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# DESIGN OF TOPOLOGICAL INDICES. PART 12.[1]

## PARAMETERS FOR VERTEX- AND EDGE-WEIGHTED MOLECULAR GRAPHS

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The weighted molecular matrices are the source of important graph theoretic descriptors of the chemical structure. Such descriptors can be used in structure-property studies and in measuring the chemical similarity and diversity of the compounds from chemical databases. Five approaches are presented for the calculation of atom and bond parameters for heteroatom-containing organic compounds represented as vertex- and edge-weighted molecular graphs. The first two weighting schemes compute the atom and bond weights on the basis of the relative atomic mass, using carbon as standard. The other three systems use the relative atom polarizability, radius, and electronegativity to compute atom and bond weights, again with the carbon atom as standard. The new parameter sets can be used to compute the adjacency matrix, the distance matrix, other molecular graph matrices and graph structural descriptors derived therefrom.

## INTRODUCTION

Molecular graph descriptors are currently used to develop structure-property models and to measure the similarity and diversity of the compounds from chemical databases. Although the graph model of the chemical structure does not consider the information regarding the three-dimensional structure of the molecule, the molecular graph descriptors are effective parameters in modeling various physical, chemical, and biological properties of organic compounds. Among the large class of molecular graph invariants used to express in a numerical form the chemical structure, we mention here graph theoretic polynomials and spectra, spectral moments, topological indices, distances, walks and paths in graphs, topological indices.[2-10]

In this paper chemical structures are represented as molecular graphs. By removing all hydrogen atoms from the chemical formula of a compound containing covalent bonds one obtains the hydrogen-depleted (or hydrogen-suppressed) molecular graph of that compound, whose vertices correspond to non-hydrogen atoms and whose edges correspond to covalent bonds. In this study such expressions as "molecular graph" and "molecule", "vertex" and "atom", "edge" and "bond" are used interchangeably.

Chemical compounds containing multiple or aromatic bonds, or heteroatoms are represented as vertex- and edge-weighted (VEW) molecular graphs. The computation of structural descriptors and topological indices from vertex- and edge-weighted molecular graphs requires the development of special parameters. A widely used set of parameters for VEW graphs was developed by Trinajstić and coworkers[11] by weighting the contributions of atoms and bonds with parameters based on the atomic number $Z$ and the topological bond order. In the atomic number weighting scheme $Z$ the vertex parameter $Vw(Z)_i$ of the vertex $v_i$ (representing atom $i$ from a molecule) is defined by the following equation:

$$Vw(Z)_i = 1 - Z_C/Z_i = 1 - 6/Z_i, \quad (1)$$

where $Z_i$ is the atomic number $Z$ of the atom $i$ and $Z_C = 6$ is the atomic number $Z$ of carbon. The edge parameter $Ew(Z)_{ij}$ that characterizes the bond between atoms $i$ and $j$ (represented in the molecular graph by the edge $e_{ij}$ between vertices $v_i$ and $v_j$), is defined as:

$$Ew(Z)_{ij} = Z_C Z_C / Bo_{ij} Z_i Z_j = 6 \cdot 6 / Bo_{ij} Z_i Z_j, \quad (2)$$

where $Bo_{ij}$ is the topological bond order of the edge between vertices $v_i$ and $v_j$. The topological bond order takes the value 1 for single bonds, 2 for double bonds, 3 for triple bonds and 1.5 for aromatic bonds.

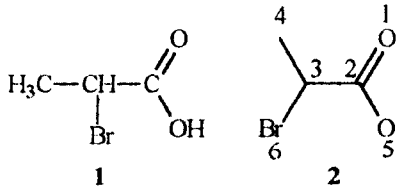
The $Z$ weighting scheme was applied with good results in various QSAR studies.[12-14] There exist other methods for computing heteroatom parameters,[15] and weights for chemical bonds.[16] A different approach for considering heteroatoms was developed for the Balaban index $J$, considering electronegativity or covalent radii.[17,18] The extended index $J$ was applied in QSAR studies.[19] Using the parameters developed for the Balaban index $J$, two general weighting schemes for the molecular matrices were proposed: $X$, the relative electronegativity scheme, and $Y$, the relative covalent radii scheme.[20]

In this paper five approaches are presented for the calculation of atom and bond parameters in heteroatom-containing organic compounds represented as vertex- and edge-weighted molecular graphs. The first two weighting schemes compute the atom and bond weights on the basis of relative atomic mass, using carbon as standard. The remaining three systems use the relative atom polarizability, radius, and electronegativity to compute atom and bond weights, again with the carbon atom as standard. The new parameter sets can be used to compute the adjacency matrix, the distance matrix, other molecular graph matrices, graph structural descriptors, and topological indices derived from them.

## Parameters for molecular graphs

The weighting schemes defined in the present paper will be applied to the computation of some molecular graph descriptors with graph operators. Three molecular matrices will be used to compute graph invariants: the adjacency matrix **A**, the distance matrix **D**, and the reciprocal distance matrix **RD**.[21-23] An operator uses some mathematical operations performed on a certain molecular matrix computed with a weighting scheme. The operatorial notation of the graph invariants offers a simple way to indicate the weighting scheme and to denote similar descriptors computed with the same mathematical procedure from different molecular matrices.

The characteristic polynomial operator **Ch**(**M**,$w$,$G$) is the characteristic polynomial for the matrix **M** of the molecular graph $G$ computed with the weighting scheme $w$. The graph spectrum operator **Sp**(**M**,$w$,$G$) is the set of eigenvalues for the matrix **M** of the molecular graph $G$ computed with the weighting scheme $w$, or the set of zeros of the characteristic polynomial, **Ch**(**M**,$w$,$G$) = 0.




1 2

As examples of structural descriptors computed with the $Z$ weighting scheme we give the characteristic polynomials and spectra for the adjacency, distance, and reciprocal distance matrices of 2-bromopropanoic acid **1** whose molecular graph is represented as graph **2**.

$$\mathbf{Ch}(\mathbf{A},Z,2) = x^6 - 1.329x^5 - 2.256x^4 + 3.378x^3 - 0.377x^2 - 0.660x + 0.146$$

$$\mathbf{Ch}(\mathbf{D},Z,2) = x^6 - 1.329x^5 - 34.505x^4 - 64.729x^3 - 29.331x^2 + 4.461x + 2.029$$

$$\mathbf{Ch}(\mathbf{RD},Z,2) = x^6 - 1.329x^5 - 48.791x^4 - 19.138x^3 + 287.493x^2 + 212.640x + 37.251$$

**Sp(A,*Z*,2)** = {1.596, 0.840, 0.629, 0.250, –0.449, –1.537}

**Sp(D,*Z*,2)** = {7.322, 0.257, –0.245, –0.884, –1.305, –3.815}

**Sp(RD,*Z*,2)** = {7.454, 2.666, –0.288, –0.460, –2.602, –5.442}.

The vertex sum operator for the vertex $v_i$ in a graph $G$, $\mathbf{VS}(\mathbf{M},w,G)_i$, is defined as the sum of the elements in the column $i$, or row $i$, of the molecular matrix $\mathbf{M}(w) = \mathbf{M}(w,G)$ computed with the weighting scheme $w$:

$$\mathbf{VS}(\mathbf{M},w,G) = \sum_{j=1}^{N}[\mathbf{M}(w)]_{ij} = \sum_{j=1}^{N}[\mathbf{M}(w)]_{ji}. \tag{3}$$

If **M** is the distance matrix, the operator is identical with the distance sum $\mathbf{DS}(w,G)$, while if **M** is the reciprocal distance matrix **RD**, this operator gives the reciprocal distance sum $\mathbf{RDS}(w,G)$.[22]

The Wiener operator, $\mathbf{Wi}(\mathbf{M},w,G)$, computed from the molecular matrix **M** with the weighting scheme $w$ is defined with the equation:

$$\mathbf{Wi}(\mathbf{M},w,G) = \sum_{i=1}^{N}\sum_{j=1}^{N}[\mathbf{M}(w)]_{ij}. \tag{4}$$

If **M** is the **D** matrix, the Wiener operator gives the Wiener index $W$,[24,25] while if **M** is the **RD** matrix, the Wiener operator gives the Harary index.[22,23]

**The *A* Weighting Scheme**. The atomic mass weighting scheme $A$ uses the atomic mass $A$ to define the vertex parameter $Vw(A)_i$ for the atom $i$:

$$Vw(A)_i = 1 - A_C/A_i = 1 - 12.011/A_i \tag{5}$$

and the edge parameter $Ew(A)_{ij}$ for the bond between atoms $i$ and $j$:

$$Ew(A)_{ij} = A_C A_C/Bo_{ij}A_iA_j = 12.011 \cdot 12.011/Bo_{ij}A_iA_j, \tag{6}$$

where $A_i$ is the atomic mass of atom $i$, $A_j$ is the atomic mass of atom $j$, and $A_C = 12.011$ is the atomic mass for carbon. Selected values for the atomic mass $A$, used in eqs. (5) and (6), are presented in Table 1, column 3.

*Table 1*

Selected set of atomic properties used with different weighting schemes: atomic number $Z$, atomic mass $A$, polarizability $\alpha_v$ (Å$^3$), radius $r_\alpha$ (Å), and electronegativity $\chi_\alpha$

| Element | $Z$ | $A$ | $\alpha_v$ | $r_\alpha$ | $\chi_\alpha$ |
|---|---|---|---|---|---|
| B | 5 | 10.811 | 3.03 | 1.45 | 2.02 |
| C | 6 | 12.011 | 1.76 | 1.21 | 2.55 |
| N | 7 | 14.007 | 1.10 | 1.03 | 3.12 |
| O | 8 | 15.999 | 0.802 | 0.93 | 3.62 |
| F | 9 | 18.998 | 0.557 | 0.82 | 4.23 |
| Si | 14 | 28.086 | 5.38 | 1.75 | 1.87 |
| P | 15 | 30.974 | 3.63 | 1.54 | 2.22 |
| S | 16 | 32.066 | 2.90 | 1.43 | 2.49 |
| Cl | 17 | 35.453 | 2.18 | 1.30 | 2.82 |
| As | 33 | 74.922 | 4.31 | 1.63 | 2.11 |
| Se | 34 | 78.960 | 3.77 | 1.56 | 2.31 |
| Br | 35 | 79.904 | 3.05 | 1.45 | 2.56 |
| Te | 52 | 127.60 | 5.5 | 1.77 | 2.08 |
| I | 53 | 126.90 | 4.7 | 1.68 | 2.27 |

*Table 2*

Vertex parameters *Vw* computed with different weighting schemes: *Vw*(*Z*), based on the atomic number *Z*; *Vw*(*A*), based on the atomic mass *A*; *Vw*(*P*), based on the atomic polarizability $\alpha_v$; *Vw*(*R*), based on the atomic radius $r_\alpha$; *Vw*(*E*), based on the atomic electronegativity $\chi_a$

| Atom | *Vw*(*Z*) | *Vw*(*A*) | *Vw*(*P*) | *Vw*(*R*) | *Vw*(*E*) |
|---|---|---|---|---|---|
| B | 0.200 | 0.111 | 0.419 | 0.166 | 0.262 |
| C | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| N | 0.143 | 0.143 | 0.600 | 0.175 | 0.183 |
| O | 0.250 | 0.249 | 1.195 | 0.301 | 0.296 |
| F | 0.333 | 0.368 | 2.160 | 0.476 | 0.397 |
| Si | 0.571 | 0.572 | 0.673 | 0.309 | 0.364 |
| P | 0.600 | 0.612 | 0.515 | 0.214 | 0.149 |
| S | 0.625 | 0.625 | 0.393 | 0.154 | 0.024 |
| Cl | 0.647 | 0.661 | 0.193 | 0.069 | 0.096 |
| As | 0.818 | 0.840 | 0.592 | 0.258 | 0.209 |
| Se | 0.824 | 0.848 | 0.533 | 0.224 | 0.104 |
| Br | 0.829 | 0.850 | 0.423 | 0.166 | 0.004 |
| Te | 0.885 | 0.906 | 0.680 | 0.316 | 0.226 |
| I | 0.887 | 0.905 | 0.626 | 0.280 | 0.123 |

Table 2 gives in column 3 the values for the vertex parameters *Vw*(*A*) computed from the atomic mass weighting scheme *A*. For boron the *Vw*(*A*) parameter has a negative value because its atomic mass is lower than that of carbon. Carbon has a *Vw*(*A*) parameter equal to zero, while for the remaining atoms from Table 2 one can observe a steady increase of the *Vw*(*A*) weight with the increase of the corresponding atomic mass. A comparison with the corresponding parameters obtained with the *Z* weighting scheme, presented in column 2 of Table 2, shows that the *Vw*(*A*) parameters are close in numerical value to the *Vw*(*Z*) parameters because the ratio *Z*/*A* is approximately constant for the atoms presented in Table 2. The edge parameters *Ew*(*A*) computed for a selected set of bonds with the atomic mass *A* weighting scheme are given in Table 3. For a pair of bonded atoms *i* and *j* the *Ew*(*A*) parameter decreases with the increase of the atomic mass of the two atoms, as one may see in the series of single bonds C–F, C–Cl, C–Br, C–I.

*Table 3*

Edge parameters *Ew*(*A*) computed with the atomic mass weighting scheme *A*

| $Atom_i$ | $Atom_j$ | single | double | triple | aromatic |
|---|---|---|---|---|---|
| C | C | 1.000 | 0.500 | 0.333 | 0.667 |
| C | N | 0.857 | 0.429 | 0.286 | 0.572 |
| C | O | 0.751 | 0.375 | | |
| C | F | 0.632 | | | |
| C | Si | 0.428 | | | |
| C | P | 0.388 | | | |
| C | S | 0.375 | 0.187 | | 0.250 |
| C | Cl | 0.339 | | | |
| C | Se | 0.152 | | | |
| C | Br | 0.150 | | | |
| C | Te | 0.094 | | | |
| C | I | 0.095 | | | |
| N | N | 0.735 | 0.368 | | 0.490 |
| N | O | 0.644 | 0.322 | | 0.429 |
| O | S | 0.281 | 0.141 | | |

*Table 4*

The vertex- and edge-weighted distance matrix **D**(*A*,**2**) for the molecular graph of 2-bromopropanoic acid **2** computed with the *A* weighting scheme

| | **D**(*A*,**2**) | | | | | |
|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 0.249 | 0.375 | 1.375 | 2.375 | 1.126 | 1.526 |
| 2 | 0.375 | 0.000 | 1.000 | 2.000 | 0.751 | 1.150 |
| 3 | 1.375 | 1.000 | 0.000 | 1.000 | 1.751 | 0.150 |
| 4 | 2.375 | 2.000 | 1.000 | 0.000 | 2.751 | 1.150 |
| 5 | 1.126 | 0.751 | 1.751 | 2.751 | 0.249 | 1.901 |
| 6 | 1.526 | 1.150 | 0.150 | 1.150 | 1.901 | 0.850 |

As an example of computation of the vertex- and edge-weighted distance matrix with the *A* weighting scheme we present in Table 4 the distance matrix **D**(*A*,**2**) for the molecular graph of 2-bromopropanoic acid **2**. The vertex sum vector of the graph **2** is **VS(D**,*A*,**2**) = {7.027, 5.276, 5.276, 9.276, 8.529, 6.727}. The sum of the elements from the upper triangle and the main diagonal of the distance matrix **D**(*A*,**2**) gives the Wiener index, **Wi(D**,*A*,**2**) = 21.730. We present below some characteristic polynomials and spectra computed with the *A* weighting scheme for the **A**, **D**, and **RD** matrices of the molecular graph **2**:

$$\mathbf{Ch(A},A,\mathbf{2}) = x^6 - 1.348x^5 - 2.241x^4 + 3.429x^3 - 0.402x^2 - 0.673x + 0.149$$

$$\mathbf{Ch(D},A,\mathbf{2}) = x^6 - 1.348x^5 - 34.263x^4 - 62.882x^3 - 26.107x^2 + 6.377x + 2.331$$

$$\mathbf{Ch(RD},A,\mathbf{2}) = x^6 - 1.348x^5 - 59.063x^4 - 18.574x^3 + 379.874x^2 + 273.629x + 46.311$$

$$\mathbf{Sp(A},A,\mathbf{2}) = \{1.593, 0.857, 0.634, 0.249, -0.450, -1.536\}$$

$$\mathbf{Sp(D},A,\mathbf{2}) = \{7.293, 0.297, -0.245, -0.882, -1.303, -3.812\}$$

$$\mathbf{Sp(RD},A,\mathbf{2}) = \{8.126, 2.801, -0.273, -0.460, -2.599, -6.247\}$$

**The *AH* Weighting Scheme.** The structural invariants computed from hydrogen-depleted molecular graphs do not reflect in an explicit way the number of hydrogen atoms attached to a certain atom. In order to define a weighting scheme based on the atomic mass *A* that gives atom and bond parameters different from those of the *Z* scheme, we consider the mass of a non-hydrogen atom together with that of the hydrogen atoms connected to it. The *AH* weighting scheme uses the following equation to define the vertex parameter $Vw(AH)_i$ for the non-hydrogen atom *i*:

$$Vw(AH)_i = 1 - A_C/(A_i + NoH_iA_H) = 1 - 12.011/(A_i + 1.0079NoH_i). \quad (7)$$

The edge parameter $Ew(AH)_{ij}$ for the bond between atoms *i* and *j* is defined with the equation:

$$Ew(AH)_{ij} = A_CA_C/Bo_{ij}(A_i + NoH_iA_H)(A_j + NoH_jA_H) =$$
$$= 12.011 \cdot 12.011/Bo_{ij}(A_i + 1.0079NoH_i)(A_j + 1.0079NoH_j), \quad (8)$$

where $A_C = 12.011$ is the atomic mass for carbon, $A_H = 1.0079$ is the atomic mass for hydrogen, $NoH_i$ is the number of hydrogen atoms bonded to the heavy atom *i*, and $NoH_j$ is the number of hydrogen atoms bonded to the heavy atom *j*.

Table 5 presents a set of vertex $Vw(AH)$ group parameters computed with the $AH$ weighting scheme. Heavy atoms without adjacent hydrogen atoms have $Vw(AH)$ parameters identical with the corresponding $Vw(A)$ parameters presented in Table 2 column 3. An inspection of the values shows that equation (7) gives parameters that do not parallel the $Vw(A)$ values. A selected set of edge parameters $Ew(AH)$ computed with the $AH$ weighting scheme is given in Table 6. Bonds between atoms that do not have adjacent hydrogen atoms have $Ew(AH)$ parameters equal to the corresponding $Ew(A)$ parameters presented in Table 3.

*Table 5*

Vertex parameters $Vw(AH)$ computed with the $AH$ weighting scheme. Vertices representing atoms not bonded to hydrogen atoms have $Vw(AH)$ parameters identical with the corresponding $Vw(A)$ parameters presented in Table 2

| Group | $Vw(AH)$ | Group | $Vw(AH)$ |
|---|---|---|---|
| $CH_3$ | 0.201 | NH | 0.200 |
| $CH_2$ | 0.144 | OH | 0.294 |
| CH | 0.077 | $PH_2$ | 0.636 |
| $NH_2$ | 0.250 | PH | 0.624 |

*Table 6*

Edge parameters $Ew(AH)$ computed with the $AH$ weighting scheme. Edges representing bonds between atoms not bonded to hydrogen atoms have $Ew(AH)$ parameters identical with the corresponding $Ew(A)$ parameters presented in Table 3

| Bond | $Ew(AH)$ | Bond | $Ew(AH)$ |
|---|---|---|---|
| $CH_3$–$CH_2$ | 0.684 | N–$CH_2$ | 0.734 |
| $CH_3$–CH | 0.737 | N–CH | 0.791 |
| $CH_3$–C | 0.799 | NH=CH | 0.369 |
| $CH_2$–$CH_2$ | 0.733 | NH=C | 0.400 |
| $CH_2$–CH | 0.790 | N=CH | 0.396 |
| $CH_2$–C | 0.856 | OH–$CH_2$ | 0.605 |
| CH–CH | 0.851 | OH–CH | 0.652 |
| CH–C | 0.923 | OH–C | 0.706 |
| $CH_2$=CH | 0.395 | O–$CH_3$ | 0.600 |
| $CH_2$=C | 0.428 | O–$CH_2$ | 0.643 |
| CH≡C | 0.308 | O–CH | 0.693 |
| $NH_2$–$CH_2$ | 0.642 | O=CH | 0.346 |
| $NH_2$–CH | 0.692 | $PH_2$–$CH_2$ | 0.312 |
| $NH_2$–C | 0.750 | $PH_2$–CH | 0.336 |
| NH–$CH_3$ | 0.639 | $PH_2$–C | 0.364 |
| NH–$CH_2$ | 0.685 | PH–$CH_3$ | 0.300 |
| NH–CH | 0.738 | PH–$CH_2$ | 0.322 |
| NH–C | 0.800 | PH–CH | 0.346 |
| N–$CH_3$ | 0.685 | PH–C | 0.376 |

As an example of application of the $AH$ weighting scheme to the computation of molecular matrices, we give in Table 7 the distance matrix $\mathbf{D}(AH,2)$ and reciprocal distance matrix $\mathbf{RD}(AH,2)$ for the molecular graph of 2-bromopropanoic acid **2**. From the two matrices one obtains the following vertex sum vectors: $\mathbf{VS(D},AH,2) = \{6.476, 4.725, 4.802, 7.874, 7.844, 6.129\}$, and $\mathbf{VS(RD},AH,2) = \{5.796, 6.709, 11.113, 4.216, 4.237, 11.407\}$. The Wiener operator applied to the above matrices gives the Wiener indices $\mathbf{Wi(D},AH,2) = 19.761$ and $\mathbf{Wi(RD},AH,2) = 22.574$. The polynomials and spectra

*Table 7*

The vertex- and edge-weighted distance matrix **D**(*AH*,**2**) and reciprocal distance matrix **RD**(*AH*,**2**) for the molecular graph of 2-bromopropanoic acid **2** computed with the A weighting scheme

**D**(*AH*,**2**)

| | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| 1 | 0.249 | 0.375 | 1.298 | 2.035 | 1.082 | 1.437 |
| 2 | 0.375 | 0.000 | 0.923 | 1.660 | 0.706 | 1.061 |
| 3 | 1.298 | 0.923 | 0.077 | 0.737 | 1.629 | 0.139 |
| 4 | 2.035 | 1.660 | 0.737 | 0.201 | 2.366 | 0.876 |
| 5 | 1.082 | 0.706 | 1.629 | 2.366 | 0.294 | 1.768 |
| 6 | 1.437 | 1.061 | 0.139 | 0.876 | 1.768 | 0.850 |

**RD**(*AH*,**2**)

| | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| 1 | 0.249 | 2.664 | 0.770 | 0.491 | 0.925 | 0.696 |
| 2 | 2.664 | 0.000 | 1.084 | 0.603 | 1.416 | 0.942 |
| 3 | 0.770 | 1.084 | 0.077 | 1.357 | 0.614 | 7.211 |
| 4 | 0.491 | 0.603 | 1.357 | 0.201 | 0.423 | 1.142 |
| 5 | 0.925 | 1.416 | 0.614 | 0.423 | 0.294 | 0.566 |
| 6 | 0.696 | 0.942 | 7.211 | 1.142 | 0.566 | 0.850 |

computed for the molecular graph **2** with the *AH* weighting scheme are:

$$\mathbf{Ch(A},AH,\mathbf{2}) = x^6 - 1.671x^5 - 1.115x^4 + 2.782x^3 - 0.950x^2 - 0.163x + 0.064$$

$$\mathbf{Ch(D},AH,\mathbf{2}) = x^6 - 1.671x^5 - 26.197x^4 - 35.341x^3 - 8.381x^2 + 4.800x + 1.233$$

$$\mathbf{Ch(RD},AH,\mathbf{2}) = x^6 - 1.671x^5 - 68.781x^4 - 17.519x^3 + 463.509x^2 + 323.459x + 50.760$$

$$\mathbf{Sp(A},AH,\mathbf{2}) = \{1.463, 0.856, 0.621, 0.259, -0.250, -1.278\}$$

$$\mathbf{Sp(D},AH,\mathbf{2}) = \{6.535, 0.348, -0.240, -0.701, -0.975, -3.296\}$$

$$\mathbf{Sp(RD},AH,\mathbf{2}) = \{8.906, 2.855, -0.238, -0.474, -2.612, -6.766\}.$$

The static electric dipole polarizability is an atomic property that can be experimentally determined and theoretically computed. Recently a relationship was presented between atomic polarizability and electronegativity, leading to a new set of electronegativities for the elements in the periodic table.[26] A set of atomic radii was also computed from the atomic polarizabilities. Using the values for polarizability, electronegativity, and radius, we define the following three weighting schemes.

**The *P* Weighting Scheme**. The polarizability weighting scheme *P* uses the polarizability[26] $\alpha$ to define the vertex parameter $Vw(P)_i$ for the atom *i*:

$$Vw(P)_i = 1 - \alpha_C/\alpha_i = 1 - 1.76/\alpha_i. \tag{9}$$

The bond between atoms *i* and *j* has an edge parameter $Ew(P)_{ij}$ computed with the equation:

$$Ew(P)_{ij} = \alpha_C\alpha_C/Bo_{ij}\alpha_i\alpha_j = 1.76 \cdot 1.76/Bo_{ij}\alpha_i\alpha_j, \tag{10}$$

where $\alpha_C = 1.76$ is the carbon polarizability, $\alpha_i$ and $\alpha_j$ are the polarizabilities of atoms $i$ and $j$, respectively. Some values for the polarizability $\alpha$ that may be used in eqs. (9) and (10) are presented in Table 1, column 4.[26] Values for the vertex parameters $Vw(P)$ computed with the polarizability weighting scheme $P$ are given in Table 2, column 4. For the elements with a polarizability lower than that of carbon (N, O, and F in Table 1), the corresponding $Vw(P)$ values are negative, while for the elements with $\alpha$ greater than $\alpha_C$ the $Vw(P)$ parameters are positive. From the definition of the $P$ weighting scheme it is clear that the parameter $Vw(P)$ captures the periodicity of the polarizability. Selected values for the edge parameters $Ew(P)$ computed with the polarizability weighting scheme $P$ are presented in Table 8. Several $Ew(P)$ parameters for single bonds have values greater than 1, i.e. C–N, C–O, C–F, N–N, N–O, and O–S. Table 8 presents also several examples of double and aromatic bonds with $Ew(P)$ values greater than 1.

*Table 8*

Edge parameters $Ew(P)$ computed with the molecular polarizability weighting scheme $P$

| $Atom_i$ | $Atom_j$ | single | double | triple | aromatic |
|---|---|---|---|---|---|
| C | C | 1.000 | 0.500 | 0.333 | 0.667 |
| C | N | 1.600 | 0.800 | 0.533 | 1.067 |
| C | O | 2.195 | 1.097 | | |
| C | F | 3.160 | | | |
| C | Si | 0.327 | | | |
| C | P | 0.485 | | | |
| C | S | 0.607 | 0.303 | | 0.405 |
| C | Cl | 0.807 | | | |
| C | Se | 0.467 | | | |
| C | Br | 0.577 | | | |
| C | Te | 0.320 | | | |
| C | I | 0.374 | | | |
| N | N | 2.560 | 1.280 | | 1.707 |
| N | O | 3.511 | 1.756 | | 2.341 |
| O | S | 1.332 | 0.666 | | |

*Table 9*

The vertex- and edge-weighted distance matrix $\mathbf{D}(P,2)$ for the molecular graph of 2-bromopropanoic acid **2** computed with the $P$ weighting scheme

| | $\mathbf{D}(P,2)$ | | | | | |
|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | -1.195 | 1.097 | 2.097 | 3.097 | 3.292 | 2.674 |
| 2 | 1.097 | 0.000 | 1.000 | 2.000 | 2.195 | 1.577 |
| 3 | 2.097 | 1.000 | 0.000 | 1.000 | 3.195 | 0.577 |
| 4 | 3.097 | 2.000 | 1.000 | 0.000 | 4.195 | 1.577 |
| 5 | 3.292 | 2.195 | 3.195 | 4.195 | -1.195 | 3.772 |
| 6 | 2.674 | 1.577 | 0.577 | 1.577 | 3.772 | 0.423 |

The polarizability weighting scheme $P$ was used to compute the distance matrix of the molecular graph **2**; the matrix $\mathbf{D}(P,2)$, presented in Table 9, offers the vertex invariants $\mathbf{VS}(\mathbf{D},P,2)$, $\mathbf{VS}(\mathbf{D},P,2) =$ $= \{11.063, 7.869, 7.869, 11.869, 15.452, 10.600\}$, and the Wiener index, $\mathbf{Wi}(\mathbf{D},P,2) = 31.378$. Some polynomials and spectra of the graph **2** computed with the polarizability weighting scheme $P$ are:

$$\mathbf{Ch}(\mathbf{A},P,2) = x^6 + 1.966x^5 - 7.936x^4 - 9.976x^3 + 9.758x^2 + 8.246x - 3.041$$

$$\mathbf{Ch}(\mathbf{D},P,2) = x^6 + 1.966x^5 - 90.913x^4 - 552.991x^3 - 1055.969x^2 - 741.117x - 147.939$$

**Ch(RD,*P*,2)** = $x^6 + 1.966x^5 - 7.468x^4 - 25.497x^3 - 25.295x^2 - 8.660x - 0.752$

**Sp(A,*P*,2)** = {2.308, 1.001, 0.302, –1.120, –1.195, –3.261}

**Sp(D,*P*,2)** = {11.259, –0.328, –0.979, –1.600, –4.137, –6.180}

**Sp(RD,*P*,2)** = {3.331, –0.130, –0.457, –1.341, –1.621, –1.749}.

**The *R* Weighting Scheme**. The atomic radius weighting scheme *R* uses the atomic radius $r_\alpha$ computed from the atomic polarizability[26] to define the vertex parameter $Vw(R)_i$ for the atom *i*:

$$Vw(R)_i = 1 - r_C/r_i = 1 - 1.21/r_i \tag{11}$$

and an edge parameter $Ew(R)_{ij}$ computed for the bond between atoms *i* and *j*:

$$Ew(R)_{ij} = r_C r_C/Bo_{ij} r_i r_j = 1.21 \cdot 1.21/Bo_{ij} r_i r_j, \tag{12}$$

where $r_C$ = 1.21 is the carbon radius, $r_i$ and $r_j$ are the atomic radii of atoms *i* and *j*, respectively. Selected values for the atomic radius *r* that may be used in eqs. (11) and (12) are reported in Table 1, column 5;[26] these values were used to compute the vertex parameters $Vw(R)$ from Table 2, column 5. The $Vw(R)$ parameters may have negative values, as is the case with N, O, and F. Using formula (12) one may obtain the edge parameters $Ew(R)$ included in Table 10. The same six single bonds that have $Ew(P)$ parameters greater than 1 have also $Ew(R)$ parameters greater than 1. On the other hand, the variation of $Ew(R)$ parameters does not parallel that of $Ew(P)$ parameters; for example, while $Ew(P)$ is greater than 1 for the bonds C=O, N=N, and N=O, the parameter $Ew(R)$ is lower than 1 for the same set of bonds.

*Table 10*

Edge parameters $Ew(R)$ computed with the atomic radius weighting scheme *R*

| $Atom_i$ | $Atom_j$ | single | double | triple | aromatic |
|---|---|---|---|---|---|
| C | C | 1.000 | 0.500 | 0.333 | 0.667 |
| C | N | 1.175 | 0.587 | 0.392 | 0.783 |
| C | O | 1.301 | 0.651 | | |
| C | F | 1.476 | | | |
| C | Si | 0.691 | | | |
| C | P | 0.786 | | | |
| C | S | 0.846 | 0.423 | | 0.564 |
| C | Cl | 0.931 | | | |
| C | Se | 0.776 | | | |
| C | Br | 0.834 | | | |
| C | Te | 0.684 | | | |
| C | I | 0.720 | | | |
| N | N | 1.380 | 0.690 | | 0.920 |
| N | O | 1.528 | 0.764 | | 1.019 |
| O | S | 1.101 | 0.550 | | |

An example of a molecular matrix computed with the *R* weighting scheme is presented in Table 11; the distance matrix **D**(*R*,**2**) for the molecular graph of 2-bromopropanoic acid **2** is used to compute the vertex sum vector **VS(D**,*R*,2) = {9.087, 6.786, 6.786, 10.786, 11.689, 10.290}, and the Wiener index **Wi(D**,*R*,2) = 27.494. Using the **A**, **D**, and **RD** matrices of the molecular graph **2** and the

*Table 11*

The vertex- and edge-weighted distance matrix **D**(*R*,2) for the molecular graph of 2-bromopropanoic acid **2** computed with the *R* weighting scheme

| | **D**(*R*,**2**) | | | | | |
|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | -0.301 | 0.651 | 1.651 | 2.651 | 1.952 | 2.485 |
| 2 | 0.651 | 0.000 | 1.000 | 2.000 | 1.301 | 1.834 |
| 3 | 1.651 | 1.000 | 0.000 | 1.000 | 2.301 | 0.834 |
| 4 | 2.651 | 2.000 | 1.000 | 0.000 | 3.301 | 1.834 |
| 5 | 1.952 | 1.301 | 2.301 | 3.301 | -0.301 | 3.136 |
| 6 | 2.485 | 1.834 | 0.834 | 1.834 | 3.136 | 0.166 |

*R* weighting scheme one obtains the following characteristic polynomials and spectra:

$$\mathbf{Ch(A},R,\mathbf{2}) = x^6 + 0.437x^5 - 4.821x^4 - 1.594x^3 + 3.650x^2 + 0.760x - 0.105$$

$$\mathbf{Ch(D},R,\mathbf{2}) = x^6 + 0.437x^5 - 61.310x^4 - 279.460x^3 - 460.116x^2 - 302.458x - 64.628$$

$$\mathbf{Ch(RD},R,\mathbf{2}) = x^6 + 0.437x^5 - 8.559x^4 - 14.596x^3 - 5.939x^2 + 1.245x + 0.798$$

$$\mathbf{Sp(A},R,\mathbf{2}) = \{1.931, 0.900, 0.096, -0.301, -1.027, -2.035\}$$

$$\mathbf{Sp(D},R,\mathbf{2}) = \{9.575, -0.419, -0.843, -1.757, -2.335, -4.659\}$$

$$\mathbf{Sp(RD},R,\mathbf{2}) = \{3.432, 0.323, -0.469, -0.680, -1.283, -1.760\}.$$

**The *E* Weighting Scheme**. The electronegativity weighting scheme *E* uses the atomic electronegativity[26] $\chi$ to define the vertex parameter $Vw(E)$ for atom $i$:

$$Vw(E)_i = 1 - \chi_C/\chi_i = 1 - 2.55/\chi_i \quad (13)$$

The bond between atoms $i$ and $j$ has an edge parameter $Ew(E)_{ij}$ computed with the formula:

$$Ew(E)_{ij} = \chi_C\chi_C/Bo_{ij}\chi_i\chi_j = 2.55 \cdot 2.55/Bo_{ij}\chi_i\chi_j, \quad (14)$$

where $\chi_C = 2.55$ is the carbon electronegativity, $\chi_i$ and $\chi_j$ are the electronegativities of atoms $i$ and $j$, respectively. Values for the electronegativity $\chi$ that may be used to compute vertex and edge parameters $Vw(E)$ and $Ew(E)v$ are presented in Table 1, column 6;[26] using these values one obtains the vertex parameters $Vw(E)$ from Table 2, column 6 and the edge parameters $Ew(E)$ presented in Table 12. All ele-

*Table 12*

Edge parameters $Ew(E)$ computed with the atomic electronegativity weighting scheme *E*

| $Atom_i$ | $Atom_j$ | Single | double | triple | aromatic |
|---|---|---|---|---|---|
| C | C | 1.000 | 0.500 | 0.333 | 0.667 |
| C | N | 0.817 | 0.409 | 0.272 | 0.545 |
| C | O | 0.704 | 0.352 | | |
| C | F | 0.603 | | | |
| C | Si | 1.364 | | | |
| C | P | 1.149 | | | |
| C | S | 1.024 | 0.512 | | 0.683 |
| C | Cl | 0.904 | | | |
| C | Se | 1.104 | | | |
| C | Br | 0.996 | | | |
| C | Te | 1.226 | | | |
| C | I | 1.123 | | | |
| N | N | 0.668 | 0.334 | | 0.445 |
| N | O | 0.576 | 0.288 | | 0.384 |
| O | S | 0.721 | 0.361 | | |

ments with electronegativity lower than that of carbon have negative values for the $Vw(E)$ parameters; Table 2 presents several such cases, namely B, Si, P, S, As, Se, Te and I. All other heteroatoms from Table 2 have positive $Vw(E)$ values. The closer the electronegativity of an atom to that of carbon, the closer to zero the corresponding $Vw(E)$ parameter. A number of single bond $Ew(E)$ parameters for have values greater than 1, i.e. C–Si, C–P, C–S, C–Se, C–Te, and C–I. For the same set of bonds, the $Ew(Z)$, $Ew(A)$, $Ew(P)$, and $Ew(R)$ parameters have values lower than 1, showing that the electronegativity weighting scheme $E$ gives a numerical representation of the chemical structure different from that of the other schemes.

*Table 13*

The vertex- and edge-weighted distance matrix **D**($E$,**2**) for the molecular graph of 2-bromopropanoic acid **2** computed with the $E$ weighting scheme

**D**($E$,**2**)

| | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| 1 | 0.296 | 0.352 | 1.352 | 2.352 | 1.057 | 2.348 |
| 2 | 0.352 | 0.000 | 1.000 | 2.000 | 0.704 | 1.996 |
| 3 | 1.352 | 1.000 | 0.000 | 1.000 | 1.704 | 0.996 |
| 4 | 2.352 | 2.000 | 1.000 | 0.000 | 2.704 | 1.996 |
| 5 | 1.057 | 0.704 | 1.704 | 2.704 | 0.296 | 2.701 |
| 6 | 2.348 | 1.996 | 0.996 | 1.996 | 2.701 | 0.004 |

We have to mention here that whereas the atom and bond parameters computed the $Z$ and $A$ weighting schemes show a monotonous variation with the atomic number $Z$ or with the atomic mass, the new parameter scales $P$, $E$, and $R$ show a periodicity in their variation.

The distance matrix of the molecular graph **2**, **D**($R$,**2**), computed with the electronegativity $E$ weighting scheme, is presented in Table 13; the sum of the elements on its columns (or rows) give the vertex invariants **VS(D**,$E$,**2)**, **VS(D**,$E$,**2)** = {7.757, 6.053, 6.053, 10.053, 9.166, 10.041}, while the sum of the application of the formula (4) gives the Wiener index, **Wi(D**,$E$,**2)** = 24.859. Some polynomials and spectra of the graph **2** computed with the electronegativity weighting scheme $E$ are:

$$\mathbf{Ch(A},E,\mathbf{2}) = x^6 - 0.595x^5 - 3.523x^4 + 1.962x^3 + 0.969x^2 - 0.367x + 0.001$$

$$\mathbf{Ch(D},E,\mathbf{2}) = x^6 - 0.595x^5 - 46.996x^4 - 149.490x^3 - 164.036x^2 - 68.456x - 8.138$$

$$\mathbf{Ch(RD},E,\mathbf{2}) = x^6 - 0.595x^5 - 16.169x^4 - 18.386x^3 + 5.339x^2 + 10.864x + 2.776$$

**Sp(A**,$E$,**2)** = {1.813, 0.768, 0.296, 0.002, –0.497, –1.786}

**Sp(D**,$E$,**2)** = {8.488, –0.194, –0.627, –0.958, –1.994, –4.120}

**Sp(RD**,$E$,**2)** = {4.746, 0.776, –0.450, –0.499, –1.214, –2.764}.

The Wiener operator is used to compute a series of topological indices with the $Z$, $A$, $P$, $R$, and $E$ weighting schemes. Table 14 presents the Wiener indices computed from the distance matrix **D** for butane and related molecules with the molecular graph CCCHet, where Het represents a heteroatom, while Table 15 presents the Wiener indices computed from the reciprocal distance matrix **RD** for the same set of compounds. The inspection of the values in Tables 14 and 15 shows that **Wi(D**,$Z$**)** and **Wi(D**,$A$**)** increase with increasing atomic number, while **Wi(RD**,$Z$**)** and **Wi(RD**,$A$**)** decrease with increasing atomic number. The topological indices computed with the $P$, $R$, and $E$ weighting schemes show a periodicity in their values; obviously, the three weighting schemes can generate molecular descriptors which express both the effect of topology and of polarizability, atomic radii, or electronega-

*Table 14*

Topological indices computed with the Wiener operator for the distance matrix and the *Z*, *A*, *P*, R, and *E* weighting schemes

| Compound | Wi(D,*Z*) | Wi(D,*A*) | Wi(D,*P*) | Wi(D,*R*) | Wi(D,*E*) |
|---|---|---|---|---|---|
| $CH_3-CH_2-CH_2-CH_3$ | 10.000 | 10.000 | 10.000 | 10.000 | 10.000 |
| $CH_3-CH_2-CH_2-SiH_3$ | 8.857 | 8.855 | 8.654 | 9.383 | 10.727 |
| $CH_3-CH_2-CH_2-NH_2$ | 9.714 | 9.715 | 11.200 | 10.350 | 9.635 |
| $CH_3-CH_2-CH_2-PH_2$ | 8.800 | 8.776 | 8.970 | 9.571 | 10.297 |
| $CH_3-CH_2-CH_2-AsH_2$ | 8.364 | 8.321 | 8.817 | 9.485 | 10.417 |
| $CH_3-CH_2-CH_2-OH$ | 9.500 | 9.501 | 12.389 | 10.602 | 9.409 |
| $CH_3-CH_2-CH_2-SH$ | 8.750 | 8.749 | 9.214 | 9.692 | 10.048 |
| $CH_3-CH_2-CH_2-SeH$ | 8.353 | 8.304 | 8.934 | 9.551 | 10.208 |
| $CH_3-CH_2-CH_2-TeH$ | 8.231 | 8.188 | 8.640 | 9.367 | 10.452 |
| $CH_3-CH_2-CH_2-F$ | 9.333 | 9.264 | 14.320 | 10.951 | 9.206 |
| $CH_3-CH_2-CH_2-Cl$ | 8.706 | 8.678 | 9.615 | 9.862 | 9.809 |
| $CH_3-CH_2-CH_2-Br$ | 8.343 | 8.301 | 9.154 | 9.669 | 9.992 |
| $CH_3-CH_2-CH_2-I$ | 8.226 | 8.189 | 8.749 | 9.440 | 10.247 |

*Table 15*

Topological indices computed with the Wiener operator for the reciprocal distance matrix and the *Z*, *A*, *P*, *R*, and *E* weighting schemes

| Compound | Wi(RD,*Z*) | Wi(RD,*A*) | Wi(RD,*P*) | Wi(RD,*R*) | Wi(RD,*E*) |
|---|---|---|---|---|---|
| $CH_3-CH_2-CH_2-CH_3$ | 4.333 | 4.333 | 4.333 | 4.333 | 4.333 |
| $CH_3-CH_2-CH_2-SiH_3$ | 6.517 | 6.523 | 7.413 | 5.218 | 3.590 |
| $CH_3-CH_2-CH_2-NH_2$ | 4.698 | 4.697 | 3.187 | 3.951 | 4.811 |
| $CH_3-CH_2-CH_2-PH_2$ | 6.731 | 6.830 | 6.154 | 4.906 | 4.005 |
| $CH_3-CH_2-CH_2-AsH_2$ | 10.123 | 10.902 | 6.666 | 5.043 | 3.883 |
| $CH_3-CH_2-CH_2-OH$ | 5.018 | 5.016 | 2.313 | 3.705 | 5.172 |
| $CH_3-CH_2-CH_2-SH$ | 6.940 | 6.944 | 5.547 | 4.729 | 4.277 |
| $CH_3-CH_2-CH_2-SeH$ | 10.300 | 11.254 | 6.262 | 4.937 | 4.099 |
| $CH_3-CH_2-CH_2-TeH$ | 13.421 | 15.421 | 7.494 | 5.246 | 3.849 |
| $CH_3-CH_2-CH_2-F$ | 5.308 | 5.442 | 1.091 | 3.394 | 5.564 |
| $CH_3-CH_2-CH_2-Cl$ | 7.145 | 7.287 | 4.841 | 4.503 | 4.571 |
| $CH_3-CH_2-CH_2-Br$ | 10.476 | 11.337 | 5.678 | 4.762 | 4.343 |
| $CH_3-CH_2-CH_2-I$ | 13.592 | 15.362 | 6.945 | 5.117 | 4.058 |

tivity. For the elements in the first row of the Periodic System, **Wi(D,*P*)**, **Wi(D,*R*)**, and **Wi(RD,*E*)** increase, whereas **Wi(D,*E*)**, **Wi(RD,*P*)**, and **Wi(RD,*R*)** decrease from carbon to fluorine. For the halogen series, **Wi(D,*E*)**, **Wi(RD,*Z*)**, **Wi(RD,*A*)**, **Wi(RD,*P*)**, and **Wi(RD,*R*)** increase and **Wi(D,*Z*)**, **Wi(D,*A*)**, **Wi(D,*P*)**, **Wi(D,*R*)**, and **Wi(RD,*E*)** decrease from fluorine to iodine.

We have presented five new approaches for the calculation of atom and bond parameters in organic compounds containing multiple bonds and heteroatoms. The first two weighting schemes compute the atom and bond weights on the basis of relative atomic mass, using carbon as standard. The remaining three systems use the relative atom polarizability, radii, and electronegativity to compute atom and bond weights, again with the carbon atom as standard. The new parameter sets may be used to compute molecular graph matrices such as the adjacency matrix, the distance matrix, or the reciprocal distance matrix. With these molecular matrices one may compute a large number of descriptors that express in a numerical form the molecular structure. Such descriptors may be polynomials, spectra, spectral moments, walk counts, or various topological indices.

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