Algebraic Forms

Three different algebraic forms can be calculated from input structures, namely quadratic, linear and bilinear maps. Shortly, if a molecule consists of *n* atoms (*vector of* $\Re^n$), then the k^{th} *total* (whole) *quadratic, bilinear* and *linear indices* are calculated as quadratic, bilinear and linear forms on $\Re^n$, respectively, in canonical basis set. Specifically, the k^{th} *non-stochastic atom-based quadratic, bilinear* and *linear indices* for a molecule, $q_k(\bar{x},\bar{x})$, $b_k(\bar{x},\bar{y})$ and $f_k(\bar{x})$, respectively, are computed from these k^{th} *non-stochastic graph–theoretic electronic-density matrices* (duplex), $\mathbf{M}^{k}$ as shown in Eqs. **1-3**, correspondingly:

$$q_k(\bar{x}) = \sum_{i=1}^{n} \sum_{j=1}^{n} {}^{k}m_{ij} x^i x^j = [\mathrm{X}]^t \mathbf{M}^{k} [\mathrm{X}] \qquad (\mathbf{1})$$

$$b_k(\bar{x},\bar{y}) = \sum_{i=1}^{n} \sum_{j=1}^{n} {}^{k}m_{ij} x^i y^j = [\mathrm{X}]^t \mathbf{M}^{k} [\mathrm{Y}] \qquad (\mathbf{2})$$

$$f_k(\bar{x}) = \sum_{i=1}^{n} f_k(\bar{x}_i) = [\mathrm{u}]^t \mathbf{M}^{k} [\mathrm{X}] \qquad (\mathbf{3})$$

where, *n* is the number of atoms (atomic nuclei) of the molecule, and $x^1,\ldots,x^n$ and $y^1,\ldots,y^n$ are the coordinates or components of the molecular vectors $\bar{x}$ and $\bar{y}$ in a system of canonical ('natural') basis vectors of $\Re^n$. In this basis system, the coordinates [($x^1,\ldots,x^n$) and ($y^1,\ldots,y^n$)] of any molecular vectors ($\bar{x}$ and $\bar{y}$) coincide with the components of the vectors [($x_1,\ldots,x_n$) and ($y_1,\ldots,y_n$)]. For this reason, these coordinates can be considered as weights (atomic labels) of the vertices of the molecular pseudo graph. $[\mathrm{u}]^t$ is an *n*-dimensional unitary row vector. The coefficients ${}^{k}m_{ij}$ are the elements of the k^{th} power of the matrix **M**(G), correspondingly, of the molecular pseudo graph.