Proof

Herein it is proven that any benzenoid composed of $h$ benzene rings can be enumerated in the specific isosceles trapezoid as described in the Section Methodologies. The length of each leg ($m$) of the trapezoid is:

$$m = \left\lfloor \frac{2h+1}{3} \right\rfloor$$

where, $h$ is the number of hexagons of each enumerated benzenoid; $m$ is the integer part of the quotient of $(2h+1)/3$. The lengths of the two bases are $h$ and $h-m+1$.

In a hexagonal lattice, a benzenoid of size $h$ can be regarded as planar connected polyhexes, called $h$ continuous hexagons here. The proof based on pure graph theory is introduced as follows.

A coordinate system $(x, \gamma)$ in a hexagonal lattice is shown in Figure 1. In the system, every hexagon in the grid can be represented by a unique coordinate.

![Figure 1. An $xy$ coordinate system in a hexagonal lattice](image)

Then a third axis is introduced as shown in Figure 2. Every hexagon still has a unique coordinate. And for every coordinate $(x, \gamma, z)$, it is easy to find that the equation $x + \gamma = z$ is always correct. For example, the coordinates of four grey hexagons in Figure 2 are $(0, 0, 0), (1, 1, 2), (1, 2, 3)$ and $(2, 2, 4)$. 
**Lemma 1:** If \( h-1 \) continuous hexagons are added (the hexagon added one by one) from a starting hexagon \((x_0, y_0, z_0)\), \( z \) of any hexagon is less than \( z_0+h \).

**Proof**

Every hexagon has six neighbors next to it, and if the coordinate of a hexagon is \((x, y, z)\), the coordinates of its six neighbors are \((x, y+1, z+1)\), \((x, y, z+1)\), \((x, y-1, z)\), \((x, y-1, z-1)\), \((x+1, y, z+1)\) and \((x-1, y+1, z)\). In this case, any neighbor \((x_n, y_n, z_n)\) satisfies: \( z_n \leq z+1 \). Thus, if \( h-1 \) continuous hexagons are added one by one from a starting hexagon \((x_0, y_0, z_0)\), \( z \) of any hexagon is less than \( z_0+h \).

**Lemma 2:** If \( h-1 \) continuous hexagons are added one by one from a starting hexagon \((x_0, y_0, z_0)\) and the coordinate \( y \) of one added hexagon is 0, the value of \( z \) of any added hexagon is less than \( z_0+h-y_0 \), i.e., \( z \leq z_0+h-y_0 \).

**Proof**

For a hexagon \((x, y, z)\), there are six neighbors as above. The coordinates \( y \) of two neighbors decrease, and their coordinates are \((x+1, y-1, z)\) and \((x, y-1, z-1)\). It can be found that the coordinates satisfy: \( z_0 \leq z \). When the coordinate of starting hexagon is \((x_0, y_0, z_0)\) and the coordinate \( y \) of one added hexagon is 0, at least \( y_0 \) hexagons satisfying \( y_0 = y-1 \) need be added, that is, at least \( y_0 \) hexagons are added, but \( z \) doesn’t
increase. In this case, if \( h-1 \) continuous hexagons are added from the starting hexagon, based on lemma 1 the coordinate of any added hexagon satisfy: \( z-\alpha_0 < h-1 \), that is, the value of \( z \) of any added hexagon is less than \( h-1+\alpha_0 \). i.e., \( z < h-1+\alpha_0 \).

**Lemma 3:** Any benzenoid composed of \( h \) hexagons can be placed in an equilateral triangular area whose edge consists of \( h \) hexagons.

**Proof**

An equilateral triangular area (the length of any edge is \( h \)) on hexagonal lattice is shown in Figure 3 and the coordinate of \( O \) is the origin \((0, 0, 0)\). Any benzenoid composed of \( h \) hexagons placed on the grid is required to follow two predefined rules:

1) For the coordinate \((x, y, z)\) of any hexagon, there must be \( x \geq 0 \) and \( y \geq 0 \);

2) At least one hexagon is placed on \( x \)-axis and one hexagon is on \( y \)-axis.

It is easy to find that each hexagon on the line DE satisfies the condition \( z=h-1 \). In this case, if \( z < h \) can be proved for every hexagon \((x, y, z)\) contained in any benzenoid size of \( h \), lemma 3 is proved.

The coordinate of hexagon A is \((0, |OA|, |OA|)\) and the coordinate of hexagon B is \((|OB|, 0, |OB|)\). When hexagon A is regarded as starting hexagon, the remaining \( h-1 \) hexagons were added one by one, and \( z \) of any added hexagon is less than \( h-|OA|+|OA|=h \) based on lemma 2 \((z < h-1+\alpha_0)\). Thus, it is proved that \( z < h \).

![Figure 3. An equilateral triangular area on hexagonal lattice](image-url)
**Lemma 4:** Any benzenoid composed of \( h \) benzene rings can be placed in an isosceles trapezoidal area with the parameters: the length of each leg is 

\[ m = \left\lfloor \frac{2h + 1}{3} \right\rfloor; \]

the lengths of the two bases are \( h \) and \( h - m + 1 \).

**Proof**

A benzenoid can be rotated in 2D space, and the different poses require different size of trapezoidal area. As an example of a benzenoid shown in Figure 4, there are six ways to place a benzenoid and all the six trapezoidal areas have the same number of hexagons (\( h \)) along the lower base, which is in accordance with Lemma 3.

![Figure 4. Six poses of a benzenoid and the corresponding trapezoidal area](image)

The ranges of coordinates \((x, y, z)\) of a benzenoid are illustrated in Figure 5. In Figure 5, \( x_{\text{min}} \) denotes the minimum value of all the \( x \) of all the hexagons in a benzenoid, \( x_{\text{max}} \) denotes the maximum of these \( x \); and \( y_{\text{max}}, y_{\text{min}}, z_{\text{max}} \) and \( z_{\text{min}} \) denotes the corresponding maximum and minimum values of \( y \) and \( z \). If \( X = x_{\text{max}} - x_{\text{min}}, Y = y_{\text{max}} - y_{\text{min}}, Z = z_{\text{max}} - z_{\text{min}} \), the value of \( \min(X, Y, Z) + 1 \) is the number of the layers of hexagons in the trapezoidal area are really required.

The benzenoid that looks like a clover has the largest value of \( \min(X, Y, Z) \) of all the benzenoids with a certain number of hexagons. In order to get this benzenoid a hexagon is added to one of the leaves circling around the central hexagon every time.
The procedure of adding hexagons is shown in Figure 6, and herein \(X = \min(X, Y, Z)\).

Figure 5. The ranges of coordinates of a benzenoid

Figure 6. The procedure of adding hexagons to the benzenoid that have the
Figure 7 shows that how the value of min(X, Y, Z) changes when hexagons are added one by one.

**Figure 7. The values of min(X, Y, Z) as hexagons are added one by one**

Thus, the equation to calculate min(X, Y, Z) is:

\[
\text{min}(X, Y, Z) = \left\lfloor \frac{(h-1)}{3} \right\rfloor \times 2 + a \quad \begin{cases} 
(\text{if } (h-1) \mod 3 = 2, \ a = 1 \\
\text{else}, \ a = 0 
\end{cases}
\]

The number of hexagons along the legs of the trapezoidal area is:

\[
m = \text{min}(X, Y, Z) + 1 \\
m = \left\lfloor \frac{(h-1)}{3} \right\rfloor \times 2 + 1 + a \quad \begin{cases} 
(\text{if } (h-1) \mod 3 = 2, \ a = 1 \\
\text{else}, \ a = 0 
\end{cases}
\]

The equation can be simplified as:

\[
m = \left\lfloor \frac{2h+1}{3} \right\rfloor
\]

It can be found in Figure 3 that if \(m=2\), the upper base of trapezoid is \(h-1\). Further,
it can be found that the length upper base is $h-m+1$. 