = 6m + 1 \qquad \text{(H)}$$

$$[2m+2,0,0,m-1] \Rightarrow s = 6m - 2 \qquad \text{(L)}$$

$$[2m+1,1,0,m-1] \Rightarrow s = 6m - 1 \qquad \text{(L)}$$

$$[2m+1,0,1,\underline{m-1}] \Rightarrow s = 6m \qquad \text{(C)}$$

and, due to equality A,

$$[2m,2,0,\underline{m-1}] \Rightarrow s = 6m \qquad \text{(C)}$$

$d_{max}(r=0)$ if $n = 3m + 2$

if $n = 3m + 2$, $s = 2n - 2 = 6m + 2$

$$[2m+2,0,0,\underline{m}] \Rightarrow s = 6m + 2 \qquad \text{(C)}$$

$a_{max}(r=0)$

$$[n,0,0,0] \Rightarrow s = n \qquad \text{(L)}$$

Since this s is much too low, we make a rough assumption that gets s up to the vicinity of the correct value while diminishing a to the least possible extent.

$$[2n/3,0,0,n/3] \Rightarrow s = 2n$$

Clearly, we must deal separately with $n = 3m$, $n = 3m + 1$, and $n = 3m + 2$.

$a_{max}(r=0)$ if $n = 3m$

if $n = 3m$, $s = 2n - 2 = 6m - 2$

$$[2m+1,0,0,m-1] \Rightarrow s = 6m - 3 \qquad \text{(L)}$$

$$[2m,0,0,m] \Rightarrow s = 6m \qquad \text{(H)}$$

$$[2m,0,1,m-1] \Rightarrow s = 6m - 1 \qquad \text{(H)}$$

$$[\underline{2m},1,0,m-1] \Rightarrow s = 6m - 2 \qquad \text{(C)}$$

and, due to equality B,

$$[\underline{2m},0,2,m-2] \Rightarrow s = 6m - 2 \qquad \text{(C)}$$

$a_{max}(r=0)$ if $n = 3m + 1$

if $n = 3m + 1$, $s = 2n - 2 = 6m$

$$[2m+2,0,0,m-1] \Rightarrow s = 6m - 2 \qquad \text{(L)}$$

$$[2m+1,0,0,m] \Rightarrow s = 6m + 1 \qquad \text{(H)}$$

$$[\underline{2m+1},0,1,m-1] \Rightarrow s = 6m \qquad \text{(C)}$$

$a_{max}(r=0)$ if $n = 3m + 2$

since $n = 3m + 2$, $s = 2n - 2 = 6m + 2$

$$[\underline{2m+2},0,0,m] \Rightarrow s = 6m + 2 \qquad \text{(C)}$$

Having derived all the maximal degree distributions for $r = 0$, we compare them with one another in order to determine whether any appears more than once, in which event it contains more than one maximal term. We do indeed find some maximal degree distributions which contain both a_{max} and d_{max}. Clearly, there is compatibility between a_{max} and d_{max}, regardless of the type of n. The extent of mutual dependence between a_{max} and d_{max} is difficult to summarize and is best seen from Table I.

Table I summarizes all the results for $r = 0$. These are then applied in Table II, which provides a listing of the numerical values for a_{max}, b_{max}, c_{max}, and d_{max} for $r = 0$ and n from 2 to 22. Since, as n increases, the maximal values produce a predictable pattern unique for the carbon atoms of each degree, one may extend Table II *ad infinitum* simply by continuing the four progressions. In order to obtain numerical values for

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Table I. Maximal Degree Distributions in Terms of n, or a Surrogate of n, for $r = 0$ [a]

maximal term	nature of n	maximal degree distributions $[a,b,c,d]$
b_{max}	any	$[2,\mathbf{n-2},0,0]$
c_{max}	$n = 2p$	$[p+1,0,\mathbf{p-1},0]$
c_{max}	$n = 2p + 1$	$[p+1,1,\mathbf{p-1},0]$
a_{max}, d_{max}	$n = 3m$	$[\mathbf{2m},1,0,\mathbf{m-1}]$
		$[\mathbf{2m},0,2,m-2]$
a_{max}, d_{max}	$n = 3m + 1$	$[\mathbf{2m+1},0,1,\mathbf{m-1}]$
		$[2m,2,0,\mathbf{m-1}]$
a_{max}, d_{max}	$n = 3m + 2$	$[\mathbf{2m+2},0,0,\mathbf{m}]$

[a] These distributions are constrained by $s = 2(n - 1 + r) = 2n - 2$. Maximal values are boldfaced.

Table IV. Maximal Degree Distributions in Terms of n, or a Surrogate of n, for $r = 2$ [a]

maximal term	nature of n	maximal degree distributions $[a,b,c,d]$
b_{max}	any	$[0,\mathbf{n-1},0,1]$
c_{max}	$n = 2p$	$[p-1,0,\mathbf{p+1},0]$
c_{max}	$n = 2p + 1$	$[p-1,1,\mathbf{p+1},0]$
a_{max}, d_{max}	$n = 3m$	$[\mathbf{2m-1},0,1,\mathbf{m}]$
		$[2m-2,2,0,\mathbf{m}]$
a_{max}, d_{max}	$n = 3m + 1$	$[\mathbf{2m},0,0,\mathbf{m+1}]$
a_{max}, d_{max}	$n = 3m + 2$	$[\mathbf{2m},1,0,\mathbf{m+1}]$
		$[\mathbf{2m},0,2,m]$

[a] These distributions are constrained by $s = 2(n - 1 + r) = 2n + 2$. Maximal values are boldfaced.

Table II. Maxima of Primary, Secondary, Tertiary, and Quaternary Carbons in Acyclic Simple Skeletons from $n = 2$ to 22

n	a_{max}	b_{max}	c_{max}	d_{max}
2	2	0	0	0
3	2	1	0	0
4	3	2	1	0
5	4	3	1	1
6	4	4	2	1
7	5	5	2	1
8	6	6	3	2
9	6	7	3	2
10	7	8	4	2
11	8	9	4	3
12	8	10	5	3
13	9	11	5	3
14	10	12	6	4
15	10	13	6	4
16	11	14	7	4
17	12	15	7	5
18	12	16	8	5
19	13	17	8	5
20	14	18	9	6
21	14	19	9	6
22	15	20	10	6

Chart I

```
      IMPLICIT REAL*8(A-H,O-Z)
      IMPLICIT INTEGER*4(I-N)
c     Routine to determine degree-distributions for isomers
c     ix    number of skeletal atoms in the molecule
c     irmax  maximum in number of rings: program evaluates isomers
c            with 0 rings (acyclic), 1 ring, 2 rings ... up to irmax rings
    2 continue
      read(5,10)ix,irmax
      if(ix.eq.0)go to 9999
      write(6,5)ix,irmax
      irtop=irmax+1
c     sum over different ring configurations
      do 26 ir=1,irtop
      inring=ir-1
      write(6,6)inring
      iring=(inring-1)*2
      itest=ix+iring
c     restrict sums using max. possible b,c,d
      ifct=2*ix+iring
c     determine limits for b,c,d: max possible values
      cutb=(dfloat(ifct)/2.0d00)
      cutc=(dfloat(ifct)/3.0d00)
      cutd=(dfloat(ifct)/4.0d00)
c     Vax Fortan real-to-integer truncation function
      ibmx=1+jidint(cutb)
      icmx=1+jidint(cutc)
      idmx=1+jidint(cutd)
      if(ibmx.gt.ix)ibmx=ix
      if(icmx.gt.ix)icmx=ix
      if(idmx.gt.ix)idmx=ix
      write(6,7)
c     tabulate # of isomer domains and determine degree distributions
      iclass=0
      DO 23 ib=0,ibmx
      iab=ix-ib
      DO 23 ic=0,icmx
      iac=iab-ic
      DO 23 id=0,idmx
      ia=iac-id
c     no negative coeff. allowed
      if(ia.lt.0) go to 23
c     coef. cannot be greater than the number of atoms
      if(ia.gt.ix) go to 23
      itst=ib+(2*ic)+(3*id)
      if(itst.eq.itest)write(6,10)ia,ib,ic,id
      if(itst.ne.itest)go to 23
      iclass=iclass+1
   23 continue
      write(6,12)iclass
   26 continue
      write(6,*)' tabulation completed'
      write(6,*) '   *********************************************'
      write(6,*) '   *********************************************   '
      go to 2
    5 format(3x,' tabulation of DD isomer domains: # of atoms ',i5,
     1'::: max. number of rings ',i5)
    6 format(' number of rings = ',i5)
    7 format('    a ** b ** c ** d  ')
   10 FORMAT(1515)
   11 FORMAT(5F10.4)
   12 format(3x,i5,' domains ******')
   13 FORMAT(25x,'********',15I2)
 9999 continue
      STOP
      END
```

Table III. Maximal Degree Distributions in Terms of n, or a Surrogate of n, for $r = 1$ [a]

maximal term	nature of n	maximal degree distributions $[a,b,c,d]$
b_{max}	any	$[0,\mathbf{n},0,0]$
c_{max}	$n = 2p$	$[p,0,\mathbf{p},0]$
c_{max}	$n = 2p + 1$	$[p,1,\mathbf{p},0]$
a_{max}, d_{max}	$n = 3m$	$[\mathbf{2m},0,0,\mathbf{m}]$
a_{max}, d_{max}	$n = 3m + 1$	$[\mathbf{2m},1,0,\mathbf{m}]$
		$[\mathbf{2m},0,2,m-1]$
a_{max}, d_{max}	$n = 3m + 2$	$[\mathbf{2m+1},0,1,\mathbf{m}]$
		$[2m,2,0,\mathbf{m}]$

[a] These distributions are constrained by $s = 2(n-1+r) = 2n$. Maximal values are boldfaced.

some very large n, it is, however, preferable to work directly from Table I.

For any other r maximal degree distributions variable in n or a surrogate of n are readily derived following the process demonstrated for $r = 0$. Tables III and IV show the results for $r = 1$ and $r = 2$, respectively.

CONCLUDING REMARKS

We have presented a computer program for generating degree distributions for carbon skeletons. In addition, we have shown that maximal degree distributions, i.e. degree distributions in which at least one of the four terms is maximal, are readily derived as functions of n, the number of carbon atoms.

ACKNOWLEDGMENT

Table V. Degree Distributions (DD Isomer Domains) for *n* = 5–12 Skeletal Atoms: No-Ring (Acyclic), One-Ring, and Two-Ring Systems

No. of Atoms = 5

No. of Rings = 0, 3 Domains

a b c d	a b c d	a b c d
4 0 0 1	3 1 1 0	2 3 0 0

No. of Rings = 1, 5 Domains

a b c d	a b c d	a b c d
3 0 1 1	2 1 2 0	2 2 0 1
1 3 1 0	0 5 0 0	

No. of Rings = 2, 6 Domains

a b c d	a b c d	a b c d
2 0 2 1	2 1 0 2	1 1 3 0
1 2 1 1	0 3 2 0	0 4 0 1

No. of Atoms = 6

No. of Rings = 0, 4 Domains

a b c d	a b c d	a b c d
4 0 2 0	4 1 0 1	3 2 1 0
2 4 0 0		

No. of rings = 1, 7 Domains

a b c d	a b c d	a b c d
4 0 0 2	3 0 3 0	3 1 1 1
2 2 2 0	2 3 0 1	1 4 1 0
0 6 0 0		

No. of Rings = 2, 8 Domains

a b c d	a b c d	a b c d
3 0 1 2	2 0 4 0	2 1 2 1
2 2 0 2	1 2 3 0	1 3 1 1
0 4 2 0	0 5 0 1	

No. of Atoms = 7

No. of Rings = 0, 5 Domains

a b c d	a b c d	a b c d
5 0 1 1	4 1 2 0	4 2 0 1
3 3 1 0	2 5 0 0	

No. of Rings = 1, 8 Domains

a b c d	a b c d	a b c d
4 0 2 1	4 1 0 2	3 1 3 0
3 2 1 1	2 3 2 0	2 4 0 1
1 5 1 0	0 7 0 0	

No. of Rings = 2, 10 Domains

a b c d	a b c d	a b c d
4 0 0 3	3 0 3 1	3 1 1 2
2 1 4 0	2 2 2 1	2 3 0 2
1 3 3 0	1 4 1 1	0 5 2 0
0 6 0 1		

No. of Atoms = 8

No. of Rings = 0, 7 Domains

a b c d	a b c d	a b c d
6 0 0 2	5 0 3 0	5 1 1 1
4 2 2 0	4 3 0 1	3 4 1 0
2 6 0 0		

No. of Rings = 1, 10 Domains

a b c d	a b c d	a b c d
5 0 1 2	4 0 4 0	4 1 2 1
4 2 0 2	3 2 3 0	3 3 1 1
2 4 2 0	2 5 0 1	1 6 1 0
0 8 0 0		

No. of Rings = 2, 12 Domains

a b c d	a b c d	a b c d
4 0 2 2	3 0 5 0	4 1 0 3
3 1 3 1	3 2 1 2	2 2 4 0
2 3 2 1	2 4 0 2	1 4 3 0
1 5 1 1	0 6 2 0	0 7 0 1

No. of Atoms = 9

No. of Rings = 0, 8 Domains

a b c d	a b c d	a b c d
6 0 2 1	6 1 0 2	5 1 3 0
5 2 1 1	4 3 2 0	4 4 0 1
3 5 1 0	2 7 0 0	

No. of Rings = 1, 12 Domains

a b c d	a b c d	a b c d
6 0 0 3	5 0 3 1	5 1 1 2
4 1 4 0	4 2 2 1	4 3 0 2
3 3 3 0	3 4 1 1	2 5 2 0
2 6 0 1	1 7 1 0	0 9 0 0

No. of Rings = 2, 14 Domains

a b c d	a b c d	a b c d
5 0 1 3	4 0 4 1	4 1 2 2
3 1 5 0	4 2 0 3	3 2 3 1
3 3 1 2	2 3 4 0	2 4 2 1
2 5 0 2	1 5 3 0	1 6 1 1
0 7 2 0	0 8 0 1	

No. of Atoms = 10

No. of Rings = 0, 10 Domains

a b c d	a b c d	a b c d
7 0 1 2	6 0 4 0	6 1 2 1
6 2 0 2	5 2 3 0	5 3 1 1
4 4 2 0	4 5 0 1	3 6 1 0
2 8 0 0		

No. of Rings = 1, 14 Domains

a b c d	a b c d	a b c d
6 0 2 2	5 0 5 0	6 1 0 3
5 1 3 1	5 2 1 2	4 2 4 0
4 3 2 1	4 4 0 2	3 4 3 0
3 5 1 1	2 6 2 0	2 7 0 1
1 8 1 0	0 10 0 0	

No. of Rings = 2, 17 Domains

a b c d	a b c d	a b c d
6 0 0 4	5 0 3 2	4 0 6 0
5 1 1 3	4 1 4 1	4 2 2 2
3 2 5 0	4 3 0 3	3 3 3 1
3 4 1 2	2 4 4 0	2 5 2 1
2 6 0 2	1 6 3 0	1 7 1 1
0 8 2 0	0 9 0 1	

No. of Atoms = 11

No. of Rings = 0, 12 Domains

a b c d	a b c d	a b c d
8 0 0 3	7 0 3 1	7 1 1 2
6 1 4 0	6 2 2 1	6 3 0 2
5 3 3 0	5 4 1 1	4 5 2 0
4 6 0 1	3 7 1 0	2 9 0 0

No. of Rings = 1, 16 Domains

a b c d	a b c d	a b c d
7 0 1 3	6 0 4 1	6 1 2 2
5 1 5 0	6 2 0 3	5 2 3 1
5 3 1 2	4 3 4 0	4 4 2 1
4 5 0 2	3 5 3 0	3 6 1 1
2 7 2 0	2 8 0 1	1 9 1 0
0 11 0 0		

No. of Rings = 2, 19 Domains

a b c d	a b c d	a b c d
6 0 2 3	5 0 5 1	6 1 0 4
5 1 3 2	4 1 6 0	5 2 1 3
4 2 4 1	4 3 2 2	3 3 5 0
4 4 0 3	3 4 3 1	3 5 1 2
2 5 4 0	2 6 2 1	2 7 0 2
1 7 3 0	1 8 1 1	0 9 2 0
0 10 0 1		

No. of Atoms = 12

No. of Rings = 0, 14 Domains

a b c d	a b c d	a b c d
8 0 2 2	7 0 5 0	8 1 0 3
7 1 3 1	7 2 1 2	6 2 4 0
6 3 2 1	6 4 0 2	5 4 3 0
5 5 1 1	4 6 2 0	4 7 0 1
3 8 1 0	2 10 0 0	

No. of Rings = 1, 19 Domains

a b c d	a b c d	a b c d
8 0 0 4	7 0 3 2	6 0 6 0
7 1 1 3	6 1 4 1	6 2 2 2
5 2 5 0	6 3 0 3	5 3 3 1
5 4 1 2	4 4 4 0	4 5 2 1
4 6 0 2	3 6 3 0	3 7 1 1
2 8 2 0	2 9 0 1	1 10 1 0
0 12 0 0		

No. of Rings = 2, 22 Domains

a b c d	a b c d	a b c d
7 0 1 4	6 0 4 2	5 0 7 0
6 1 2 3	5 1 5 1	6 2 0 4
5 2 3 2	4 2 6 0	5 3 1 3
4 3 4 1	4 4 2 2	3 4 5 0
4 5 0 3	3 5 3 1	3 6 1 2
2 6 4 0	2 7 2 1	2 8 0 2
1 8 3 0	1 9 1 1	0 10 2 0
0 11 0 1		

APPENDIX A

The Fortran program which generates degree distributions for a given number of skeletal atoms and a given number of rings is given in Chart I.

APPENDIX B

Degree distributions (DD isomer domains) for *n* = 5–12 skeletal atoms are given in Table V.

REFERENCES AND NOTES

(1) Bondy, J. A.; Murty, U. S. R. *Graph Theory with Applications*; North-Holland: New York, 1976; p 25.

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