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.


\[
\text{LDM} = \begin{bmatrix}
\Lambda(\Omega_1) & \delta(\Omega_1, \Omega_2)/2 & \cdots & \delta(\Omega_1, \Omega_n)/2 \\
\delta(\Omega_2, \Omega_1)/2 & \Lambda(\Omega_2) & \cdots & \delta(\Omega_2, \Omega_n)/2 \\
& \cdots & \ddots & \cdots \\
\delta(\Omega_n, \Omega_1)/2 & \delta(\Omega_n, \Omega_2)/2 & \cdots & \Lambda(\Omega_n)
\end{bmatrix}
\]

\[
\sum_{\text{row}} = N(\Omega_i) = N
\]

\[
\sum_{\text{column}} = N(\Omega_i) = N
\]

\[
\sum_{i=1}^{n} N(\Omega_i) = N
\]

\[
\text{tr} (\zeta) = N_{\text{loc}}
\]

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