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QSPR ANALYSIS OF POWER INDICES OF POLYCYCLIC AROMATIC HYDROCARBONS

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Abstract. In this paper, we present two new degree-based topological indices, the First Power Index $FPI(G)$ and the Second Power Index $SPI(G)$. We provided explicit formulae for $FPI(G)$ and $SPI(G)$ for some standard graphs. We also discussed the quantitative structure-property relationship (QSPR) of polycyclic aromatic hydrocarbons (PAHs). This study shows a strong connection between the physical and chemical properties of PAHs and the First Power Index $FPI(G)$ and Second Power Index $SPI(G)$, which are related to the way these molecules are structured in graphs. Additionally, the paper calculated the Hyper Zagreb Index $HZI(G)$, Randic Index $RI(G)$, and Sum Connectivity Index $SCI(G)$ for the PAH graph structure, which all showed a stronger connection to the physical and chemical properties of PAHs. Finally, the paper presented a linear regression between the considered molecular descriptors and the physicochemical properties of PAHs.

Keywords. Maximum degree, Minimum degree, Topological indices, QSPR analysis.

AMS (MOS) subject classification: 05C90, 05C92, 05C07, 05C38.

1 Introduction

Graph theory is a branch of applied mathematics and has a wide range of applications in solving real-life problems. It offers feasible solutions in ar-