Localization-delocalization matrices: Bridging QTAIM and chemical graph theory

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Chemical graph theory (CGT) defines matrices that represent the molecular graph based on connectivity. In CGT one then extracts numbering/labeling-independent matrix invariants to be used as molecular descriptors in empirical quantitative structure/property to activity relationships (QSAR/QSPR). A matrix representations of molecular structure is proposed as a more powerful alternative to connectivity graphs. The localization and delocalization indices calculated within the framework of the quantum theory of atoms in molecules (QTAIM) are used to construct a matrix representation of the molecular graph, a “fuzzy” graph, whereby an edge exists between any pair of atoms in the molecules (bonded (i.e. share a bond path) or not) weighted by the delocalization index between them. Such a fuzzy graph is represented by what we term electron “localization-delocalization matrix (or LDM)”. We show that the LDM representations of a series of molecules provide a powerful tool for robust QSAR/QSPR modeling. This approach has potential applications e.g. predicting physicochemical properties of homologous series of molecules, corrosion protective abilities (and identifying active corrosion protective species), ribotoxicity, pKa’s, aromaticity, and more.


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