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Localization-delocalization matrices: Bridging QTAIM and chemical graph theory

Chérif Matta[1], Ronal Cook[2], Ismat Sumar[3], Paul Ayers[1]
[1]*Dept. Chemistry And Physics, Mount Saint Vincent University, Halifax, Canada,* [2]*TDA Research, Denver, Colorado, United States,* [3]*Saint Mary's University, Halifax, NS, Canada*
E-mail: cherif.matta@msvu.ca

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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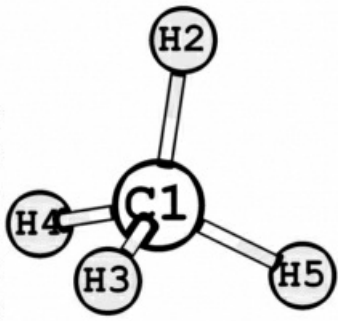
$$\mathrm{LDM} \equiv \begin{bmatrix} \Lambda(\Omega_1) & \delta(\Omega_1,\Omega_2)/2 & \cdots & \delta(\Omega_1,\Omega_n)/2 \\ \delta(\Omega_2,\Omega_1)/2 & \Lambda(\Omega_2) & \cdots & \delta(\Omega_2,\Omega_n)/2 \\ \vdots & \vdots & \ddots & \vdots \\ \delta(\Omega_n,\Omega_1)/2 & \delta(\Omega_n,\Omega_2)/2 & \cdots & \Lambda(\Omega_n) \end{bmatrix}_{n\times n} \begin{matrix} \sum_{\text{row}} \\ = N(\Omega_1) \\ = N(\Omega_2) \\ \vdots \\ = N(\Omega_n) \end{matrix} \Bigg\} \sum_{i=1}^{n} N(\Omega_i) = N$$

$$\sum_{\text{column}} \underbrace{= N(\Omega_1) \quad = N(\Omega_2) \quad \cdots \quad = N(\Omega_n)}_{\sum_{i=1}^{n} N(\Omega_i) = N} \qquad tr(\zeta) = N_{\text{loc}}$$

$$\mathrm{LDM}_{CH_4} = \begin{array}{c} \\ \mathrm{C1} \\ \mathrm{H2} \\ \mathrm{H3} \\ \mathrm{H4} \\ \mathrm{H4} \\ \sum \end{array} \begin{array}{c} \begin{array}{ccccc} \mathrm{C1} & \mathrm{H2} & \mathrm{H3} & \mathrm{H4} & \mathrm{H5} \end{array} \\ \begin{pmatrix} 4.040 & 0.492 & 0.492 & 0.492 & 0.492 \\ 0.492 & 0.444 & 0.021 & 0.021 & 0.021 \\ 0.492 & 0.021 & 0.444 & 0.021 & 0.021 \\ 0.492 & 0.021 & 0.021 & 0.444 & 0.021 \\ 0.492 & 0.021 & 0.021 & 0.021 & 0.444 \\ 6.007 & 0.998 & 0.998 & 0.998 & 0.998 \end{pmatrix} \end{array} \begin{array}{c} \sum \\ 6.007 \\ 0.998 \\ 0.998 \\ 0.998 \\ 0.998 \\ 10.000 \end{array}$$



Keywords: Quantum theory of atoms in molecules, chemical graph theory, fuzzy molecular graphs