

DESIGN OF TOPOLOGICAL INDICES. PART 5.
PRECISION AND ERROR IN COMPUTING GRAPH THEORETIC INVARIANTS
FOR MOLECULES CONTAINING HETEROATOMS AND MULTIPLE BONDS¹

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The precision of computing several Graph Theoretic Invariants (GTI's) was examined for molecular graphs containing multiple bonds and heteroatoms. A large variety of GTI's were computed: adjacency and distance matrix spectra, characteristic, acyclic, and distance polynomials, as well as three new topological indices based on these GTI's. All of them exhibit a significant dependence on the precision of computing the weighting parameters. A standardization for the computation of GTI's is proposed, aimed to improve their use in chemical similarity and identity asserting, and QSAR.

1. INTRODUCTION

Molecular topology determines a large number of molecular properties ranging from physico-chemical and thermodynamic properties to chemical reactivity and biological activity. In this respect, chemical applications of graph theory have undergone dramatic expansions in recent years.²⁻⁷

From the practical point of view, an efficient way of coding the topology of a chemical compound is represented by the topological indices (TI's).⁸⁻¹² A TI is a numerical quantity obtained after a matricial, polynomial, or combinatorial manipulation of the molecular graph.

A theoretical interpretation of TI's was offered by Klein^{13,14} in the framework of graph cluster expansion theory: TI's represent a low-order expansion of the chemical structure in terms of the subgraphs of the molecular graph. The characterization of the chemical structure by using Graph Theoretical Invariants (GTI's) may be viewed as discrete analogues of Taylor series expansions. A GTI is termed multiplicative if

$$GTI(G_1 \cup G_2) = GTI(G_1) \cdot GTI(G_2)$$

where $G_1 \cup G_2$ denotes the graph composed of two disconnected components G_1 and G_2 . Such applications relating a physico-chemical property in terms of connected-subgraph cluster expansions have been made to a wide variety of properties, including boiling points, refractive indices, solubilities, heats of atomization and formation, and liquid densities.

By removing all hydrogen atoms from the chemical formula

of a chemical compound containing covalent bonds we obtain the hydrogen-depleted graph (or molecular graph) of that compound, whose vertices correspond to non-hydrogen atoms. One has to note that the molecular graph of a saturated hydrocarbon is a graph, while the molecular graph of an unsaturated hydrocarbon is a multigraph, and that of a molecule with heteroatoms is represented by a general graph. Some definitions concerning molecular graphs will follow.

Let $G = (V, E)$ be a graph G with the vertex set $V = V(G)$ and the edge set $E = E(G)$. A general graph $G = (V, L, E, Lw, Ew)$ is a graph with loops and multiple edges, with the vertex set $V = V(G)$, the loop set $L = L(G)$, the edge set $E = E(G)$, the loop weight set $Lw = Lw(G)$ and the edge weight set $Ew = Ew(G)$. In a molecular graph the atoms are represented by the vertex set V , and the chemical bonds are represented by the edge set E . Conventionally, the loop weight of a carbon atom equals zero, while the edge weight of an aliphatic C-C bond is equal to one.

The presence of multiple or aromatic bonds or heteroatoms in the molecular graphs requires the development of special parameters.

One approach was developed by Trinajstić and coworkers.^{15,16} These authors defined the loop weight of a heteroatom as follows:

$$Lw_i = 1 - 6/Z_i \quad (1)$$

where Z_i is the number of all electrons in atom i . A few values of Lw for various elements are presented in Table I. The edge weight is defined as:

$$Ew_{ij} = \frac{36}{bz_i Z_j} \quad (2)$$

Table I. Calculated loop-weights
for various chemical elements.

Atom	Lw
C	0.
N	0.143
O	0.250
P	0.600
S	0.625
F	0.333
Cl	0.647
Br	0.829
I	0.887

Table II. Calculated edge-weights
for various chemical bonds.

Bond	Ew
C-C	1.
C=C	0.500
C≡C	0.333
aromatic CC bond	0.667
C-N	0.857
C=N	0.429
C≡N	0.286
aromatic CN bond	0.571
C-O	0.750
C=O	0.375
C-F	0.667
C-Cl	0.353
C-Br	0.171
C-I	0.113

where b is the bond order, which takes the value 1 for single bonds, 2 for double bonds, 3 for triple bonds and 1.5 for aromatic bonds. A few values for E_w for various bonds are presented in Table II.

A different approach for considering heteroatoms was devised by Balaban,¹⁷ taking into account the periodicity of two chemical properties: electronegativity and covalent radii. Recently, Tvaruzek and Komenda¹⁸ devised another electronegativity-based method for computing vertex- and edge-weight in the molecular graph. A different approach is the one of Lall and Srivastava,¹⁹ who defined the edge-weight of a heteroatom-containing molecular graph being equal to the Hückel MO parameters for hetero bonds.

The application of TI's spans correlations between chemical structure and physical, chemical, and biological properties, similarity indices, codification and retrieval of chemical compounds in databases, computer-assisted organic synthesis, computer generation of classes of organic compounds.

In computing the TI's, the weightings for heteroatoms and multiple bonds may be considered with different degrees of accuracy, thus leading to different values of the same TI for a given molecular graph. This situation may lead to a number of disagreements in various applications of TI's:

- (i) The correlations with graph theoretical descriptors in Quantitative Structure-Activity Relationships (QSAR) may lead to different mathematical models and predictions.
- (ii) The codification and retrieval of molecules in chemical databases using TI's may fail, owing to the fact that a molecular structure may be characterized by different values for the same TI.

- (iii) The generation of classes of chemical compounds may lead to erroneous multiple generation of the same structure.
- (iv) The results reported in the literature concerning TI's are irreproducible if no standardisation in computing TI's is considered.

In order to investigate how the accuracy of computing the parameters of multiple bonds and heteroatoms is reflected in the value of selected GTI's and TI's, we will consider the weighting parameters defined by equations (1) and (2). The computations will be done with increasing accuracy of the weightings, beginning with two decimal positions, increasing up to six decimal positions, and finally, by computing the loop and edge weights with the highest precision of the computer (i.e. in DOUBLE PRECISION), and with at least ten reliable decimal positions. The programs were written in FORTRAN 77 and run on a IBM PC compatible computer.

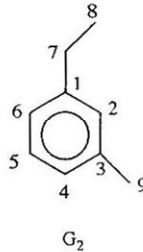
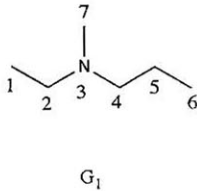
Computations will be done for a large variety of GTI's: adjacency and distance matrix spectra, characteristic, acyclic, and distance polynomials, and TI's based on all these invariants. We made this choice because we expect that the effect of the accuracy of weights will be more pronounced on this set of multiplicative GTI's.

2. ADJACENCY MATRIX SPECTRUM

The topology of a chemical structure can be coded in matrix form by the use of the adjacency matrix. The adjacency matrix of a general graph G with N vertices, $A(G)=A$, is the square $N \times N$ symmetric matrix which contains information about the connectivity of vertices in G . Its entries are defined as:

$$(A)_{ij} = \begin{cases} Lw_i & \text{for } i = j \\ Ew_{ij} & \text{for vertices } i, j \text{ adjacent} \\ 0 & \text{otherwise} \end{cases}$$

As example, the molecular graph and the adjacency matrix of ethyl-methyl-propylamine (G_1), and 1-ethyl-3-methylbenzene (G_2) are given below.



$$A(G_1) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0.857 & 0 & 0 & 0 & 0 \\ 0 & 0.857 & 0.143 & 0.857 & 0 & 0 & 0.857 \\ 0 & 0 & 0.857 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0.857 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$A(G_2) = \begin{bmatrix} 0 & 0.667 & 0 & 0 & 0 & 0 & 0.667 & 1 & 0 & 0 \\ 0.667 & 0 & 0.667 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.667 & 0 & 0.667 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0.667 & 0 & 0.667 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.667 & 0 & 0.667 & 0 & 0 & 0 & 0 \\ 0.667 & 0 & 0 & 0 & 0.667 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Lovasz and Pelikan²⁰ proposed the largest eigenvalue, X_1 , of the adjacency matrix as a measure of molecular branching.

In the present investigation we adopt the Jacobi method to calculate the adjacency spectra of graphs.

Tables III and IV present the adjacency matrix spectrum of ethyl-methyl-propylamine, and 1-ethyl-3-methylbenzene, respectively. As it is apparent from the tables, the computations using a precision of three decimal positions for the weighting parameters, as usually used, provides unreliable results, when compared with the computation with the highest precision. On the other hand, computations with weighting parameters with a precision of five and six decimal positions give results whose precision is up to five decimal positions precision.

Table III. Adjacency matrix spectrum of ethyl-methyl-propylamine.

LW	EW
.14	.86
.143	.857
.1429	.8571
.14286	.85714
.142857	.857143
1-6/7	6/7

1.82805066	-1.74482871	1.27394634	-1.25575055	0.67899202	-0.64040977	0
1.82514228	-1.74058183	1.27363999	-1.25488536	0.67889103	-0.63920611	0
1.82523913	-1.74072293	1.27365025	-1.25491438	0.67889439	-0.63924645	0
1.82527787	-1.74077938	1.27365435	-1.25492599	0.67889573	-0.63926258	0
1.82528078	-1.74078362	1.27365465	-1.25492686	0.67889583	-0.63926379	0
1.82528064	-1.74078342	1.27365464	-1.25492682	0.67889583	-0.63926373	0

Table IV. Adjacency matrix spectrum of 1-ethyl-3-methylbenzene.

EW
.66
.666
.6666
.66666
.666666
1/1.5

1.68447633	-1.34336884	1.34336884	0.85507137	-0.85507137	-0.49025769	0.49025769	0
1.69156129	-1.69156129	-1.34715339	1.34715340	0.86084112	-0.86084112	-0.49405132	0.49405132
1.69227557	-1.69227557	-1.34752998	1.34752998	0.86141686	-0.86141686	-0.49442970	0.49442970
1.69234705	-1.69234705	-1.34756762	1.34756762	0.86147442	-0.86147442	-0.49446752	0.49446752
1.69235420	-1.69235420	-1.34757138	1.34757138	0.86148017	-0.86148017	-0.49447131	0.49447131
1.69235499	-1.69235499	-1.34757180	1.34757180	0.86148081	-0.86148081	-0.49447173	0.49447173

3. DISTANCE MATRIX SPECTRUM

The distance matrix of a general graph G with N vertices, $D(G) = D$, is a square $N \times N$ symmetric matrix, whose entries, $(D)_{ij}$, are equal to the minimum sum of the weights of the edges on a path between vertices i and j . In the recent literature, there are many efficient algorithms available for computing the distance matrix for any molecular graph.²¹⁻²⁴ The numerous applications of the distance matrix to various branches of chemistry were recently surveyed.²⁵ The distance matrix of the graph G_1 is shown below:

$$D(G_1) = \begin{bmatrix} 0 & 1 & 1.857 & 2.714 & 3.714 & 4.714 & 2.714 \\ 1 & 0 & 0.857 & 1.714 & 2.714 & 3.714 & 1.714 \\ 1.857 & 0.857 & 0.143 & 0.857 & 1.857 & 2.857 & 0.857 \\ 2.714 & 1.714 & 0.857 & 0 & 1 & 2 & 1.714 \\ 3.714 & 2.714 & 1.857 & 1 & 0 & 1 & 2.714 \\ 4.714 & 3.714 & 2.857 & 2 & 1 & 0 & 3.714 \\ 2.714 & 1.714 & 0.857 & 1.714 & 2.714 & 3.714 & 0 \end{bmatrix}$$

Applications of the distance matrix spectrum were published recently.²⁶

The distance matrix spectra of graphs G_1 and G_2 are presented in Tables V and VI, computed with the same series of weighting parameters. Again, when the precision of the weights increases, we observe an increase in the precision of distance spectra of the matrices. We have to point out that even if the weights are considered with six decimal positions, the results are different from the most exact ones starting with the seventh decimal position.

The distance spectra of graphs was computed using the Jacobi method.

4. CHARACTERISTIC POLYNOMIAL

The characteristic or spectral polynomial $\text{Ch}(G,x)$ of the molecular graph G is the characteristic polynomial of its adjacency matrix:²⁷

$$\text{Ch}(G,x) = \det (xI - A) \quad (3)$$

where I is the $N \times N$ unit matrix. The characteristic polynomial of a graph is most often given in the following form:

$$\text{Ch}(G,x) = \sum_{n=0}^N c_n x^{N-n} \quad (4)$$

In the present investigation the characteristic polynomial of graphs was calculated using the Le Verrier-Fadeev-Frame method.²⁸⁻³⁰

The sum of the absolute values of the coefficients a_{2k} appearing alternatively in the characteristic polynomial (i.e. every second, or even, term) is defined as the stability index, \tilde{Z} :³¹⁻³³

$$\tilde{Z} = \sum_{k=0}^L |c_{2k}| \quad (5)$$

where L is defined as the integer smaller or equal to $[N/2]$. Another form of the stability index may be expressed as:

$$\tilde{Z} = i^{-N} \text{Ch}(G,i) \quad (6)$$

where $i = (-1)^{1/2}$. In the case of benzenoid hydrocarbons, the index \tilde{Z} has been found to be related to the total π -electron energy. We must note that the \tilde{Z} index was computed considering the weight of an aromatic carbon-carbon bond

Table VII. The coefficients of the characteristic polynomial of ethyl-methyl-propylamine.

Lw	Ew	c ₀	c ₁	c ₂	c ₃	c ₄	c ₅	c ₆	c ₇
.14	.86	1	-0.14000000	-5.21880000	0.42000000	7.17720000	-0.28000000	-2.21880000	0
.143	.857	1	-0.14300000	-5.20334700	0.42900000	7.14114300	-0.28600000	-2.20334700	0
.1429	.8571	1	-0.14290000	-5.20386123	0.42870000	7.14234287	-0.28590000	-2.20386123	0
.14286	.85714	1	-0.14286000	-5.20406694	0.42858000	7.14282286	-0.28572000	-2.20406694	0
.142857	.857143	1	-0.14285700	-5.20408237	0.42857100	7.14285886	-0.28571400	-2.20408237	0
1-6/7	6/7	1	-0.14285714	-5.20408163	0.42857143	7.14285714	-0.28571429	-2.20408163	0

Table VIII. The coefficients of the characteristic polynomial of 1-ethyl-3-methylbenzene.

Ew	c ₀	c ₁	c ₂	c ₃	c ₄	c ₅	c ₆	c ₇	c ₈	c ₉
.66	1	0	-5.613600	0	9.806126	0	-5.790426	0	0.899858	0
.666	1	0	-5.661336	0	9.980461	0	-5.961529	0	0.939290	0
.6666	1	0	-5.666133	0	9.998045	0	-5.978867	0	0.943311	0
.66666	1	0	-5.666613	0	9.999804	0	-5.980603	0	0.943714	0
.666666	1	0	-5.666661	0	9.999980	0	-5.980776	0	0.943754	0
1/1.5	1	0	-5.666667	0	10.000000	0	-5.980786	0	0.943759	0

equal to 1.

The coefficients of the characteristic polynomial of graphs G_1 and G_2 are presented in Tables VII and VIII, computed with the same set of increasing precision of loop and edge weights. As expected for a multiplicative GTI, the precision of the weights has an important effect on the values of the coefficients of the characteristic polynomial.

5. ACYCLIC POLYNOMIAL

The acyclic (matching) polynomial of a graph G is defined as:^{34,35}

$$Ac(G, x) = \sum_{k=0}^L (-1)^k M(G, k) x^{N-2k} = \sum_{n=0}^N \alpha_n x^{N-n} \quad (7)$$

where $M(G, k)$ is the number of k -matchings of G , i.e. the number of selections of k mutually non-adjacent edges in G . By definition, $M(G, 0)=1$ and $M(G, 1)$ is equal to the number of edges. The set of numbers $M(G, k)$ can easily be obtained by the aid of the Z-counting polynomial:

$$Q(G, x) = \sum_{k=0}^L M(G, k) \cdot x^k \quad (8)$$

The Hosoya Z index of a graph G is given by:³⁶⁻⁴³

$$Z = \sum_{k=0}^L M(G, k) \quad (9)$$

The computation of the Hosoya index using Eq. (9) is a tedious task, due to the long time for the combinatorial generation of all k -matchings of G .

An interesting property of the acyclic (matching) polynomial is that the sum of its coefficients equals the Hosoya index Z . This property allows the computation of the Z index using algorithms and computer programs^{44,45} devised for the computation of the acyclic polynomial, or recurrence relationships for the acyclic polynomial.^{46,47}

The Hosoya Z index was applied to various correlations with theoretical and experimental molecular properties: Coulson and Pauling bond order, boiling point, absolute entropy of acyclic saturated hydrocarbons. Various relations and formulas enabling the computation of the Z index were obtained.⁴⁸⁻⁵² Again, we must point out that the Z index was computed considering the weight of an aromatic carbon-carbon bond equal to 1.

We adopt an algorithm similar to the one proposed by Ramaraj and Balasubramanian⁴⁴ to calculate the acyclic polynomials of vertex- and edge-weighted graphs.

The coefficients of the acyclic polynomials for the graph G_2 are presented in Table IX. Computations were done with a weight of an aromatic carbon-carbon bond equal to $1/1.5$, with increasing precision, as stated in Table IX.

From the values of the coefficients of the acyclic polynomial we observe that the usual precision of three decimal positions used in computing the weights is not sufficient, giving numerical values far from the "exact" ones.

Table IX. The coefficients of the acyclic polynomial of 1-ethyl-3-methylbenzene.

E_w	a_0	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	a_9
.66	1	0	-5.613600	0	9.806126	0	-5.625118	0	0.734550	0
.666	1	0	-5.661336	0	9.980461	0	-5.786997	0	0.764758	0
.6666	1	0	-5.666133	0	9.998045	0	-5.803389	0	0.767833	0
.66666	1	0	-5.666613	0	9.999804	0	-5.805030	0	0.768141	0
.666666	1	0	-5.666661	0	9.999980	0	-5.805194	0	0.768172	0
1/1.5	1	0	-5.666667	0	10.000000	0	-5.805213	0	0.768176	0

Table X. Coefficients of the distance polynomial of ethyl-methyl-propylamine.

L_w	E_w	d_0	d_1	d_2	d_3	d_4	d_5	d_6	d_7
.14	.86	1	-0.14000000	-126.58000000	-720.96710400	-1515.58697088	-1422.14521856	-593.31402752	-87.26569984
.143	.857	1	-0.14300000	-126.14245000	-716.90302591	-1503.44672244	-1406.84237917	-584.83419101	-85.56373154
.1429	.8571	1	-0.14290000	-126.15702050	-717.03825111	-1503.85032747	-1407.35064596	-585.11554413	-85.62013502
.14286	.85714	1	-0.14286000	-126.16284898	-717.09234590	-1504.01179012	-1407.55988792	-585.22811059	-85.64270275
.142857	.857143	1	-0.14285700	-126.16328612	-717.09640311	-1504.02390029	-1407.56923998	-585.23655366	-85.64439548
1-6/7	6/7	1	-0.14285714	-126.16326531	-717.09620991	-1504.02332362	-1407.56851312	-585.23615160	-85.64431487

6. DISTANCE POLYNOMIAL

The distance polynomial of the molecular graph G is the characteristic polynomial of its distance matrix:

$$\text{Dis}(G,x) = \det (xI - D) = \sum_{n=0}^N d_n x^{N-n} \quad (10)$$

The sum of the absolute values of the coefficients of the distance polynomial is defined as the Hosoya Z' index:

$$Z' = \sum_{n=0}^N |d_n| \quad (11)$$

A computer program was developed to compute distance polynomials of graphs containing up to 200 vertices.⁵³

In the present investigation the distance polynomial of graphs was calculated using the Le Verrier-Fadeev-Frame method.²⁸⁻³⁰

The coefficients of the distance polynomials of graphs G_1 and G_2 are presented in Tables X and XI, respectively. In the case of the distance polynomials, the effect of increasing precision of the weighting parameters has the more dramatic effects.

Table XI. The coefficients of the distance polynomial of 1-ethyl-3-methylbenzene.

Ew	d ₀	d ₁	d ₂	d ₃	d ₄	d ₅	d ₆	d ₇	d ₈	d ₉
.66	1	0	-163.86200	-1194.318048	-3354.757759	-4331.934225	-2550.003794	-549.784351	0	0
.666	1	0	-165.385832	-1211.023182	-3416.765723	-4430.439908	-2618.660604	-566.957055	0	0
.6666	1	0	-165.538578	-1212.702232	-3423.009471	-4440.376452	-2625.598659	-568.695491	0	0
.66666	1	0	-165.553858	-1212.870222	-3423.634276	-4441.370970	-2626.293192	-568.869547	0	0
.666666	1	0	-165.555386	-1212.887022	-3423.696761	-4441.470430	-2626.362652	-568.886955	0	0
1/1.5	1	0	-165.555556	-1212.888889	-3423.703704	-4441.481481	-2626.370370	-568.888889	0	0

Table XII. Topological indices Z_a and Z_d of ethyl-methyl-propylamine.

Lw	Ew	Z _a	Z _d
.14	.86	16.45480000	4466.99902080
.143	.857	16.40583700	4424.87550007
.1429	.8571	16.40746533	4426.27482419
.14286	.85714	16.40811674	4426.88464626
.142857	.857143	16.40816560	4426.87663564
1-6/7	6/7	16.40816326	4426.87463557

Table XIII. Topological indices Z_a, Z_c and Z_d of 1-ethyl-3-methylbenzene.

Ew	Z _a	Z _c	Z _d
.66	22.779394	23.110010	12145.661377
.666	23.193552	23.542616	12410.232304
.6666	23.235400	23.586356	12436.920883
.66666	23.239588	23.590734	12439.592065
.666666	23.240007	23.591171	12439.859206
1/1.5	23.240056	23.591222	12439.888889

7. TOPOLOGICAL INDICES BASED ON GRAPH THEORETICAL POLYNOMIALS

In the definitions of the TI's Z , \tilde{Z} , and Z' , the parameters of vertex- and edge-weighted graphs were not considered. As stated above, when the above indices were computed for benzenoid hydrocarbons, an aromatic C-C weight equal to 1 was considered.

For the vertex- and edge-weighted graphs we define the general index

$$Z_{\rho} = \sum_{n=0}^N |p_n| \quad (12)$$

where $\rho = a$ for the acyclic polynomial, $\rho = c$ for the characteristic polynomial, and $\rho = d$ for the distance polynomial, respectively.

Using the coefficients of the polynomials in Tables VIII-XI, we have computed the TI's Z_a and Z_d for the graph G_1 , and the TI's Z_a , Z_c , and Z_d for the graph G_2 , respectively. The corresponding numerical values are presented in Tables XII and XIII.

The values of the TI's present a steady increase with increasing precision of the weights, with the largest effect on the Z_d . Again, the precision of three decimal positions gives poor results when compared with the most precise ones.

8. CONCLUSIONS

The precision of computing several graph theoretic invariants (GTI's) was examined for molecular graphs containing multiple bonds and heteroatoms, using a weighting procedure based mainly on the atomic number Z .^{15,16} The atom and bond weights were computed with increasing accuracy, up to the highest precision of the computer, and a large variety of GTI's were computed: adjacency and distance matrix spectra, characteristic, acyclic, and distance polynomials, as well as three new defined TI's defined on weighted graph theoretical polynomials, namely Z_{α} , Z_c , and Z_d , respectively.

All of the GTI's under examination exhibit a significant dependence on the precision of computing the weighting parameters, the most sensitive being the invariants computed on the basis of the distance matrix.

The usual precision of three decimal positions for the weighting parameters gives completely unreliable results.

A conclusion emerges from the computations in the present investigation concerning the applications of GTI's: if one expects to obtain reliable results, the highest precision of the computer must be used in computing the weighting parameters. The main drawback of such an approach is that the results will be machine and language dependent.

We propose that for any table of TI the numerical value of each TI should include information on the decimal place accuracy of that value. Also, one should include information on the decimal place accuracy of the atom and bond weights used in computing each TI.

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