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Vukicevic, Boskovic: Adriatic graphs - mathematical properties and applications to correct NIST database

Let F be a family of graphs. Adriatic graph $A(F)$ is a graph which vertices are ordered pairs of graphs in F that have the same number of vertices. Two vertices (G_1, G_2) and (H_1, H_2) are adjacent if: there is a non-pendant vertex v_i in graph G_i which all neighbors except one are leaves, $i = 1, 2$; v_1 and v_2 have the same degrees; and graph obtained by replacing one pendant vertex of v_i by path of length two is isomorphic to H_i , $i = 1, 2$. Mathematical properties of these graphs and their application in chemistry will be discussed.