Core Electrons and Hydrogen Atoms in Chemical Graph Theory

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Abstract

A new algorithm for the δ^v number, which is able to 'graph' encode the core electrons of the atoms in a molecule, as well as the number of hydrogen atoms in a molecule, is proposed. The new δ^v algorithm is based on two mathematical concepts: the general graph or pseudograph and the complete graph. The concept of pseudograph is used to encode into the δ^v number the single bond, the multiple bonds as well as the non-bonding electrons. The concept of complete graph is instead used to encode into the δ^v number the core electrons. This last encoding is achieved by the aid of two characteristics of complete graphs: the order, and the regularity. The hydrogen atoms, which are normally suppressed in chemical graph theory, are encoded by an extended use of the two already cited graph concepts. Actually, the hydrogen encoding could be read as a kind of 'graph' perturbation inserted into the δ^v number. The δ^v algorithm is now able to differentiate among compounds which have a differing number of bonded hydrogen atoms like BHF_2 and CH_2F_2, as well as to differentiate among compounds, which have atoms that differ only by their principal quantum number, like CH_2F_2 and CH_2Cl_2. The proposed algorithm has been tested with different properties of different classes of compounds and the obtained results tell us that odd complete graphs are better suited to encode the core electrons of atoms. The same results tell us also that the hydrogen perturbation is not always constant throughout the model of the different properties, and that in some cases the perturbation depends on the number of compounds of a class.