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Energies of graphs by means of splitting and shadow graph operations

S. V. S. K. Samarasinghe[1*] and K. K. K. R. Perera[2]

[1]Faculty of Science, University of Kelaniya, Sri Lanka
[2]Department of Mathematics, University of Kelaniya, Sri Lanka
savini.kusalka@gmail.com*

Chemical applications of graph theory were presented by Hückel in his molecular orbital theory. In mathematical chemistry, the skeleton of non-saturated hydrocarbon is represented by a graph which is called the molecular graph. The energy levels of electrons are eigenvalues of the graph, and the strength of particles is closely identified with the spectrum of its graph. The sum of the absolute values of eigenvalues of the adjacency matrix of a simple, finite, and undirected graph G was defined as the energy of G. After the success of this theory, numerous various graph energies were introduced, using different matrices other than adjacency matrix, such as Laplacian energy and Randić energy from Laplacian and Randić matrices respectively. Applications of graph energy appeared in quantum chemistry to determine different characteristics of molecules. Graph energy is related to π-electron energy of a molecule, the generalized ABC energy is related to the polarization of bonds in a molecule, and the harmonic energy is a useful tool in predicting the boiling point, heats of vaporization, surface tensions and critical temperature of alkanes with high correlation coefficient values. There are many graph operations such as graph union, graph intersection, graph join, that can be used to obtain different graphs from a given graph. In this study, splitting and shadow graph operations will be discussed. These two graph operations enable us to acquire bigger graphs from a given graph. The objective of this research is to find generalized ABC energy, sum-connectivity energy and harmonic energy of much bigger graphs acquired from the given graph using the above graph operations. This allows us to obtain ABC energy, sum-connectivity energy and harmonic energy of bigger graphs using those energies of rather small graphs. Direct relationship between the original graph various energy and the relevant energy of the larger graph can be observed from the results. In this research, ABC energy of the splitting graph and shadow graph of any k-regular graph, and the sum-connectivity energy and harmonic energy of the shadow graph of any graph were obtained. These results were novel and verified through the simulations.

Keywords: Generalized ABC Energy, Harmonic Energy, Sum-Connectivity Energy, Splitting Graph, Shadow Graph