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Hexagonal Arrangements in the Plane.

In Chemistry, Polycyclic Aromatic Hydrocarbons (PAHs) are modeled by connected graphs formed by adjoining identical hexagons, where each hexagon must share an edge with at least one other hexagon. We will focus on PAHs whose graphs live strictly in the plane. An exact formula for the number of such PAHs whose graphs are composed of n hexagons is extremely unlikely, but we prove that this number has exponential growth as well as provide lower and upper bounds. Moreover, we look at which PAHs have graphs maximizing/minimizing the Wiener index, a topological index which has been well-studied for many types of graphs and which has been shown in the case of alkanes to be highly correlated to properties such as boiling point, surface tension, and density. (Received February 10, 2018)