Simplified Nomenclature of a Hexagonal Tessellation Lattice Using a Dimension-Increasing Transformation

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A technique for correlating the lattice points in a hexagaonal tessellation of the plane with a three-dimensional Cartesian coordinate system is proposed. By this procedure, a means for canonically naming the set of polycyclic aromatic compounds formed by the edge fusion of six-membered rings is created.

In most of the important mathematical transformations that have found use in science the objective is to create a simplified representation of the original system by formulating a related system that is of lower dimension than the original. Examination of the image system so created is usually more amenable to analysis. Two such familiar imaging systems are the modern day interpretation of the Mercator projection in cartography[1] and the Schlegel projection in chemistry.[2] In each instance the dimension of the object (three) is one higher than the dimension of the image (two).

In the present study, a reverse type of transformation is developed: namely, a transformation that relates an over-determined, and thus often contradictory, set of coordinate axes to a familiar, albeit higher dimensional, coordinate system. From such a seemingly ambiguous system, we are able to derive consistent information by establishing an algorithm that selects the canonical name of each multinamed lattice point from the various names assigned to each module. In this way we are able to optimize the description in a consistent manner. In order to develop an efficient nomenclature for the class of polycyclic aromatic hydrocarbons formed by the edge fusion of benzene modules—referred to by various authors as benzenoid polycyclic hydrocarbons,[3] polybenzenes,[4] polyhexes,[5] PAH6s,[6] etc., we wish to create a canonical ordering of the lattice points in a hexagonal tessellation of a plane. Toward this end, we note that very many interesting protocols have already been developed using the unique properties that such a tessellation of the plane has. A few representative examples are given in ref 7.

Consider a hexagonal tessellation of the plane in which regular hexagons are oriented so that a set of parallel sides are drawn vertically. This corresponds to Patterson's rules for standardizing the drawing of chemical molecules[8] (Figure 1). The central point of each hexagon now forms a two-dimensional lattice (Figure 2), to which we may assign a canonical name for each lattice point. Note that the *x*-axis of a Cartesian coordinate system imposed on the lattice would now correspond to the "principal axis" of the hexagonal tessellation system. Now, instead of the Cartesian positioning of the *y*-axis perpendicular to the *x*-axis, let us consider that the angle between the axes is 60°. In other words, just as the *x*-axis ran through the centers of a set of hexagons, similarly, so shall the *y*-axis. Next, rather than using
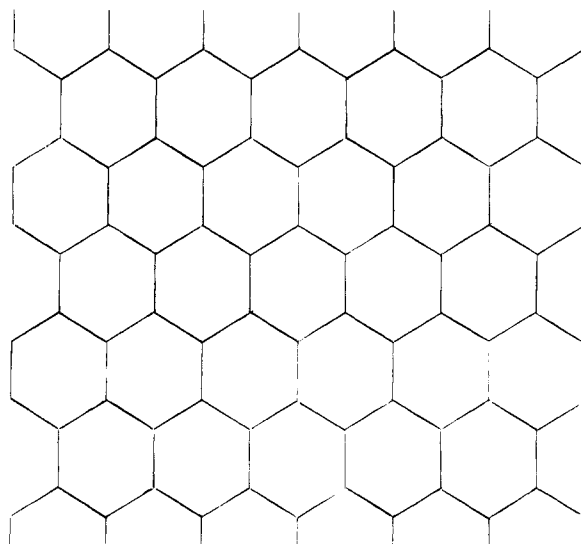

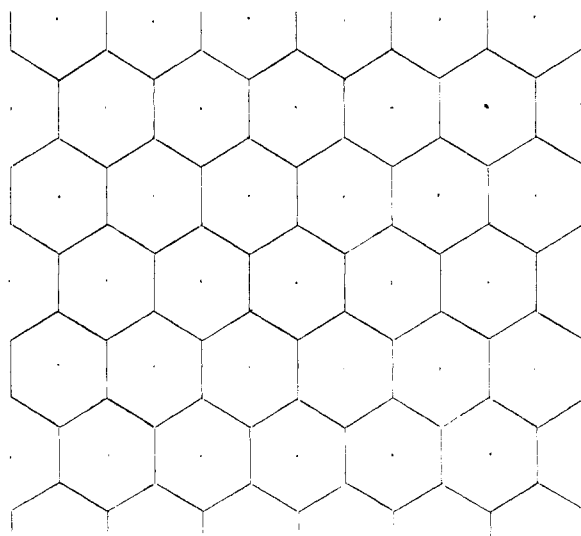**Figure 1.** Hexagonal tesselation of the plane using Patterson's orientation.

Figure 2. Two-dimensional lattice formed from Figure 1.

contravariant coordinates and thus assigning a unique name to each point of the lattice,[9] we note the existence of a third (albeit dependent) axis, set at an additional 60° from the *y*-axis, that also passes through the center of hexagons. This we shall call the *z*-axis. The three axes, which form an overdetermined set of coordinates, may be superimposed on the hexagonal tessellation of the plane. This is shown in
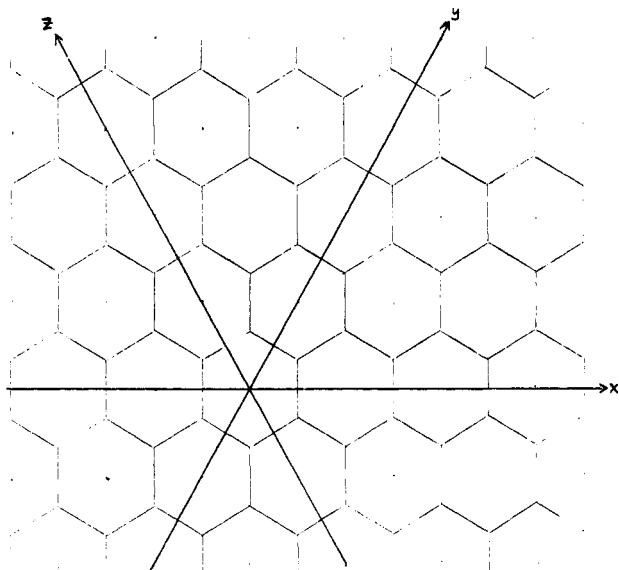
Figure 3. Overdetermined coordinate system superimposed on Figure 2.

Figure 4. Nonorthogonal x-y coordinate system.

Figure 3. Furthermore, we observe that any hexagon could have been selected as the origin of this coordinate system and that if we were to form the coordinate system to accommodate a given polycyclic aromatic hydrocarbon system, 12 possible orientations exist, each of which can be used with any of the hexagons that make up the molecule as the origin.[10]

Having selected the coordinate system that shall be used to nomenclate a given molecule, we begin to assign names to the lattice points as follows.

1. The origin will be named (0,0,0), and each point on the x-axis will have the name $(x,0,0)$ where x is the (signed) distance from the origin, with $+$ being to the right, as is traditional.

2. Next, assign the name of $(x,1,0)$ to the lattice point (hexagon) one unit above and to the right of point named $(x,0,0)$ and $(x,-1,0)$ to the lattice point one unit below and to the left of $(x,0,0)$. Similarly, we may name each lattice point (hexagon) that is diagonally right and up y units or diagonally down and left starting from the named point on the x-axis (Figure 4).

3. In a similar manner, each point along the y-axis could have been named $(0,y,0)$ or each point along the z-axis $(0,0,z)$.

4. If we now focus attention on the two remaining set of two axes (x-z and y-z) and assign names to lattice points based on these axes, we create the lattice names shown in Figures 5 and 6, respectively.

Notice that, although the above choices of lattice names always contained at least one coordinate equal to zero, this is an idiosyncracy of the method of naming chosen. We might just as easily start from any previously named lattice point and moving in the direction of any axis ($+$ or $-$) name the next lattice point by incrementing the applicable coordinate. For example, in Figure 4, we see that the origin could have been named $(1,-1,1)$ by starting from $(1,-1,0)$ and moving one unit in the positive z direction or else as $(-1,1,-1)$ by starting from $(-1,1,0)$ and moving one unit in the negative z direction. Similarly, using Figure 5, we created the same names for the origin by moving in the negative y direction from $(1,0,1)$ and from $(-1,0,-1)$ in the positive y direction; also, using Figure 6 by moving from the adjacent
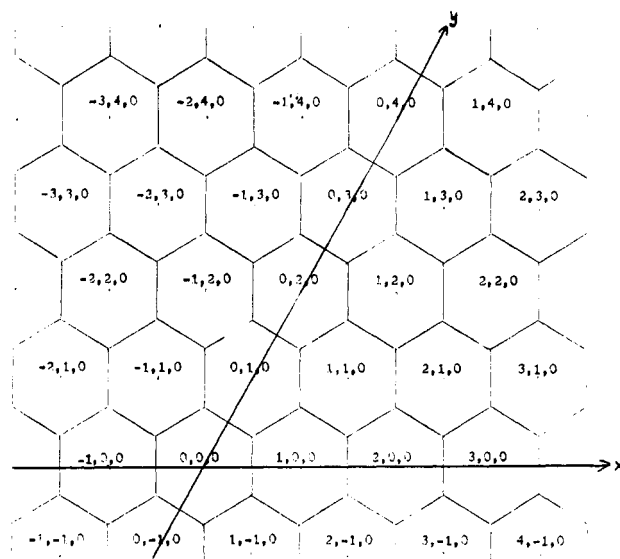

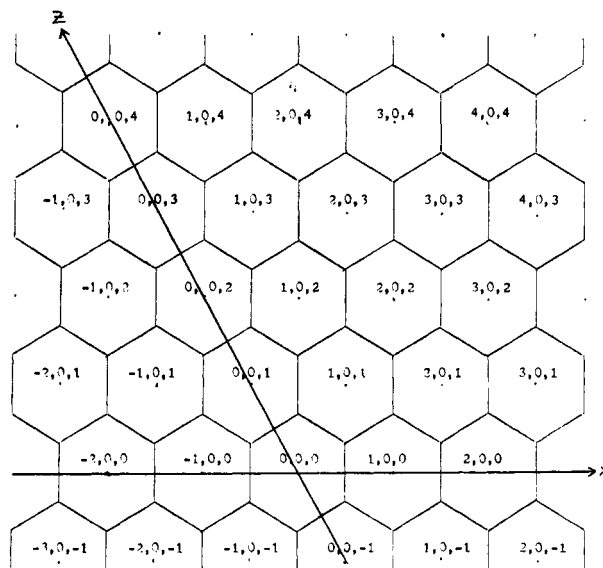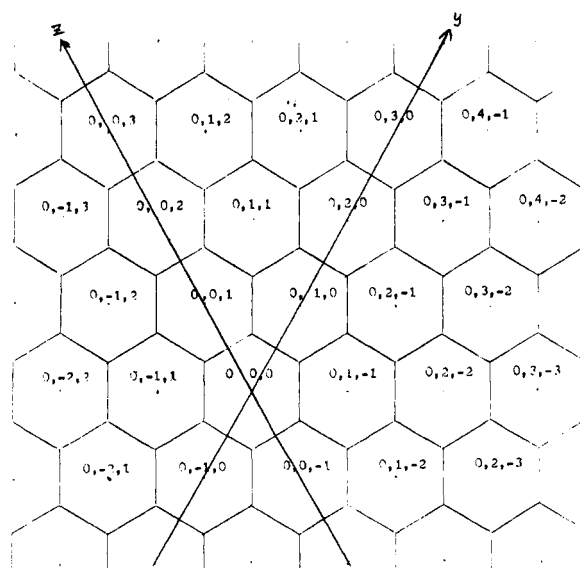**Figure 5.** Nonorthogonal x-z coordinate system.

Figure 6. Nonorthogonal y-z coordinate system.

hexagon in the positive and negative x directions. Furthermore, we note that we could assign an infinite number of
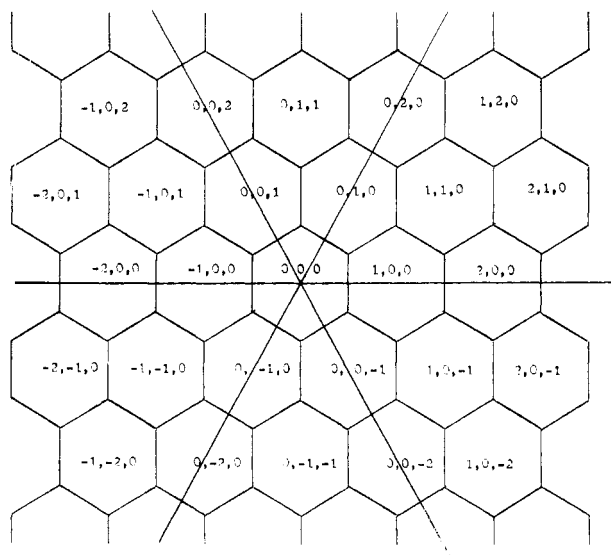
Figure 7. Proposed lattice labeling system (formed by fusion of the three nonorthognal coordinate systems).

names to each lattice point, such as $(-6,6,-6)$ to the origin, etc.

5. Because there exists an infinite number of names for each lattice point, in order to introduce standardization, we wish to superimpose some preselected criterion to use in assigning the "optimal" name from this overdetermined set. In doing so we also want to characterize the different regions of the plane that have been so designated. The criterion that seems most efficient to us is to minimize the sum of the absolute values of the coordinates (Figure 7). By such a choice, we note that in the upper right "hextant" (in which all three coordinates are non-negative), the coordinate with $z = 0$ is the desired name, also in the lower left hextant. Similarly, in the upper and the lower central hextants the coordinate with $x = 0$ is the desired name and in the upper left and lower right hextants the coordinate with $y = 0$.

By the above choice of the coordinate system, we have generated a relatively efficient system for nomenclating most coplanar molecules that are likely to be of interest, with the added property that by minimizing the sum of the absolute values of the coordinates we have effectively given a centering algorithm. Note that if we set s equal to the sum of absolute values of the three coordinates in Figure 7; i.e., $(s = |x| + |y| + |z|)$, then the set formed with a given numerical value for s is the one-hexagon wide perimeter shell, a shell which circumscribes the set of hexagons whose coordinates sum to $s - 1$, etc. In other words,

$s = 0$ corresponds to a single hexagon;

$s = 1$ to a set of six hexagons surrounding this $s = 0$ set

for a total of seven hexagons in the area covered

$s = 2$ to a set of $6 \times 2 = 12$ hexagons surround the $s = 1$ set,

for a total of 19 hexagons in the area covered

$s = n$ to a set of $6n$ hexagons surrounding the $s = n - 1$ "core", etc.

Furthermore, we note that the number of hexagon modules in the core is given by $(s + 1)^3 - s^3$; namely

$$1^3 - 0^3 = 1$$

$$2^3 - 1^3 = 7$$

$$3^3 - 2^3 = 19; \text{ etc.}$$

One additional idea of importance, that shall be the subject of a follow-up report, is that once we have created such a dimension-increasing transformation, the mathematical basis for creating a nomenclature for the modules that make up the diamond lattice (referred to as polymantanes[11]) by means of a transforming to a four dimensional Cartesian coordinate system is produced.

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