

UNIVERSITI TEKNOLOGI MARA

TECHNICAL REPORT

**VALENCY-BASED TOPOLOGICAL INDICES OF SOME WHEEL
RELATED GRAPHS**

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IN THE NAME OF ALLAH, THE MOST GRACIOUS, THE MOST MERCIFUL

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ABSTRACT

The study of topological indices in chemistry has a considerable influence on our comprehension of molecular connectivity and its significance in comparing the boiling points of chemical compounds. While topological indices and graph theory have been widely used in chemistry to analyse compounds and determine structure-activity relationships, there is still a knowledge gap over how to compute the first and second Zagreb indices as well as the Randić index for some wheel related graphs. Scientists have to calculate the value of these topological indices from the beginning. Degree of each vertices have to be determined in order to calculate the values of the topological indices. For graphs of big order, it will be time-consuming. This work fills this knowledge gap by advancing the understanding and offering helpful information to researchers. The objectives involve constructing wheel-related graphs, such as gear and helm graphs, using Maple software, and determining the corresponding indices by using its' definition. The main significance of the study is to provide the chemist the exact value of first and second Zagreb index and Randic index. The methodology includes an exploration of fundamental graph theory concepts, constructing graphs using Maple, determining vertex degrees by counting the number of edges that incident to the vertex, and subsequently computing the indices based on the provided definitions. The first Zagreb index is defined as sum of the squares of the degree of vertices in the graph. Meanwhile, the second Zagreb index is sum of product of the degree pairs of adjacent vertices in graph and Randić index is the sum of one divided with square root of the degree of vertices in graph. In this study, these indices of wheel, gear and helm graphs of order at most 12 are determined. This study found that the topological indices are increased when the order of the graphs are increased.