On Kites, Comets, and Stars.
Sums of Eigenvector Coefficients in (Molecular) Graphs

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Two graph invariants were encountered that form the link between (molecular) walk counts and eigenvalues of graph adjacency matrices. In particular, the absolute value of the sum of coefficients of the first or principal (normalized) eigenvector, s_1, and the analogous quantity s_n, pertaining to the last eigenvector, appear in equations describing some limits (for infinitely long walks) of relative frequencies of several walk counts. Quantity s_1 is interpreted as a measure of *mixedness* of a graph, and s_n, which plays a role for bipartite graphs only, is interpreted as a measure of the *imbalance* of a bipartite graph. Consequently, s_n is maximal for star graphs, while the minimal value of s_n is zero. Mixedness s_1 is maximal for regular graphs. Minimal values of s_1 were found by exhaustive computer search within the sample of all simple connected undirected n-vertex graphs, $n \leq 10$: They are encountered among graphs called *kites*. Within the special sample of tree graphs (searched for $n \leq 20$) so-called *double snakes* have maximal s_1, while the trees with minimal s_1 are so-called *comets*. The behaviour of stars and double snakes can be described by exact equations, while approximate equations for s_1 of kites and comets could be derived that are fully compatible with and allow to predict some pecularities of the results of the computer search. Finally, the discriminating power of s_1, determined within trees and 4-trees (alkanes), was found to be high.

Key words: Molecular Graphs; Walks; Eigenvector Coefficients.