The molecular descriptors computed with MOLGEN

General references:

· TodCon : Todeschini, R.; Consonni, V. *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim and New York, **2000**
· Trin: Trinajstić, N. *Chemical Graph Theory*, 2nd edition, CRC Press, Boca Raton, FL, **1992**

0 number of atoms

A, A (incl. H) and N_H are descriptors of the category 'arithmetic'.
Notation in text: A, $A\,(incl.H)$ and N_H
A is the number of atoms excluding H atoms. $A\,(incl.H)$ is the number of atoms including H atoms. N_H is the number of H atoms.

1 number of atoms incl. H atoms

A (incl. H) see 0.

2 number of H atoms

N_H see 0.

3 relative number of H atoms

rel. N_H, rel. N_C, rel. N_O, rel. N_N, rel. N_S, rel. N_F, rel. N_Cl, rel. N_Br, rel. N_I and rel. N_P are descriptors of the category 'arithmetic'.
Notation in text: $rel.N_H$, $rel.N_C$, $rel.N_O$, $rel.N_N$, $rel.N_S$, $rel.N_F$, $rel.N_{Cl}$, $rel.N_{Br}$, $rel.N_I$ and $rel.N_P$
Relative means divided by the number of atoms (inclusive H atoms):

$$rel.N_H = \frac{N_H}{A\,(incl.H)}$$

Correspondingly $rel.N_H$, $rel.N_C$, $rel.N_O$, $rel.N_N$, $rel.N_S$, $rel.N_F$, $rel.N_{Cl}$, $rel.N_{Br}$, $rel.N_I$ and $rel.N_P$.
For N_H see 2, for $A\,(incl.H)$ see 1.

4 number of C atoms

N_C, N_O, N_N, N_S, N_F, N_Cl, N_Br, N_I and N_P are descriptors of the category 'arithmetic'.
Notation in text: N_C, N_O, N_N, N_S, N_F, N_{Cl}, N_{Br}, N_I and N_P
N_C is the number of C atoms in a molecule.
Correspondingly N_O, N_N, N_S, N_F, N_{Cl}, N_{Br}, N_I and N_P.

5 relative number of C atoms

rel. N_C see 3.

6 number of O atoms

N_O see 4.

7 relative number of O atoms
rel. N_O see 3.

8 number of N atoms
N_N see 4.

9 relative number of N atoms
rel. N_N see 3.

10 number of S atoms
N_S see 4.

11 relative number of S atoms
rel. N_S see 3.

12 number of F atoms
N_F see 4.

13 relative number of F atoms
rel. N_F see 3.

14 number of Cl atoms
N_Cl see 4.

15 relative number of Cl atoms
rel. N_Cl see 3.

16 number of Br atoms
N_Br see 4.

17 relative number of Br atoms
rel. N_Br see 3.

18 number of I atoms
N_I see 4.

19 relative number of I atoms
rel. N_I see 3.

20 number of P atoms
N_P see 4.

21 relative number of P atoms
rel. N_P see 3.

22 number of bonds
B and B (incl. H) are descriptors of the category 'arithmetic'.

Notation in text: B , $B(incl.H)$
B is the number of bonds in the H-suppressed molecule. $B(incl.H)$ is the number of bonds in a molecule containing H atoms.

23 number of bonds (incl. H atoms)

B (incl. H) see 22.

24 number of localized bonding electron pairs

loc. B and loc. B (incl. H) are descriptors of the category 'arithmetic'.
Notation in text: $loc.B$ and $loc.B(incl.H)$
$loc.B$ is the number of localized bonding electron pairs in an H-suppressed molecule. Aromatic π-electrons are delocalized and therefore not counted here.
$loc.B(incl.H)$ is analogous to $loc.B$ but includes bonds to H atoms.

25 number of localized bonding electron pairs (incl. H)

loc. B (incl. H) see 24.

26 number of single bonds

n- and n- (incl. H) are descriptors of the category 'arithmetic'.
Notation in text: $n-$ and $n-(incl.H)$
$n-$ is the number of single bonds in an H-suppressed molecule. $n-(incl.H)$ is analogous to $n-$ but includes bonds to H atoms.

27 rel. number of single bonds

rel. n- and rel n- (incl. H) are descriptors of the category 'arithmetic'.
Notation in text: $rel.n-$ and $rel.n-(incl.H)$
rel. n- is relative to the number of bonds of an H-suppressed molecule:

$$rel.n- = \frac{n-}{B}$$

Analogous is:

$$rel.n-(incl.H) = \frac{n-(incl.H)}{B\,(incl.H)}$$

For $n-$ see 26, for B see 22, for $n-(incl.H)$ see 28 and for $B(incl.H)$ see 23.

28 number of single bonds (incl. H atoms)

n- (incl. H) see 26.

29 rel. number of single bonds (incl. H atoms)

rel. n- (incl. H) see 27.

30 number of double bonds

n=, n# and n aromatic are descriptors of the category 'arithmetic'.
Notation in text: $n=$, $n\equiv$ and n_{aroma}
$n=$ is the number of double bonds, $n\equiv$ the number of triple bonds and n_{aroma} is the number of aromatic bonds.

31 relative number of double bonds

rel. n=, rel. n= (incl. H) , rel. n#, rel. n# (incl. H), rel. n aromatic and rel. n aromatic (incl. H) are descriptors of the category 'arithmetic'.
Notation in text: $rel.n=$, $rel.n=(incl.H)$, $rel.n\equiv$, $rel.n\equiv(incl.H)$, $rel.n_{aroma}$ and $rel.n_{aroma}(incl.H)$
$rel.n=$ is relative to the number of bonds in an H-suppressed molecule.
$rel.n=(incl.H)$ is relative to the number of bonds in a molecule with H atoms.
Correspondingly $rel.n\equiv$, $rel.n\equiv(incl.H)$, $rel.n_{aroma}$ and $rel.n_{aroma}(incl.H)$.

32 relative number of double bonds (incl. H atoms)

rel. n= (incl. H) see 31.

33 number of triple bonds

n# see 30.

34 relative number of triple bonds

rel. n# see 31.

35 relative number of triple bonds (incl. H atoms)

rel. n# (incl. H) see 31.

36 number of aromatic bonds

n aromatic see 30.

37 relative number of aromatic bonds

rel. n aromatic see 31.

38 relative number of aromatic bonds (incl. H atoms)

rel. n aromatic (incl. H) see 31.

39 cyclomatic number

C is a descriptor of the category 'arithmetic'.
Notation in text: C
For molecules (connected graphs) C is defined as:

$$C = B - A + 1$$

For A see 0, for B see 22.

40 molecular weight

MW and MW (incl. H) are descriptors of the category 'arithmetic'.
Notation in text: MW and $MW(incl.H)$
MW is the sum of the atomic weights in an H-suppressed molecule. The atomic weight is that of the natural abundance isotope mixture. $MW(incl.H)$ takes account of the H atoms.
Source:
- TodCon, page 332

41 mean atomic weight (or average atomic weight)

mean AW and mean AW (incl. H) are descriptors of the category 'arithmetic'.
Notation in text: $\overline{AW}$ and $\overline{AW}(incl.H)$
mean AW is defined as:

$$\overline{AW} = \frac{MW}{A}$$

Analogous $\overline{AW}(incl.H)$:

$$\overline{AW}(incl.H) = \frac{MW(incl.H)}{A(incl.H)}$$

For MW and $MW(incl.H)$ see 40 and 42. For A and $A(incl.H)$ see 0 and 1.

42 molecular weight (incl. H atoms)

MW (incl. H) see 40.

43 mean atomic weight (incl. H atoms)

mean AW (incl. H) see 41.

44 Wiener index

W is a descriptor of the category 'topological'.
Notation in text: W
W is the half-sum of the entries of the distance-matrix of the H-suppressed molecule:

$$W = \frac{1}{2} \cdot \sum_{i=1}^{A} \sum_{j=1}^{A} D_{ij} = \sum_{i=1}^{A} \sum_{j=i+1}^{A} D_{ij}$$

where A is the number of non-H atoms and D_{ij} is the entry in the ith row and the jth column of the distance matrix.
For A see 0 and for D_{ij} see distance matrix.

Source:

- Wiener, H. Structural Determination of Paraffin Boiling Points. *J. Am. Chem. Soc.* **1947**, *69*, 17-20
- TodCon, page 497

45 1st Zagreb index

M_1 is a descriptor of the category 'topological'.
Notation in text: M_1
M_1 is the sum over the squares of the vertex degree of each atom in an H-suppressed molecule:

$$M_1 = \sum_{i=1}^{A} (\delta_i)^2$$

where A is the number of non-H atoms and δ_i is the number of neighbours of atom i in an H-suppressed molecule.
For A see 0. For δ_i see vertex degree.

Source:

- Gutman, I.; Ruščić, B.; Trinajstić, N.; Wilcox, C. F. Graph Theory and Molecular Orbitals. XII. Acyclic Polyenes. *J. Chem. Phys.* **1975**, *62*, 3399-3405

· TodCon, page 509
· Trin, page 226

46 2nd Zagreb index

M_2 is a descriptor of the category 'topological'.
Notation in text: M_2

M_2 is the following sum over all edges:

$$M_2 = \sum_{edge(i,j)} (\delta_i \cdot \delta_j)$$

where δ_i is the number of neighbours of atom i in an H-suppressed molecule.

For δ_i see vertex degree.

Source:

· Gutman, I.; Ruščić, B.; Trinajstić, N.; Wilcox, C. F. Graph Theory and Molecular Orbitals. XII. Acyclic Polyenes. *J. Chem. Phys.* **1975**, *62*, 3399-3405
· TodCon, page 509
· Trin, page 226

47 1st modified Zagreb index

m^M_1 and m^M_2 are descriptors of the category 'topological'.
Notation in text: ${}^mM_1$ and ${}^mM_2$

${}^mM_1$ is the sum over the squares of the reciprocal vertex degree of each atom in an H-suppressed molecule:

$${}^mM_1 = \sum_{i=1}^{A} \left(\frac{1}{\delta_i} \right)^2$$

${}^mM_2$ is defined as the following sum over all edges:

$${}^mM_2 = \sum_{edge(i,j)} \left(\frac{1}{\delta_i \cdot \delta_j} \right)$$

where A is the number of non-H atoms and δ_i is the number of neighbours of atom i in an H-suppressed molecule. m stands for modified.
For A see 0. For δ_i see vertex degree.

Source:

· Nikolić, S.; Kovačević, G.; Miličević, A.; Trinajstić, N. The Zagreb Indices 30 Years After. *Croat. Chem. Acta*, **2003**, *76*, 113-124

48 2nd modified Zagreb index

m^M_2 see 47.

49 Randic index of order 0 (or connectivity index of order 0)

0^Chi is a descriptor of the category 'topological'.
Notation in text: ${}^0\chi$
This is the zeroth descriptor in the series m^Chi with m = 1, 2, 3, …
Notation in text: ${}^m\chi$

The definition of ${}^0\chi$:

$$ {}^0\chi = \sum_{i=1}^{A} \delta_i^{-1/2} $$

where A is the number of non H-atoms and δ_i is the number of neighbours of atom i in an H-suppressed molecule.
For A see 0. For δ_i see vertex degree.

The definition of ${}^m\chi$:

$$ {}^m\chi = \sum_{\substack{path\ p\ of \\ length\ m}} \left(\prod_{i=1}^{A(p)} \delta_i^{-1/2} \right) $$

with $m \in \{1, 2, 3, \ldots\}$. The sum runs over all paths of length m (this is the number of edges of the path). $A(p)$ is the number of the atoms in a path p. The product runs over all atoms of path p. δ_i is the vertex degree of the ith atom in path p.

For δ_i see vertex degree.

Source:

- Randić, M. On Characterization of Molecular Branching. *J. Am. Chem. Soc.* **1975**, *97*, 6609-6615
- Kier, L. B.; Murray, W. J.; Randić, M.; Hall, L. H. Molecular Connectivity V: Connectivity Series Applied to Density. *J. Pharm. Sci.*, **1976**, *65*, 1226-1230
- Kier, L. B.; Hall L. H. The Nature of Structure-Activity Relationships and their Relation to Molecular Connectivity. *Eur. J. Med. Chem.*, **1977**, *12*, 307-312
- Kier, L. B.; Hall L. H. *Molecular Connectivity in Structure-Activity Analysis.* Research-Studies Press - Wiley, Chichester (UK), **1986**
- TodCon, pages 84-85
- Trin, page 226

50 Randic Index of order 1

1^Chi see 49.

51 Randic Index of order 2

2^Chi see 49.

52 solvation connectivity index of order 0

0^Chi^s is a descriptor of the category 'topological'.

Notation in text: ${}^0\chi^s$

${}^0\chi^s$ is the zeroth member in the series m^Chi^s with m = 1, 2, 3, …

Notation in text: ${}^m\chi^s$

The definition of ${}^0\chi^s$:

$$ {}^0\chi^s = \frac{1}{2} \cdot \sum_{i=1}^{A} \frac{L_i}{\delta_i^{1/2}} $$

where A is the number of non-H atoms and δ_i is the number of neighbours of atom i in an H-suppressed molecule. L_i is the principal quantum number of atom i (for C, N, O, F: L=2; for Si, P, S, Cl: L=3).

For A see 0. For δ_i see vertex degree.

The definition of ${}^m\chi^s$:

$$ {}^m\chi^s = \frac{1}{2^{m+1}} \cdot \sum_{\substack{path\ p\ of \\ length\ m}} \left(\prod_{i=1}^{A(p)} \frac{L_i}{\delta_i^{1/2}} \right) $$

with $m \in \{1, 2, 3, \ldots\}$. The sum runs over all paths of length m (this is the number of edges in the path). $A(p)$ is the number of the atoms in a path p. The product runs over all atoms in path p. δ_i is the vertex degree of the ith atom in path p. L_i is the principal quantum number of atom i in path p.

For δ_i see vertex degree.

Source:

- Zefirov, N. S.; Palyulin, V. A. QSAR for Boiling Points of "Small" Sulfides. Are the "High-Quality Structure-Property-Activity Regressions" the Real High Quality QSAR Models? *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 1022-1027
- TodCon, pages 88-89

53 solvation connectivity index of order 1

1^Chi^s see 52.

54 solvation connectivity index of order 2

2^Chi^s see 52.

55 solvation connectivity index of order 3

3^Chi^s see 52.

56 solvation connectivity index for clusters

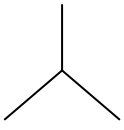
3^Chi^s (cluster) is a descriptor of the category 'topological'.

Notation in text: ${}^3\chi_C^s$

The definition of ${}^3\chi_C^s$ is:

$$ {}^3\chi_C^s = \frac{1}{2^4} \cdot \sum_{\substack{cluster\ c \\ of\ size\ 3}} \left(\prod_{i=1}^{4} \frac{L_i}{\delta_i^{1/2}} \right) $$

The sum runs over all clusters of size 3:



cluster of size 3

The product runs over all four atoms of cluster c. δ_i is the vertex degree of the ith atom in cluster c. L_i is the principal quantum number of atom i in cluster c.

For δ_i see vertex degree.

Source:

- TodCon, pages 88-89

57 Kier and Hall index of order 0

0^Chi^v is a descriptor of the category 'topological'.

Notation in text: ${}^0\chi^v$

${}^0\chi^v$ is the zeroth member of the series m^Chi with m = 1, 2, 3, …

Notation in text: ${}^m\chi^v$

The definition of ${}^0\chi^v$:

$$ {}^0\chi^v = \sum_{i=1}^{A} (\delta_i^v)^{-1/2} $$

where A is the number of non-H atoms and δ_i^v is the valence vertex degree of atom i in an H-suppressed molecule.

For A see 0. For δ_i^v see valence vertex degree.

The definition of ${}^m\chi^v$:

$$ {}^m\chi^v = \sum_{\substack{path\ p\ of \\ length\ m}} \left(\prod_{i=1}^{A(p)} (\delta_i^v)^{-1/2} \right) $$

with $m \in \{1, 2, 3, \ldots\}$. The sum runs over all paths of length m (this is the number of edges of the path). $A(p)$ is the number of atoms in a path p. The product runs over all atoms of path p.

For δ_i^v see valence vertex degree.

Source:

- Kier, L. B.; Murray, W. J.; Randić, M.; Hall, L. H. Molecular Connectivity V: Connectivity Series Applied to Density. *J. Pharm. Sci.*, **1976**, *65*, 1226-1230
- Kier, L. B.; Hall L. H. The Nature of Structure-Activity Relationships and Their Relation to Molecular Connectivity. *Eur. J. Med. Chem.* **1977**, *12*, 307-312
- TodCon, pages 85-86
- Trin, page 229

58 Kier and Hall index of order 1

1^Chi^v see 57.

Source:

- Kier, L. B.; Hall L. H. Derivation and Significance of Valence Molecular Connectivity. *J. Pharm. Sci.* **1981**, 70, 583-589
- TodCon, pages 85-86
- Trin, page 229

59 Kier and Hall index of order 2

2^Chi^v see 57.

60 Kier and Hall index of order 3

3^Chi^v see 57.

61 Kier shape index 1

1^kappa is a descriptor of the category 'topological'.

Notation in text: ${}^1\kappa$

$$ {}^1\kappa = \frac{A \cdot (A-1)^2}{B^2} $$

where A is the number of atoms and B is the number of bonds in an H-suppressed molecular graph.
For A see 0. For B see 22.
Source:

- Kier, L. B. Shape Indexes of Orders One and Three from Molecular Graphs. *Quant. Struct.-Act. Relat.* **1986**, *5*, 1-7
- Kier, L. B. Indexes of Molecular Shape from Chemical Graphs. *Acta Pharm. Jugosl.* **1986**, *36*, 171-188
- TodCon, pages 248-249

62 Kier shape index 2

2^kappa is a descriptor of the category 'topological'.
Notation in text: ${}^2\kappa$

$$ {}^2\kappa = \frac{(A-1) \cdot (A-2)^2}{({}^2P)^2} $$

where A is the number of atoms and ${}^2P$ is the number of paths of length 2 in an H-suppressed molecular graph.
For A see 0.
Source:

- Kier, L. B. A Shape Index from Molecular Graphs. *Quant. Struct.-Act. Relat.* **1985**, *4*, 109-116
- Kier, L. B. Indexes of Molecular Shape from Chemical Graphs. *Acta Pharm. Jugosl.* **1986**, *36*, 171-188
- TodCon, pages 248-249

63 Kier shape index 3

3^kappa is a descriptor of the category 'topological'.
Notation in text: ${}^3\kappa$

$$ {}^3\kappa = \begin{cases} \dfrac{(A-3) \cdot (A-2)^2}{({}^3P)^2} & \textit{for even } A\ (A>3) \\ \dfrac{(A-1) \cdot (A-3)^2}{({}^3P)^2} & \textit{for odd } A\ (A>3) \end{cases} $$

where A is the number of atoms and ${}^3P$ is the number of paths of length 3 in an H-suppressed molecular graph.
For A see 0.
Source:

- Kier, L. B. Shape Indexes of Orders One and Three from Molecular Graphs. *Quant. Struct.-Act. Relat.* **1986**, *5*, 1-7
- Kier, L. B. Indexes of Molecular Shape from Chemical Graphs. *Acta Pharm. Jugosl.* **1986**, *36*, 171-188
- TodCon, pages 248-249

64 Kier molecular flexibility index non-alpha-modified

Phi_non-alpha is a descriptor of the category 'topological'.
Notation in text: $\Phi_{\bar{\alpha}}$

$$\Phi_{\bar{\alpha}} = \frac{{}^1\kappa \cdot {}^2\kappa}{A}$$

where A is the number of atoms. ${}^1\kappa$, ${}^2\kappa$ are the Kier shape indices 1 and 2.
For ${}^1\kappa$ and ${}^2\kappa$ see 61 and 62. For A see 0.
Source:

- No source! Definition is analogous to 68 without modifying alpha.

65 Kier alpha-modified shape index 1

1^kappa_alpha is a descriptor of the category 'topological'.
Notation in text: ${}^1\kappa_\alpha$

$${}^1\kappa_\alpha = \frac{(A+\alpha)\cdot(A+\alpha-1)^2}{(B+\alpha)^2}$$

where A is the number of atoms and B is the number of bonds in an H-suppressed molecular graph. α is derived from the covalent radius of each atom.
For α see alpha. For A see 0. For B see 22.
Source:

- Kier, L. B. Distinguishing Atom Differences in a Molecular Graph Shape Index. *Quant. Struct.-Act. Relat.* **1986**, *5*, 7-12
- Kier, L. B. Shape Indexes of Orders One and Three from Molecular Graphs. *Quant. Struct.-Act. Relat.* **1986**, *5*, 1-7
- Kier, L. B. Indexes of Molecular Shape from Chemical Graphs. *Acta Pharm. Jugosl.* **1986**, *36*, 171-188
- TodCon, pages 249-250

66 Kier alpha-modified shape index 2

2^kappa_alpha is a descriptor of the category 'topological'.
Notation in text: ${}^2\kappa_\alpha$

$${}^2\kappa_\alpha = \frac{(A+\alpha-1)\cdot(A+\alpha-2)^2}{({}^2P+\alpha)^2}$$

where A is the number of atoms and ${}^2P$ is the number of paths of length 2 in an H-suppressed molecular graph. α is derived from the covalent radius of each atom.
For α see alpha. For A see 0.
Source:

- Kier, L. B. Distinguishing Atom Differences in a Molecular Graph Shape Index. *Quant. Struct.-Act. Relat.* **1986**, *5*, 7-12
- Kier, L. B. Indexes of Molecular Shape from Chemical Graphs. *Acta Pharm. Jugosl.* **1986**, *36*, 171-188
- TodCon, pages 249-250

67 Kier alpha-modified shape index 3

3^kappa_alpha is a descriptor of the category 'topological'.
Notation in text: ${}^3\kappa_\alpha$

$$ {}^3\kappa_\alpha = \begin{cases} \dfrac{(A+\alpha-3)\cdot(A+\alpha-2)^2}{({}^3P+\alpha)^2} & for\ even\ A\ (A>3) \\ \dfrac{(A+\alpha-1)\cdot(A+\alpha-3)^2}{({}^3P+\alpha)^2} & for\ odd\ A\ (A>3) \end{cases} $$

where A is the number of atoms and ${}^3P$ is the number of paths of length 3 in an H-suppressed molecular graph. α is derived from the covalent radius of each atom.
For α see alpha. For A see 0.

Source:

- Kier, L. B. Shape Indexes of Orders One and Three from Molecular Graphs. *Quant. Struct.-Act. Relat.* **1986**, *5*, 1-7
- Kier, L. B. Indexes of Molecular Shape from Chemical Graphs. *Acta Pharm. Jugosl.* **1986**, *36*, 171-188
- TodCon, pages 249-250

68 Kier molecular flexibility index

Phi is a descriptor of the category 'topological'.
Notation in text: Φ_α

$$ \Phi_\alpha = \frac{{}^1\kappa_\alpha \cdot {}^2\kappa_\alpha}{A} $$

where A is the number of atoms. ${}^1\kappa_\alpha$, ${}^2\kappa_\alpha$ are the Kier alpha-modified shape indices 1 and 2. α is derived from the covalent radius of each atom.
For ${}^1\kappa_\alpha$ and ${}^2\kappa_\alpha$ see 65 and 66. For A see 0.

Source:

- Kier, L. B. An Index of Molecular Flexibility from Kappa Shape Attributes. *Quant. Struct.-Act. Relat.* **1989**, *8*, 221-224
- TodCon, page 178

69 Platt number

F is a descriptor of the category 'topological'.
Notation in text: F

$$ F = \sum_{edge\,(i,j)} \left(N(i)+N(j)-2\right) $$

where $N(i)$ is the number of neighbours of atom i. The sum runs over all edges in an H-suppressed molecular graph.

Source:

- Platt, J. R. Influence of Neighbor Bonds on Additive Bond Properties in Paraffins. *J. Chem. Phys.* **1947**, *15*, 419-420
- Platt, J. R. Prediction of Isomeric Differences in Paraffin Properties. *J. Phys. Chem.* **1952**, *56*, 328-336
- TodCon, page 125
- Trin, page 245

70 Gordon-Scantlebury index

N_GS is a descriptor of the category 'topological'.
Notation in text: N_{GS}

N_{GS} is the number of path subgraphs of length 2 in an H-suppressed molecular graph.

Source:
- TodCon, page 125
- Trin, 245

71 Balaban index

J is a descriptor of the category 'topological'.
Notation in text: J

$$J = \frac{B}{C+1} \cdot \sum_{edge\,(i,j)} (\sigma_i \cdot \sigma_j)^{-1/2}$$

where B is the number of bonds and C is the cyclomatic number. σ_i is the i[th] vertex distance degree. The sum runs over all edges of an H-suppressed molecular graph.
For B see 22. For C see 39. For σ_i see vertex distance degree.

Source:
- Balaban, A. T. Highly Discriminating Distance-Based Topological Index. *Chem. Phys. Lett.* **1982**, *89*, 399-404
- Balaban, A. T. Topological Indices Based on Topological Distances in Molecular Graphs. *Pure Appl. Chem.* **1983**, *55*, 199-206
- TodCon, page 21
- Trin, page 246

72 unsaturated Balaban index

J_unsat is a descriptor of the category 'topological'.
Notation in text: J_{unsat}

$$J_{unsat} = \frac{B}{C+1} \cdot \sum_{edge\,(i,j)} (\hat{\sigma}_i \cdot \hat{\sigma}_j)^{-1/2}$$

where B is the number of bonds and C is the cyclomatic number. $\hat{\sigma}_i$ is the i[th] vertex unsaturated distance degree, i.e. the row sum in the unsaturated distance matrix.
For B see 22. For C see 39. For $\hat{\sigma}_i$ see vertex unsaturated distance degree.

Source:
- Balaban, A. T. Highly Discriminating Distance-Based Topological Index. *Chem. Phys. Lett.* **1982**, *89*, 399-404
- Balaban, A. T.; Filip, P. Computer Program For Topological Index J. *MATCH – Commun. Math. Comp. Chem.* **1984**, *16*, 163

73 Schultz molecular topological index

MTI is descriptor of the category 'topological'.
Notation in text: MTI
MTI is defined for an H-suppressed molecular graph:

$$MTI = \underbrace{(1,\ldots,1)}_{u^t} \cdot [A \cdot (A+D)] \cdot u = u^t \cdot (A^2 + A \cdot D) \cdot u = u^t \cdot A^2 \cdot u + \underbrace{u^t \cdot (A \cdot D) \cdot u}_{MTI'} =$$
$$= (u^t \cdot A) \cdot (A \cdot u) + MTI' = (\delta_1,\ldots,\delta_n)^t \cdot (\delta_1,\ldots,\delta_n) + MTI' = \sum_{i=1}^{n} \delta_i^2 + MTI' =$$
$$= M_1 + MTI'$$

where A is the adjacence matrix (here not the descriptor A: number of atoms), D is the distance matrix, n the number of atoms, MTI' the second MTI descriptor , δ_i is

the vertex degree of the i[th] atom and M_1 is the first Zagreb index. The letter t specifies the transposition of a vector or a matrix: $A_{ij} = A^t{}_{ji}$ in a symmetric matrix.

For A see adjacence matrix, for D see distance matrix, for MTI' see 74, for δ_i see vertex degree, for M_1 see 45.

Source:

- Schultz, H. P. Topological Organic Chemistry. 1. Graph Theory and Topological Indices of Alkanes. *J. Chem. Inf. Comput. Sci.* **1989**, *29*, 227-228
- Schultz, H. P.; Schultz, T. P. Topological Organic Chemistry. 6. Graph Theory and Molecular Topological Indices of Cycloalkanes. *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 240-244
- TodCon, page 381 (The formula given there is incorrect.)
- Trin, page 257

74 MTI'-index

MTI' is a descriptor of the category 'topological'.
Notation in text: MTI'
MTI' is defined for an H-suppressed molecular graph:

$$MTI' = \underbrace{(1,\ldots,1)}_{u^t}\cdot(A\cdot D)\cdot u = (u^t\cdot A)\cdot(D\cdot u)$$

$$= (\delta_1,\ldots,\delta_n)^t\cdot(\sigma_1,\ldots,\sigma_n) = \sum_{i=1}^{n}\delta_i\cdot\sigma_i$$

where A is the adjacence matrix (here not the descriptor A: number of atoms), D is the distance matrix, n the number of atoms, δ_i is the vertex degree of the i[th] atom, σ_i is the vertex distance degree of the i[th] atom. The letter t specifies the transposition of a vector or a matrix: $A_{ij} = A^t{}_{ji}$ in a symmetric matrix.

For A see adjacency matrix, for D see distance matrix, for δ_i see vertex degree and for σ_i see vertex distance degree.

Source:

- Müller, W. R.; Szymanski, K.; Knop, J. v.; Trinajstić, N. Molecular Topological Indices. *J. Chem. Inf. Comput. Sci.* **1990**, *30*, 160-163
- Mihalić, Z.; Nikolić, S; Trinajstić, N. Comparative Study of Molecular Descriptors Derived from the Distance Matrix. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 28-37
- TodCon, page 381

75 Harary number

H is a descriptor of the category 'topological'.
Notation in text: H
The sums run over all pairs of atoms in an H-suppressed molecular graph:

$$H = \sum_{i=1}^{A}\sum_{j=i+1}^{A}\frac{1}{D_{ij}}$$

where A is the number of non-H atoms and D_{ij} is the entry in the i[th] row and the j[th] column of the distance matrix.
For A see 0 and for D_{ij} see distance matrix.

Source:

· Ivanciuc, O.; Balaban, T.-S.; Balaban, A. T. Design of Topological Indices. Part 4. Reciprocal Distance Matrix, Related Local Vertex Invariants and Topological Indices. *J. Math. Chem.* **1993**, *12*, 309-318
· Plavsić, D.; Nikolić, S; Trinajstić, N.; Mihalić, Z. On the Harary Index for the Characterization of Chemical Graphs. *J. Math. Chem.* **1993**, *12*, 235-250
· Lucić, B.; Milicević, A.; Nikolić, S; Trinajstić, N. Harary Index – Twelve Years Later. *Croat. Chem. Acta* **2002**, *75*, 847-867
· TodCon, pages 209-210

76 total walk count

twc is a descriptor of the category 'topological'.
Notation in text: *twc*
The sum runs over all lengths (from length 1 to length $n-1$) of walks in an H-suppressed molecular graph:

$$twc = \sum_{k=1}^{n-1} mwc^{(k)}$$

where n is the number of atoms and $mwc^{(k)}$ is the molecular walk count of length k.
For $mwc^{(k)}$ see 77-83.
Source:

· Rücker, G.; Rücker, C. Counts of All Walks as Atomic and Molecular Descriptors. *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 683-695
· Rücker, G.; Rücker, C. Walk Counts, Labyrinthicity, and Complexity of Acyclic and Cyclic Graphs and Molecules. *J. Chem. Inf. Comput. Sci.* **2000**, *40*, 99-106
· Gutman, I.; Rücker, C.; Rücker, G. On Walks in Molecular Graphs *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 739-745
· Nikolić, S; Trinajstić, N.; Tolić, I. M.; Rücker, G.; Rücker, C. On Molecular Complexity Indices. Chapter 2, pages 29-89 in *Complexity in Chemistry* (Bonchev, D.; Rouvray, D. H., Eds.), Taylor and Francis, London, **2003**
· TodCon, pages 480-482

77-83 molecular walk count of length k

mwc2, **mwc3**, **mwc4**, **mwc5**, **mwc6**, **mwc7** and **mwc8** are descriptors of the category 'topological'.
Notation in text: $mwc^{(k)}$; e.g.: $mwc^{(2)}$
The sums run over all atoms in an H-suppressed molecular graph:

$$mwc^{(k)} = \sum_{i=1}^{n} \sum_{j=1}^{n} A^{(k)}{}_{ij}$$

where $A^{(k)}$ is the kth power of the adjacency matrix A (here not the descriptor A: number of atoms) and n the number of atoms.
Remark: $mwc^{(0)}$ is equal to the number of atoms, $mwc^{(1)}$ is equal to $2 \cdot B$.
For A see adjacency matrix, for B see 22.
Source:

· Rücker, G.; Rücker, C. Counts of All Walks as Atomic and Molecular Descriptors. *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 683-695
· Rücker, G.; Rücker, C. Walk Counts, Labyrinthicity, and Complexity of Acyclic and Cyclic Graphs and Molecules. *J. Chem. Inf. Comput. Sci.* **2000**, *40*, 99-106

· Gutman, I.; Rücker, C.; Rücker, G. On Walks in Molecular Graphs *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 739-745
· Nikolić, S; Trinajstić, N.; Tolić, I. M.; Rücker, G.; Rücker, C. On Molecular Complexity Indices. Chapter 2, pages 29-89 in *Complexity in Chemistry* (Bonchev, D.; Rouvray, D. H., Eds.), Taylor and Francis, London, **2003**
· TodCon, pages 480-482

84 unsaturated total walk count

twc_unsat is a descriptor of the category 'topological'.
Notation in text: twc_{unsat}
The sum runs over all lengths (from length 1 to length $n-1$) of walks in an H-suppressed molecular graph:

$$twc_{unsat} = \sum_{k=1}^{n-1} mwc_{unsat}^{(k)}$$

where n is the number of atoms and $mwc_{unsat}^{(k)}$ is the molecular walk count of length k derived from the "unsaturated" adjacency matrix, i. e. a matrix with entries >1 for multiple bonds.
For $mwc_{unsat}^{(k)}$ see 85-91. See also unsaturated adjacency matrix.
Source:
· No source. Definition is analogous to 76.

85-91 unsaturated molecular walk count of length k

mwc2_unsat, **mwc3_unsat**, **mwc4_unsat**, **mwc5_unsat**, **mwc6_unsat**, **mwc7_unsat** and **mwc8_unsat** are descriptors of the category 'topological'.
Notation in text: $mwc_{unsat}^{(k)}$; e.g.: $mwc_{unsat}^{(2)}$
The sums run over all atoms in an H-suppressed molecular graph:

$$mwc_{unsat}^{(k)} = \sum_{i=1}^{n}\sum_{j=1}^{n} \hat{A}^{(k)}{}_{ij}$$

where $\hat{A}^{(k)}$ is the kth power of the unsaturated adjacency matrix $\hat{A}$ with entries >1 for multiple bonds, and n is the number of atoms.
For $\hat{A}$ see unsaturated adjacency matrix, for B see 22.
Source:
· No source. Definition is analogous to 77-83.

92 gravitational index (pairs, topo. dist.)

G_1 (topo. dist.) is a descriptor of the category 'topological'.
Notation in text: $G_{1,topo.}$
The sum runs over all pairs of atoms in an H-suppressed molecular graph.

$$G_{1,topo.} = \sum_{i=1}^{A}\sum_{j=i+1}^{A} \frac{w_i \cdot w_j}{D_{ij}^{\ 2}}$$

where w_i is the average weight of atom i (expressed in *amu*, i.e. 12.0110 for carbon) and D_{ij} is the entry in the ith row and the jth column of the distance matrix. A is the number of atoms.
For D_{ij} see distance matrix. For A see 0.

Source:

· No source. Definition is analogous to 96 with topological distances.

93 gravitational index (pairs, topo. dist., incl. H atoms)

G_1 (topo. dist.,incl. H) is a descriptor of the category 'topological'.
Notation in text: $G_{1,topo.,H}$

The sum runs over all pairs of atoms in a molecular graph containing H atoms.

$$G_{1,topo.,H} = \sum_{i=1}^{A} \sum_{j=i+1}^{A} \frac{w_i \cdot w_j}{D_{ij}^{\ 2}}$$

where w_i is the average weight of atom i and D_{ij} is the entry in the ith row and the jth column of the distance matrix. A is the number of atoms.
For D_{ij} see distance matrix. For A see 0.

Source:

· No source. Definition is analogous to 97 with topological distances.

94 gravitational index (bonds, topo. dist.)

G_2 (topo. dist.) is a descriptor of the category 'topological'.
Notation in text: $G_{2,topo.}$

The sum runs over all edges of an H-suppressed molecular graph.

$$G_{2,topo.} = \sum_{edge\,(i,j)} w_i \cdot w_j$$

where w_i is the average weight of atom i.

Source:

· No source. Definition is analogous to 98 with topological distances.

95 gravitational index (bonds, topo. dist., incl. H atoms)

G_2 (topo. dist.,incl. H) is a descriptor of the category 'topological'.
Notation in text: $G_{2,topo.,H}$

The sum runs over all edges of a molecular graph containing H atoms.

$$G_{2,topo.,H} = \sum_{edge\,(i,j)} w_i \cdot w_j$$

where w_i is the average weight of atom i.

Source:

· No source. Definition is analogous to 99 with topological distances.

96 gravitational index (pairs, 3D-dist.)

G_1 is a descriptor of the category 'geometrical'.
Notation in text: G_1

The sum runs over all pairs of an H-suppressed molecular graph.

$$G_1 = \sum_{i=1}^{A} \sum_{j=i+1}^{A} \frac{w_i \cdot w_j}{r_{ij}^{\ 2}}$$

where w_i is the average weight of atom i and r_{ij} is the interatomic distance (expressed in Ångström Å) of atom i and atom j. A is the number of atoms.
For A see 0.

Source:
- Katritzky, A. R.; Mu L.; Lobanov, V. S.; Karelson, M. Correlation of Boiling Points with Molecular Structure. 1. A Training Set of 298 Diverse Organics and a Test Set of 9 Simple Inorganics. *J. Phys. Chem.* **1996**, *100*, 10400-10407
- TodCon, page 412

97 gravitational index (pairs, 3D-dist., incl. H atoms)

G_1 (incl. H) is a descriptor of the category 'geometrical'.
Notation in text: $G_{1,H}$

The sum runs over all pairs of atoms in a molecular graph containing H atoms.

$$G_{1,H} = \sum_{i=1}^{A} \sum_{j=i+1}^{A} \frac{w_i \cdot w_j}{r_{ij}^{\,2}}$$

where w_i is the average weight of atom i and r_{ij} is the interatomic distance (expressed in Ångström Å) of atom i and atom j. A is the number of atoms.
For A see 0.
Source:
- Katritzky, A. R.; Mu L.; Lobanov, V. S.; Karelson, M. Correlation of Boiling Points with Molecular Structure. 1. A Training Set of 298 Diverse Organics and a Test Set of 9 Simple Inorganics. *J. Phys. Chem.* **1996**, *100*, 10400-10407
- TodCon, page 412

98 gravitational index (bonds, 3D-dist.)

G_2 is a descriptor of the category 'geometrical'.
Notation in text: G_2

The sum runs over all edges of an H-suppressed molecular graph.

$$G_2 = \sum_{edge\,(i,j)} \frac{w_i \cdot w_j}{r_{ij}^{\,2}}$$

where w_i is the average weight of atom i and r_{ij} is the interatomic distance (expressed in Ångström Å) of atom i and atom j.
Source:
- Katritzky, A. R.; Mu L.; Lobanov, V. S.; Karelson, M. Correlation of Boiling Points with Molecular Structure. 1. A Training Set of 298 Diverse Organics and a Test Set of 9 Simple Inorganics. *J. Phys. Chem.* **1996**, *100*, 10400-10407
- TodCon, page 412

99 gravitational index (bonds, 3D-dist., incl. H atoms)

G_2 (incl. H) is a descriptor of the category 'geometrical'.
Notation in text: $G_{2,H}$

The sum runs over all edges of a molecular graph containing H atoms.

$$G_{2,H} = \sum_{edge\,(i,j)} \frac{w_i \cdot w_j}{r_{ij}^{\,2}}$$

where w_i is the average weight of atom i and r_{ij} is the interatomic distance (expressed in Ångström Å) of atom i and atom j.
Source:

· Katritzky, A. R.; Mu L.; Lobanov, V. S.; Karelson, M. Correlation of Boiling Points with Molecular Structure. 1. A Training Set of 298 Diverse Organics and a Test Set of 9 Simple Inorganics. *J. Phys. Chem.* **1996**, *100*, 10400-10407
· TodCon, page 412

100 Hosoya Z-index

Z is a descriptor of the category 'topological'.
Notation in text: Z

$$Z = \sum_{k=0}^{\lfloor A/2 \rfloor} a_k; \quad with \ \lfloor A/2 \rfloor = \begin{cases} A/2 & for\ even\ A \\ (A-1)/2 & for\ odd\ A \end{cases}$$

where A is the number of atoms in the H-suppressed molecular graph and a_k is the number of sets of k mutually non-adjacent edges. $a_0 = 1$, $a_1 = B$.

For A see 0, for B see 22.
Source:

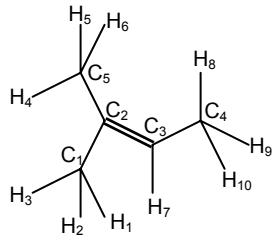
· Hosoya, H. Topological Index. A Newly Proposed Quantity Characterizing the Topological Nature of Structural Isomers of Saturated Hydrocarbons. *Bull. Chem. Soc. Jpn.* **1971**, *44*, 2332-2339
· TodCon, page 215
· Trin, page 132

101 Basak information content of order 0

IC_0, IC_1, IC_2, TIC_0, TIC_1, TIC_2, CIC_0, CIC_1, CIC_2, N*CIC_0, N*CIC_1, N*CIC_2, SIC_0, SIC_1, SIC_2, N*SIC_0, N*SIC_1, N*SIC_2, BIC_0, BIC_1, BIC_2, N*BIC_0, N*BIC_1 and N*BIC_2 are descriptors of the category 'topological'.
Notation in text: IC_0, IC_1, IC_2, TIC_0, TIC_1, TIC_2, CIC_0, CIC_1, CIC_2, $N \cdot CIC_0$, $N \cdot CIC_1$, $N \cdot CIC_2$, SIC_0, SIC_1, SIC_2, $N \cdot SIC_0$, $N \cdot SIC_1$, $N \cdot SIC_2$, BIC_0, BIC_1, BIC_2, $N \cdot BIC_0$, $N \cdot BIC_1$, $N \cdot BIC_2$
For calculating these descriptors a molecular graph inclusive H atoms is considered.

$$IC_r = \sum_{g=1}^{G} \frac{A_g^r}{A^r} \cdot \log_2 \frac{A_g^r}{A^r}$$

Explanation:



Every atom is characterized by itself and its neighbours. Here the characterization of the i[th] atom itself depends on the atom number a_i and on the number of bonding electron pairs δ_i (without H atoms). The characterization of the neighbourhood depends on the depth r of the neighbourhood (e.g. $r = 1$ for the next neighbours) and the characterization of the connected atoms and their bond multiplicities:
To calculate IC_0 only the characterization of the atoms is needed: C_1, C_2, C_3, C_4, C_5 are C-atoms and have all

$$TIC_r = A(incl.H) \cdot IC_r$$
$$CIC_r = \log_2 A(incl.H) - IC_r$$

$$N \cdot CIC_r = A(incl.H) \cdot CIC_r$$
$$SIC_r = \frac{IC_r}{\log_2 A(incl.H)}$$
$$N \cdot SIC_r = A(incl.H) \cdot SIC_r$$
$$BIC_r = \frac{IC_r}{\log_2 B(incl.H)}$$
$$N \cdot BIC_r = A(incl.H) \cdot BIC_r$$

with $A(incl.H)$ is the number of atoms and $B(incl.H)$ is the number of bonds.
For $A(incl.H)$ see 1, for $B(incl.H)$ see 23.
Source:

- Basak, S. C. Information Theoretic Indices of Neighborhood Complexity and Their Applications, chapter 12 in *Topological Indices and Related Descripors in QSAR and QSPR* (Devillers, J.; Balaban, A. T., Eds.) Gordon and Breach, Amsterdam, **1999**
- Basak, S. C. Use of Molecular Complexity Indices in Predictive Pharmacology and Toxicology: A QSAR Approach. *Med. Sci. Res.* **1987**, *15*, 605-609
- Basak, S. C.; Gute, B. D. Characterization of Molecular Structures Using Topological Indices. *SAR QSAR Environ. Res.* **1997**, *7*, 1-21

102 Basak total information content of order 0

TIC_0 see 101.

103 Basak complementary information content of order 0

CIC_0 see 101.

104 total complementary information content of order 0

N*CIC_0 see 101.

105 Basak structural information content of order 0

SIC_0 see 101.

106 total structural information content of order 0

N*SIC_0 see 101.

107 bonding information content of order 0

BIC_0 see 101.

108 total bonding information content of order 0

N*BIC_0 see 101.

109 Basak information content of order 1

IC_1 see 101.

110 Basak total information content of order 1

TIC_1 see 101.

111 Basak complementary information content of order 1
CIC_1 see 101.

112 total complementary information content of order 1
N*CIC_1 see 101.

113 Basak structural information content of order 1
SIC_1 see 101.

114 total structural information content of order 1
N*SIC_1 see 101.

115 bonding information content of order 1
BIC_1 see 101.

116 total bonding information content of order 1
N*BIC_1 see 101.

117 Basak information content of order 2
IC_2 see 101.

118 Basak total information content of order 2
TIC_2 see 101.

119 Basak complementary information content of order 2
CIC_2 see 101.

120 total complementary information content of order 2
N*CIC_2 see 101.

121 Basak structural information content of order 2
SIC_2 see 101.

122 total structural information content of order 2
N*SIC_2 see 101.

123 bonding information content of order 2
BIC_2 see 101.

124 total bonding information content of order 2
N*BIC_2 see 101.

125 mean square distance index
MSD is a descriptor of the category 'topological'.
Notation in text: *MSD*
The sums run over all atoms of an H-suppressed molecular graph:

$$MSD = \left(\frac{\sum_{i=1}^{A} \sum_{j=1}^{A} (D_{ij})^2}{A \cdot (A-1)} \right)^{1/2}$$

where A is the number of non-H atoms and D_{ij} is the entry in the i[th] row and the j[th] column of the distance matrix.
For A see 0 and for D_{ij} see distance matrix.

Source:
- Balaban, A. T. Topological Indices Based on Topological Distances in Molecular Graphs. *Pure Appl. Chem.* **1983**, *55*, 199-206
- TodCon, page 113 (The formula given there is incorrect.)

126 detour index

w is a descriptor of the category 'topological'.
Notation in text: w
The sums run over all atoms of an H-suppressed molecular graph:

$$w = \frac{1}{2} \cdot \sum_{i=1}^{A} \sum_{j=1}^{A} \Delta_{ij} = \sum_{i=1}^{A} \sum_{j=i+1}^{A} \Delta_{ij}$$

where A is the number of non-H atoms and Δ_{ij} is the entry in the i[th] row and the j[th] column of the detour matrix.
For A see 0 and for Δ_{ij} see detour matrix.

Source:
- Ivanciuc, O.; Balaban, A. T. Design of Topological Indices. Part 8. Path Matrices and Derived Molecular Graph Invariants. *MATCH – Commun. Math. Comp. Chem.* **1994**, *30*, 141-152
- Amić, D.; Trinajstić, N. On the Detour Matrix. *Croat. Chem. Acta.* **1995**, *68*, 53-62
- Lukovits, I. The Detour Index. *Croat. Chem. Acta* **1996**, *69*, 873-882
- Lukovits, I.; Razinger, M. On Calculation of the Detour Index. *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 283-286
- TodCon, page 103

127 detour index (incl. half main diagonal)

w (incl. half diag.) is a descriptor of the category 'topological'.
Notation in text: $w_{half.diag.}$
The sums run over all atoms of an H-suppressed molecular graph:

$$w_{half.diag.} = \frac{1}{2} \cdot \sum_{i=1}^{A} \sum_{j=1}^{A} \Delta^*_{ij}$$

where A is the number of non-H atoms and Δ^*_{ij} is the entry in the i[th] row and the j[th] column of the detour matrix containing diagonal elements $\neq 0$.
For A see 0 and for Δ^*_{ij} see detour matrix.

Source:
Rücker, G.; Rücker, C. Symmetry-Aided Computation of the Detour Matrix and the Detour Index. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 710-714

128-135 total acyclic path count and molecular acyclic path counts of length k

P_acyc, **2^P_acyc**, **3^P_acyc**, **4^P_acyc**, **5^P_acyc**, **6^P_acyc**, **7^P_acyc**, **8^P_acyc**, 9^P_acyc and higher are descriptors of the category 'topological'.
Notation in text: P_{acyc}, ${}^{2}P_{acyc}$, ${}^{3}P_{acyc}$, ${}^{4}P_{acyc}$, ${}^{5}P_{acyc}$, ${}^{6}P_{acyc}$, ${}^{7}P_{acyc}$, ${}^{8}P_{acyc}$, ${}^{\geq 9}P_{acyc}$

$$P_{acyc} = \sum_{l=1}^{l_{\max}} {}^{l}P_{acyc}$$

$${}^{\geq 9}P_{acyc} = \sum_{l=9}^{l_{\max}} {}^{l}P_{acyc}$$

where ${}^{l}P_{acyc}$ is the number of paths of length l in the H-suppressed molecular graph without counting any closed paths (rings). $l_{\max}$ is the maximum length of all unclosed paths.
Source:

- Randić, M.; Brissey, G. M.; Spencer, R. B.; Wilkins, C. L. Search for All Self-Avoiding Paths for Molecular Graphs. *Comput. & Chem.* **1979**, *3*, 5-13
- Randić, M. Characterization of Atoms, Molecules, and Classes of Molecules Based on Paths Enumeration. *MATCH – Commun. Math. Comp. Chem.* **1979**, *7*, 5-64
- TodCon, page 344

136 molecular acyclic path count of length 9 and higher

9^P_acyc and higher see 128-135.

137-144 total path count and molecular path counts of length k

P, **2^P**, **3^P**, **4^P**, **5^P**, **6^P**, **7^P**, **8^P**, 9^P and higher are descriptors of the category 'topological'.
Notation in text: P, ${}^{2}P$, ${}^{3}P$, ${}^{4}P$, ${}^{5}P$, ${}^{6}P$, ${}^{7}P$, ${}^{8}P$, ${}^{\geq 9}P$

$$P = \sum_{l=1}^{l_{\max}} {}^{l}P$$

$${}^{\geq 9}P = \sum_{l=9}^{l_{\max}} {}^{l}P$$

where ${}^{l}P$ is the number of paths of length l in the H-suppressed molecular graph including closed paths (rings). $l_{\max}$ is the maximum length of all paths.
Source:

- Randić, M.; Brissey, G. M.; Spencer, R. B.; Wilkins, C. L. Search for All Self-Avoiding Paths for Molecular Graphs. *Comput. & Chem.* **1979**, *3*, 5-13
- Randić, M. Characterization of Atoms, Molecules, and Classes of Molecules Based on Paths Enumeration. *MATCH – Commun. Math. Comp. Chem.* **1979**, *7*, 5-64
- TodCon, page 344

145 molecular path count of length 9 and higher

9^P and higher see 137-144.

146-152 total ring count and molecular ring count of length k

rings, **3^rings**, **4^rings**, **5^rings**, **6^rings**, **7^rings**, **8^rings**, **9^rings and higher** are descriptors of the category 'topological'.

Notation in text: $rings$, $^{3}rings$, $^{4}rings$, $^{5}rings$, $^{6}rings$, $^{7}rings$, $^{8}rings$, $^{\geq 9}rings$

$$rings = \sum_{l=3}^{l_{\max}} {}^{l}rings$$

$$^{\geq 9}rings = \sum_{l=9}^{l_{\max}} {}^{l}rings$$

where $^{l}rings$ is the number of rings of length (size) l in the H-suppressed molecular graph. $l_{\max}$ is the maximum size of all rings.

Source:

- TodCon, page 94

153 molecular ring count of length 9 and higher

9^rings and higher see 146-152.

154 moment of inertia A

I_A, I_B, I_C are descriptors of the category 'geometrical'.

Notation in text: I_A, I_B, I_C

I_A, I_B and I_C are the three principal moments of inertia of the molecule with $I_A \leq I_B \leq I_C$.

Source:

- TodCon, page 352

155 moment of inertia B

I_B see 154.

156 moment of inertia C

I_C see 154.

157-164 topological charge index of order k

ch. G_1, **ch. G_2**, **ch. G_3**, **ch. G_4**, **ch. G_5**, **ch. G_6**, **ch. G_7**, **ch. G_8** are descriptors of the category 'topological'.

Notation in text: $ch.G_1$, $ch.G_2$, $ch.G_3$, $ch.G_4$, $ch.G_5$, $ch.G_6$, $ch.G_7$, $ch.G_8$

The sums run over all atoms in an H-suppressed molecular graph.

$$ch.G_k = \frac{1}{2} \cdot \sum_{i=1}^{A} \sum_{j=1}^{A} \left| CT_{ij} \right| \cdot \delta(k; D_{ij})$$

where CT is the charge term matrix, A is the number of atoms, D_{ij} is the distance from atom i to atom j, $k = 1, 2, \ldots$, and δ is the Kronecker delta:

$$\delta(k; D_{ij}) = \begin{cases} 1 & if\ k = D_{ij} \\ 0 & if\ k \neq D_{ij} \end{cases}$$

For A see 0, for D_{ij} see distanc matrix, for CT see charge term matrix.

Source:

- Gálvez, J.; Garcìa, R.; Salabert, M. T.; Soler, R. Charge Indexes. New Topologcal Descriptors. *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 520-525

· Gálvez , J.; Garcìa-Domenech, R.; De Julián-Ortiz, V.; Soler, R. Topological Approach to Drug Design. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 272-284
· TodCon, pages 445-446

165-172 mean topological charge index of order k

ch. J_1, **ch. J_2**, **ch. J_3**, **ch. J_4**, **ch. J_5**, **ch. J_6**, **ch. J_7**, **ch. J_8** and ch. J [5] are descriptors of the category 'topological'.
Notation in text: $ch.J_1$, $ch.J_2$, $ch.J_3$, $ch.J_4$, $ch.J_5$, $ch.J_6$, $ch.J_7$, $ch.J_8$, $ch.J[5]$

$$ch.J_k = \frac{ch.G_k}{A-1}\text{, mean topological charge index}$$

$$ch.J[5] = \sum_{k=1}^{5} ch.J_k\text{, global topological charge index}$$

where A is the number of atoms, $k = 1,2,...$, and $ch.G_k$ is the topological charge index of order k.
For $ch.G_k$ see 157, for A see 0.
Source:

· Gálvez, J.; Garcìa, R.; Salabert, M. T.; Soler, R. Charge Indexes. New Topologcal Descriptors. *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 520-525
· Gálvez , J.; Garcìa-Domenech, R.; De Julián-Ortiz, V.; Soler, R. Topological Approach to Drug Design. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 272-284
· TodCon, pages 445-446

173 global topological charge index

ch. J [5] see 165-172.

174 Crippen slog P

slog P is a descriptor of the category 'miscellaneous'.
Notation in text: $slog\,P$

$$slog\,P = \sum_k a_k \cdot N_k$$

where N_k is the number of atoms of Crippen type k, a_k is an increment for the hydrophobicity of atom type k. Structure-based types are attributed to atoms using a special table.
Source:

· Wildman, S. A.; Crippen, G. M. Prediction of Physicochemical Parameters by Atomic Contributions *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 868-873

175 Crippen sMR

sMR is a desriptor of the category 'miscellaneous'.
Notation in text: sMR

$$sMR = \sum_k a_k \cdot N_k$$

where N_k is the number of atoms of Crippen type k, a_k is an increment for the molar refractivity of atom type k. Structure-based types are attributed to atoms using a special table.
Source:

· Wildman, S. A.; Crippen, G. M. Prediction of Physicochemical Parameters by Atomic Contributions *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 868-873

176 steric energy

st. energy is a descriptor of the category 'geometrical'.
Notation in text: *st.energy*
This is the steric energy, as calculated by molecular mechanics in MOLGEN.

177 diameter

D is a descriptor of the category 'topological'.
Notation in text: D
D is the short name of the topological diameter:

$$D = \max_{1 \le i < j \le A} (D_{ij})$$

where A is the number of atoms in the H-suppressed molecular graph and D_{ij} is an entry in the distance matrix.
For A see 0 and for D_{ij} see distance matrix.

Source:
· TodCon, page 112

178-245 Crippen atom type Xxnn

at C01- at C27, **at H01- at H04**, **at O01- at O12**, **at N01- at N14**, **at Hal**, **at Cl**, **at Br**, **at I**, **at F**, **at P**, **at S01- at S03**, **at Me01**, **at Me02** are descriptors of the category 'miscellaneous'.
Notation in text: $at\,C01$, $at\,C02$, …, $at\,Hal$, …, $at\,Me02$

Source:
· Wildman, S. ; Crippen, G. M. A. Prediction of Physicochemical Parameters by Atomic Contributions *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 868-873

246 sum of subgraphs of order 0 to 8

0-8^K is a descriptor of the category 'overall'.
Notation in text: ${}^{0-8}K$

$$^{0-8}K = \sum_{i=0}^{8} {}^{i}K$$

where ${}^{i}K$ is the number of subgraphs of i edges.
For ${}^{i}K$ see 247-255.
Source:
· Bonchev, D. Novel Indices for the Topological Complexity of Molecules. *SAR QSAR Environ. Res.* **1997**, *7*, 23-43
· Rücker, G.; Rücker, C. Automatic Enumeration of All Connected Subgraphs. *MATCH – Commun. Math. Comp. Chem.* **2000**, *41*, 145-149

247-255 subgraphs of order k

0^K, **1^K**, **2^K**, **3^K**, **4^K**, **5^K**, **6^K**, **7^K** and **8^K** are descriptors of the category 'overall'.
Notation in text: ${}^{0}K$, ${}^{1}K$, …, ${}^{8}K$

$$^{i}K = \left|\{S : S\ subgraph\ of\ G; S\ has\ i\ edges\}\right|$$

where G is the H-suppressed molecular graph.
Source:

- Bonchev, D. Novel Indices for the Topological Complexity of Molecules. *SAR QSAR Environ. Res.* **1997**, *7*, 23-43
- Rücker, G.; Rücker, C. Automatic Enumeration of All Connected Subgraphs. *MATCH – Commun. Math. Comp. Chem.* **2000**, *41*, 145-149

256 eccentric connectivity index

Xi^c is a descriptor of the category 'topological'.
Notation in text: ξ^c

$$\xi^c = \sum_{i=1}^{A} \eta_i \cdot \delta_i$$

where η_i is the maximum entry in the i[th] line of the distance matrix. δ_i is the vertex degree of atom i.
For δ_i see vertex degree, for η_i see eccentricity.
Source:

- Sharma, V.; Goswami, R.; Madan, A. K. Eccentric Conectivity Index: A Novel Highly Discriminating Topological Descriptor for Structure-Property and Structure-Activity Studies *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 273-282
- TodCon, page 124

257 principal eigenvalue of A

lambda_1^A is a descriptor of the category 'topological'.
Notation in text: λ_1^A

λ_1^A is the principal eigenvalue of the adjacency matrix A.

For A see adjacency matrix.
Source:

- TodCon, page 131

258 sum of coefficents of princ. eigenvec. of A

SCA1, SCA2 and SCA3 are descriptors of the category 'topological'.
Notation in text: $SCA1$, $SCA2$, $SCA3$
The sum runs over all atoms of an H-suppressed molecule:

$$SCA1 = \sum_{i=1}^{n} c_i^{A,1}$$

$$SCA2 = \frac{SCA1}{n}$$

$$SCA3 = \frac{n}{10} \cdot \log(SCA1)$$

where n is the number of atoms, $c_i^{A,1}$ is the i[th] coefficient of the eigenvector of the principal eigenvalue of A. All coefficients in a principle eigenvector have the same sign, here always the positive sign is assumed.
The descriptors SCR2 and SCR3 are calculated analogously to VEA in TodCon, page 132.
For A see adjacency matrix.

Source:

- Rücker, G.; Rücker, C.; Gutman, I. On Kites, Comets, and Stars. Sums of Eigenvector Coefficients in (Molecular) Graphs. *Z. Naturforsch. A* **2002**, *57a*, 143-153

259 mean coefficent of princ. eigenvec. of A

SCA2 see SCA1.

260 log of sum of coeff. of princ. eigenvec. of A

SCA3 see SCA1.

261 principal eigenvalue of D

lambda_1^D is descriptor of the category 'topological'.
Notation in text: λ_1^D

λ_1^D is the principal eigenvalue of the distance matrix D.

For D see distance matrix.

Source:

- Schultz, H. P.; Schultz, E. B.; Schultz, T. P. Topological Organic Chemistry. 2. Graph Theory, Matrix Determinants and Eigenvalues, and Topological Indices of Alkanes. *J. Chem. Inf. Comput. Sci.* **1990**, *30*, 27-29
- TodCon, page 134

262 total charge

cha is a descriptor of the category 'arithmetic'.
Notation in text: *cha*
cha is the charge of the molecule.

263 number of radicals

n_rad is a descriptor of the category 'arithmetic'.
Notation in text: n_{rad}

$$n_{rad} = \left|\{i : atom\ i\ bears\ an\ unpaired\ electron\}\right|$$

n_{rad} is the number of radical sites in a molecule.

264 total Chi index

Chi_T is a descriptor of the category 'topological'.
Notation in text: Chi_T
The product runs over all atoms of an H-suppressed molecular graph.

$$Chi_T = \prod_{i=1}^{A} \delta_i^{-1/2}$$

where δ_i is the vertex degree of atom i. A is the number of atoms.

For δ_i see vertex degree, for A see 0.

Source:

- Needham, D. E.;Wei, I. C.; Seybold, P. G. Molecular Modeling of the Physical Properties of the Alkanes. *J. Am. Chem. Soc.* **1988**, *110*, 4186-4194
- TodCon, page 86

265 number of methyl groups

T_m is a descriptor of the category 'topological'.
Notation in text: T_m

$$T_m = \left|\{C : C \text{ has four neighbours; three of them are } H \text{ atoms}\}\right|$$

T_m is the number of methyl groups in a molecular graph with H atoms.

Source:

- Needham, D. E.;Wei, I. C.; Seybold, P. G. Molecular Modeling of the Physical Properties of the Alkanes. *J. Am. Chem. Soc.* **1988**, *110*, 4186-4194

266 number of pairs of methyl groups at distance 3

T_3 is a descriptor of the category 'topological'.
Notation in text: T_3

$$T_3 = \left|\{(i,j) : 1 \le i < j \le A;\ i, j \text{ are the } C \text{ atoms of methyl groups};\ D_{ij} = 3\}\right|$$

T_3 is the number of pairs of methyl groups at distance 3.

For A see 0 and for D_{ij} see distance matrix.

Source:

- Needham, D. E.;Wei, I. C.; Seybold, P. G. Molecular Modeling of the Physical Properties of the Alkanes. *J. Am. Chem. Soc.* **1988**, *110*, 4186-4194

267 number of hydrogen bond donors

HBD is a descriptor of the category 'arithmetic'.
Notation in text: *HBD*
HBD is the number of H atoms attached to O and N atoms, in accord with the ACD definition.
Source:

- *STNotes* **2002**, *28*, 3
- TodCon, page 221-222

268 number of hydrogen bond acceptors

HBA is a descriptor of the category 'arithmetic'.
Notation in text: *HBA*
HBA is the number of N and O atoms, in accord with the ACD definition.
Source:

- *STNotes* **2002**, *28*, 3
- TodCon, page 221-222

269 freely rotatable bonds

FRB is a descriptor of the category 'topological'.
Notation in text: *FRB*

$$FRB = |\{b :\ b \text{ is an acyclic single bond};\ b \text{ is not terminal in an } H-\text{supressed molecular graph},\ b \text{ is not an amide bond}\}|$$

Source:

- Veber, D. F.; Johnson, S. R.; Cheng, H.-Y.; Smith, B. R.; Ward, K. W.; Kopple, K. D. Molecular Properties that Influence the Oral Bioavailability of Drug Candidates. *J. Med. Chem.* **2002**, *45*, 2615-2623

· TodCon, page 178

270 XY shadow

SHDW1, SHDW2 , SHDW3, SHDW4, SHDW5, SHDW6, SHDW1/ SHDW2, SHDW1/ SHDW3, SHDW2/ SHDW3, ssSHDW1, ssSHDW2 , ssSHDW3, ssSHDW4, ssSHDW5, ssSHDW6, ssSHDW1/ SHDW2, ssSHDW1/ SHDW3, ssSHDW2/ SHDW3 are descriptors of the category 'geometrical'.
Notation in text: $SHDW1$, $SHDW2$, $SHDW3$, …, $ssSHDW1$, …, $ssSHDW1/SHDW3$, $ssSHDW2/SHDW3$

$SHDW1$ *is the area of the projection of the molecular surface onto the plane XY*
$SHDW2$ *is the area of the projection of the molecular surface onto the plane XZ*
$SHDW3$ *is the area of the projection of the molecular surface onto the plane YZ*

where X, Y and Z are the principle axes of inertia of the molecule (incl. H atoms). Each atom is projected using its vdw radius.

$$SHDW4 = \frac{SHDW1}{L_X \cdot L_Y}$$

$$SHDW5 = \frac{SHDW2}{L_X \cdot L_Z}$$

$$SHDW6 = \frac{SHDW3}{L_Y \cdot L_Z}$$

where L_X, L_Y and L_Z are the maximum dimension of the molecular surface in X, Y and Z direction using vdw radii.

$$SHDW1/SHDW2 = \frac{SHDW1}{SHDW2}$$

$$SHDW1/SHDW3 = \frac{SHDW1}{SHDW3}$$

$$SHDW2/SHDW3 = \frac{SHDW2}{SHDW3}$$

Source:

· Jurs, P. C.; Hasan, M. N.; Hansen, P. J.; Rohrbaugh, R. H. Prediction of Physicochemical Properties of Organic Compounds from Molecular Structure, pages 209-233 in *Physical Property Prediction* (Jochum, C., Ed.) Springer, Berlin **1988**
· Rohrbaugh, R. H.; Jurs, P. C. Description of Molecular Shape Applied in Studies of Structure/Activity and Structure/Property Relationships *Anal. Chim. Acta* **1987**, *199*, 99-109
· Rohrbaugh, R. H.; Jurs, P. C. Molecular Shape and the Prediction of HPLC Retention Indexes of Polycyclic Aromatic Hydrocarbons *Anal. Chem.* **1987**, *59*, 1048-1054
· TodCon, page 389

$$ssSHDW1 = SHDW\_I$$

$$ssSHDW2 = SHDW\_II$$

$$ssSHDW3 = SHDW\_III$$

$$ssSHDW4 = \frac{SHDW\_I}{L\_X \cdot L\_Y}$$

$$ssSHDW5 = \frac{SHDW\_II}{L\_X \cdot L\_Z}$$

$$ssSHDW6 = \frac{SHDW\_III}{L\_Y \cdot L\_Z}$$

where $SHDW\_I$ is the largest value, $SHDW\_II$ is the second largest value, and $SHDW\_III$ is the smallest value of $\{SHDW1, SHDW2, SHDW3\}$. ss stands for size-sorted.
L_X, L_Y and L_Z span the respective plane of projection.

$$ssSHDW1/ssSHDW2 = \frac{ssSHDW1}{ssSHDW2}$$

$$ssSHDW1/ssSHDW3 = \frac{ssSHDW1}{ssSHDW3}$$

$$ssSHDW2/ssSHDW3 = \frac{ssSHDW2}{ssSHDW3}$$

Source:
· TodCon, page 389

271 XZ shadow
SHDW2 see 270.

272 YZ shadow
SHDW3 see 270.

273 standardized XY shadow
SHDW4 see 270.

274 standardized XZ shadow
SHDW5 see 270.

275 standardized YZ shadow
SHDW6 see 270.

276 XY/XZ shadow
SHDW1/SHDW2 see 270.

277 XY/YZ shadow
SHDW1/SHDW3 see 270.

278 XZ/YZ shadow
SHDW2/SHDW3 see 270.

279 size sorted shadow 1
ssSHDW1 see 270.

280 size sorted shadow 2

ssSHDW2 see 270.

281 size sorted shadow 3

ssSHDW3 see 270.

282 size sorted standardized shadow 1

ssSHDW4 see 270.

283 size sorted standardized shadow 2

ssSHDW5 see 270.

284 size sorted standardized shadow 3

ssSHDW6 see 270.

285 size sorted shadow 1/2

ssSHDW1/SHDW2 see 270.

286 size sorted shadow 1/3

ssSHDW1/SHDW3 see 270.

287 size sorted shadow 2/3

ssSHDW2/SHDW3 see 270.

288 Van der Waals volume

V_vdw, density_vdw, V_vdw^s, V_cub are descriptors of the category 'geometrical'.
Notation in text: V_{vdw}, ρ_{vdw}, V^s_{vdw}, V_{cub}

V_{vdw}, ρ_{vdw}, V^s_{vdw} and V_{cub} are calculated for molecules including H atoms.

V_{vdw} *is the volume of the molecule by using vdw radii for each atom*

$$\rho_{vdw} = \frac{MW\,(incl.H)}{V_{vdw}}$$

$$V^s_{vdw} = \frac{V_{vdw}}{V_{cub}}$$

$$V_{cub} = L_X \cdot L_Y \cdot L_Z$$

where L_X, L_Y and L_Z are the maximum dimensions of the molecular surface in X, Y and Z direction by using *vdw radii*, where X, Y and Z are the principle axes of inertia of the molecule (incl. H atoms).

Source:

- TodCon, page 326

289 density by Van der Waals volume

rho_vdw see 288.

290 standardized Van der Waals volume

V_vdw^s see 288.

291 enclosing cuboid

V_cub see 288.

292-371 Sum of E-state of atomic subgraphs

S(atomic subgraph) are descriptors of the category 'electrotopol./AI';
e.g. S(sCH3) for subgraph: -CH3.
Notation in text: $S(-CH_3)$, …

$S(-CH_3)$ is the sum of electrotopological state values of all $-CH_3$ subgraphs.

The S(sCH3) is descriptor 292. Here is the list of all E-state descriptors from 292 to 371:

292	S(sCH3)	312	S(sssNH)	332	S(aaS)	352	S(ssSiH2)
293	S(dCH2)	313	S(dsN)	333	S(dssS)	353	S(sssSiH)
294	S(ssCH2)	314	S(aaN)	334	S(ddssS)	354	S(ssssSi)
295	S(tCH)	315	S(sssN)	335	S(sssssS)	355	S(sGeH3)
296	S(dsCH)	316	S(ddsN)	336	S(sCl)	356	S(ssGeH2)
297	S(aaCH)	317	S(aasN)	337	S(sSeH)	357	S(sssGeH)
298	S(sssCH)	318	S(ssssN)	338	S(dSe)	358	S(ssssGe)
299	S(ddC)	319	S(sOH)	339	S(ssSe)	359	S(sAsH2)
300	S(tsC)	320	S(dO)	340	S(aaSe)	360	S(ssAsH)
301	S(dssC)	321	S(ssO)	341	S(dssSe)	361	S(sssAs)
302	S(aasC)	322	S(aaO)	342	S(ddssSe)	362	S(sssdAs)
303	S(aaaC)	323	S(sF)	343	S(sBr)	363	S(sssssAs)
304	S(ssssC)	324	S(sPH2)	344	S(sI)	364	S(sSnH3)
305	S(sNH3)	325	S(ssPH)	345	S(sLi)	365	S(ssSnH2)
306	S(sNH2)	326	S(sssP)	346	S(ssBe)	366	S(sssSnH)
307	S(ssNH2)	327	S(dsssP)	347	S(ssssBe)	367	S(ssssSn)
308	S(dNH)	328	S(sssssP)	348	S(ssBH)	368	S(sPbH3)
309	S(ssNH)	329	S(sSH)	349	S(sssB)	369	S(ssPbH2)
310	S(aaNH)	330	S(dS)	350	S(ssssB)	370	S(sssPbH)
311	S(tN)	331	S(ssS)	351	S(sSiH3)	371	S(ssssPb)

where s means a single bond, ss two single bonds, d a double bonds, t a triple bond, a an aromatic bond, etc. connected to the specified atom, not counting the single bonds to the attached H atoms. H2 means two attached H atoms.
Source:

- Kier, L. B.; Hall, L. H. *Molecular Structure Description. The Electrotopological State.* Academic Press, San Diego (California) and London, **1999**

372 Szeged index

SZD, SZDp are indices of the category 'topological'.

Notation in text: SZD , SZD_P
The sums run over an H-suppressed molecular graph:

$$SZD = \sum_{edge(i,j)} SZ_{ij} \cdot SZ_{ji}$$

$$SZD_P = \sum_{i=1}^{A} \sum_{j=1}^{A} SZ_{ij} \cdot SZ_{ji}$$

where A is the number of atoms in the H-suppressed molecular graph and SZ is the Szeged matrix.
For A see 0 and for SZ see Szeged matrix.
Source:

- Khadikar, P. V.; Deshpande, N.V.; Kale, P. P.; Dobrynin, A.; Gutman, I.; Dömötör, G. The Szeged Index and an Analogy with the Wiener Index. *J. Chem. Inf. Comput. Sci.*, **1995**, *35*, 547-550
- Gutman, I; Klavzar, S. An Algorithm for the Calculation of the Szeged Index of Benzenoid Hydrocarbons. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 1011-1014
- Zerovnik, J. Computing the Szeged Index. *Croat. Chem. Acta.* **1996**, *69*, 837-843
- Zerovnik, J. Szeged Index of Symmetric Graphs. *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 77-80
- TodCon, page 438

373 hyper-Szeged index

SZDp see 372.

374 Van der Waals surface

S_vdw is a descriptor of the category 'geometrical'.
Notation in text: S_{vdw}
S_{vdw} is the surface of the molecule by using vdw radii for each atom.

375 solvent-accessible surface (H2O)

SASA H2O is a descriptor of the category 'geometrical'.
Notation in text: $SASA_{H_2O}$
$SASA_{H_2O}$ is the solvent accessible surface of the molecule by using vdw radii and an H_2O molecule (r = 1.5Å) as a probe.

376 solvent-accessible surface (H)

SASA H is a descriptor of the category 'geometrical'.
Notation in text: $SASA_H$
$SASA_H$ is the solvent accessible surface of the molecule by using vdw radii and an H atom (r = 1.2Å) as a probe.

377-456 AI of atomic subgraph

AI(atomic subgraph) are descriptors of the category 'electrotopol./AI';
eg. AI(sCH3) for subgraph: -CH3.
Notation in text: $AI(-CH_3)$, …
The sums run over an H-suppressed molecular graph:

$$AI(-CH_3) = m + \frac{\sum_{i=1}^{m} \delta_i^{\text{mod}} \cdot \sigma_i^{\,2}}{\sum_{i=1}^{A} \delta_i^{\text{mod}} \cdot \sigma_i^{\,2}}$$

where m is the number of $-CH_3$ subgraphs, δ_i^{mod} (or δ_i^{m}) is the modified vertex degree of atom i and σ_i is the vertex distance degree of atom i.
For the subgraphs considered see 292-371, for δ_i^{mod} see modified vertex degree and for σ_i see vertex distance degree.

The AI(sCH3) is descriptor 377. Here is the list of all AI descriptors from 377 to 456:

377	AI(sCH3)	397	AI(sssNH)	417	AI(aaS)	437	AI(ssSiH2)
378	AI(dCH2)	398	AI(dsN)	418	AI(dssS)	438	AI(sssSiH)
379	AI(ssCH2)	399	AI(aaN)	419	AI(ddssS)	439	AI(ssssSi)
380	AI(tCH)	400	AI(sssN)	420	AI(sssssssS)	440	AI(sGeH3)
381	AI(dsCH)	401	AI(ddsN)	421	AI(sCl)	441	AI(ssGeH2)
382	AI(aaCH)	402	AI(aasN)	422	AI(sSeH)	442	AI(sssGeH)
383	AI(sssCH)	403	AI(ssssN)	423	AI(dSe)	443	AI(ssssGe)
384	AI(ddC)	404	AI(sOH)	424	AI(ssSe)	444	AI(sAsH2)
385	AI(tsC)	405	AI(dO)	425	AI(aaSe)	445	AI(ssAsH)
386	AI(dssC)	406	AI(ssO)	426	AI(dssSe)	446	AI(sssAs)
387	AI(aasC)	407	AI(aaO)	427	AI(ddssSe)	447	AI(sssdAs)
388	AI(aaaC)	408	AI(sF)	428	AI(sBr)	448	AI(sssssAs)
389	AI(ssssC)	409	AI(sPH2)	429	AI(sI)	449	AI(sSnH3)
390	AI(sNH3)	410	AI(ssPH)	430	AI(sLi)	450	AI(ssSnH2)
391	AI(sNH2)	411	AI(sssP)	431	AI(ssBe)	451	AI(sssSnH)
392	AI(ssNH2)	412	AI(dsssP)	432	AI(ssssBe)	452	AI(ssssSn)
393	AI(dNH)	413	AI(sssssP)	433	AI(ssBH)	453	AI(sPbH3)
394	AI(ssNH)	414	AI(sSH)	434	AI(sssB)	454	AI(ssPbH2)
395	AI(aaNH)	415	AI(dS)	435	AI(ssssB)	455	AI(sssPbH)
396	AI(tN)	416	AI(ssS)	436	AI(sSiH3)	456	AI(ssssPb)

where s means a single bond, ss two single bonds, d a double bonds, t a triple bond, a an aromatic bond, etc. connected to the specified atom not counting the single bonds to the attached H atoms. H2 means two attached H atoms.
Source:

· Ren, B. Novel Atomic-Level-Based AI Topological Descriptors: Application to QSPR/QSAR Modeling. *J. Chem. Inf. Comput. Sci.* **2002**, *42*, 858-868
· Ren, B. Novel Atomic-Level-Based AI Topological Descriptors for Structure-Property Correlations. *J. Chem. Inf. Comput. Sci.* **2003**, *43*, 161-169
· Ren, B. Novel Atom-Type AI Indices for QSPR Studies of Alcohols. *Comput. & Chem.* **2002**, *26*, 223-235

· Ren, B. Application of Novel Atom-Type AI Topological Indices to QSPR Studies of Alkanes. *Comput. & Chem.* **2002**, *26*, 357-369

457 Xu index

Xu, Xu^m are descriptors of the category 'electrotopol./AI'.
Notation in text: Xu , Xu^m
The sum runs over all atoms of an H-suppressed molecule:

$$Xu = \sqrt{A} \cdot \log\left(\frac{\sum_{i=1}^{A} \delta_i \cdot \sigma_i^{\,2}}{\sum_{i=1}^{A} \delta_i \cdot \sigma_i}\right)$$

$$Xu^m = \sqrt{A} \cdot \log\left(\frac{\sum_{i=1}^{A} \delta_i^{\mathrm{mod}} \cdot \sigma_i^{\,2}}{\sum_{i=1}^{A} \delta_i^{\mathrm{mod}} \cdot \sigma_i}\right)$$

where A is the number of atoms in an H-suppressed molecule, δ_i is the vertex degree of the ith atom, σ_i is the vertex distance degree of the ith atom. δ_i^{mod} (or δ_i^m) is the modified vertex degree of atom i.
For A see 0, for δ_i see vertex degree, for σ_i see vertex distance degree and for δ_i^{mod} see modified vertex degree.
Source:

· Ren, B. A New Topological Index for QSPR of Alkanes. *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 139-143
· TodCon, page 507

458 modified Xu index

Xu^m see 457.

459-488 connectivity indices for substructures

m^Chi_q and **m^Chi^v_q** are descriptors of the category 'topological'. Substructures are paths, clusters, path-clusters and chains.

Available are:

459	3^Chi_p	469	6^Chi_pc	479	4^Chi^v_c
460	4^Chi_p	470	3^Chi_ch	480	5^Chi^v_c
461	5^Chi_p	471	4^Chi_ch	481	6^Chi^v_c
462	6^Chi_p	472	5^Chi_ch	482	4^Chi^v_pc
463	3^Chi_c	473	6^Chi_ch	483	5^Chi^v_pc
464	4^Chi_c	474	3^Chi^v_p	484	6^Chi^v_pc
465	5^Chi_c	475	4^Chi^v_p	485	3^Chi^v_ch
466	6^Chi_c	476	5^Chi^v_p	486	4^Chi^v_ch
467	4^Chi_pc	477	6^Chi^v_p	487	5^Chi^v_ch
468	5^Chi_pc	478	3^Chi^v_c	488	6^Chi^v_ch

Notation in text: ${}^{m}\chi_q$, ${}^{m}\chi_q^v$

$$ {}^{m}\chi_q = \sum_{k=1}^{K(m,q)} \left(\prod_{i=1}^{n} \delta_i \right)^{-1/2} $$

$$ {}^{m}\chi_q^v = \sum_{k=1}^{K(m,q)} \left(\prod_{i=1}^{n} \delta_i^v \right)^{-1/2} $$

where δ_i is the vertex degree and δ_i^v is the valence vertex degree of atom i of the subgraph of type q in the H-suppressed molecular graph. m is the order (this is also called the "size" or "the number of edges") of the subgraphs considered. q means paths, clusters, path-clusters or chains. $K(m,q)$ is the number of subgraphs of type q and size m. n is the number of atoms of the subgraph considered.

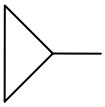
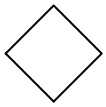
Type of subgraphs:

- If a subgraph contains a cycle it is of type chain (*ch*) for $m \geq 3$,
- otherwise if every vertex has one or more than two non-H neighbours it is of type cluster (*c*) for $m \geq 3$,
- otherwise if every vertex has one or two non-H neighbours it is of type path (*p*) for $m \geq 2$,
- otherwise it is of type path-cluster (*pc*) for $m \geq 4$. So a path-cluster has no cycles but vertices with one, two and more than two non-H neighbours.

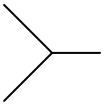
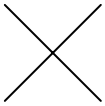
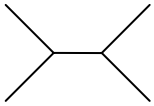
For example paths are:

path			
m	3	4	5

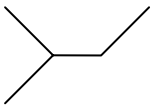
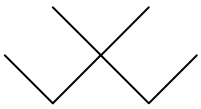
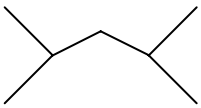
For example chains are:

chain			
m	3	4	4

For example clusters are:

cluster			
m	3	4	5

For example path-clusters are:

path-cluster			
m	4	6	6

For δ_i see vertex degree, for δ_i^v see valence vertex degree.

Source:

- Kier, L. B.; Hall L. H. The Nature of Structure-Acticity Relationships and their Relation to Molecular Connectivity. *Eur. J. Med. Chem.*, **1977**, *12*, 307-312
- Kier, L. B.; Hall L. H. *Molecular Connectivity in Structure-Activity Analysis.* Research Studies Press - Wiley, Chichester (UK), **1986**.
- TodCon, pages 84-86 and page 314

489-699 overall indices

m^TO, **m^TO***, **m^TO_q**, **m^TO*_q**, **TO**, **TO***, **TO_q**, **TO*_q** are descriptors of the category 'overall'.

Available are:

489	0^TC	542	2^TW	595	5^TC*_c	648	4^TM_2_pc
490	1^TC	543	3^TW	596	6^TC*_c	649	5^TM_2_pc
491	2^TC	544	4^TW	597	TC*_c	650	6^TM_2_pc
492	3^TC	545	5^TW	598	3^TC^v_c	651	TM_2_pc
493	4^TC	546	6^TW	599	4^TC^v_c	652	4^TM_2*_pc
494	5^TC	547	TW	600	5^TC^v_c	653	5^TM_2*_pc
495	6^TC	548	3^TC_p	601	6^TC^v_c	654	6^TM_2*_pc
496	TC	549	4^TC_p	602	TC^v_c	655	TM_2*_pc
497	1^TC*	550	5^TC_p	603	3^TM_1_c	656	4^TW_pc
498	2^TC*	551	6^TC_p	604	4^TM_1_c	657	5^TW_pc
499	3^TC*	552	TC_p	605	5^TM_1_c	658	6^TW_pc
500	4^TC*	553	3^TC*_p	606	6^TM_1_c	659	TW_pc
501	5^TC*	554	4^TC*_p	607	TM_1_c	660	3^TC_ch
502	6^TC*	555	5^TC*_p	608	3^TM_1*_c	661	4^TC_ch
503	TC*	556	6^TC*_p	609	4^TM_1*_c	662	5^TC_ch
504	0^TC^v	557	TC*_p	610	5^TM_1*_c	663	6^TC_ch
505	1^TC^v	558	3^TC^v_p	611	6^TM_1*_c	664	TC_ch
506	2^TC^v	559	4^TC^v_p	612	TM_1*_c	665	3^TC*_ch
507	3^TC^v	560	5^TC^v_p	613	3^TM_2_c	666	4^TC*_ch
508	4^TC^v	561	6^TC^v_p	614	4^TM_2_c	667	5^TC*_ch
509	5^TC^v	562	TC^v_p	615	5^TM_2_c	668	6^TC*_ch
510	6^TC^v	563	3^TM_1_p	616	6^TM_2_c	669	TC*_ch
511	TC^v	564	4^TM_1_p	617	TM_2_c	670	3^TC^v_ch
512	0^TM_1	565	5^TM_1_p	618	3^TM_2*_c	671	4^TC^v_ch
513	1^TM_1	566	6^TM_1_p	619	4^TM_2*_c	672	5^TC^v_ch
514	2^TM_1	567	TM_1_p	620	5^TM_2*_c	673	6^TC^v_ch
515	3^TM_1	568	3^TM_1*_p	621	6^TM_2*_c	674	TC^v_ch
516	4^TM_1	569	4^TM_1*_p	622	TM_2*_c	675	3^TM_1_ch
517	5^TM_1	570	5^TM_1*_p	623	3^TW_c	676	4^TM_1_ch
518	6^TM_1	571	6^TM_1*_p	624	4^TW_c	677	5^TM_1_ch
519	TM_1	572	TM_1*_p	625	5^TW_c	678	6^TM_1_ch
520	1^TM_1*	573	3^TM_2_p	626	6^TW_c	679	TM_1_ch

521	2^TM_1*	574	4^TM_2_p	627	TW_c	680	3^TM_1*_ch
522	3^TM_1*	575	5^TM_2_p	628	4^TC_pc	681	4^TM_1*_ch
523	4^TM_1*	576	6^TM_2_p	629	5^TC_pc	682	5^TM_1*_ch
524	5^TM_1*	577	TM_2_p	630	6^TC_pc	683	6^TM_1*_ch
525	6^TM_1*	578	3^TM_2*_p	631	TC_pc	684	TM_1*_ch
526	TM_1*	579	4^TM_2*_p	632	4^TC*_pc	685	3^TM_2_ch
527	1^TM_2	580	5^TM_2*_p	633	5^TC*_pc	686	4^TM_2_ch
528	2^TM_2	581	6^TM_2*_p	634	6^TC*_pc	687	5^TM_2_ch
529	3^TM_2	582	TM_2*_p	635	TC*_pc	688	6^TM_2_ch
530	4^TM_2	583	3^TW_p	636	4^TC^v_pc	689	TM_2_ch
531	5^TM_2	584	4^TW_p	637	5^TC^v_pc	690	3^TM_2*_ch
532	6^TM_2	585	5^TW_p	638	6^TC^v_pc	691	4^TM_2*_ch
533	TM_2	586	6^TW_p	639	TC^v_pc	692	5^TM_2*_ch
534	1^TM_2*	587	TW_p	640	4^TM_1_pc	693	6^TM_2*_ch
535	2^TM_2*	588	3^TC_c	641	5^TM_1_pc	694	TM_2*_ch
536	3^TM_2*	589	4^TC_c	642	6^TM_1_pc	695	3^TW_ch
537	4^TM_2*	590	5^TC_c	643	TM_1_pc	696	4^TW_ch
538	5^TM_2*	591	6^TC_c	644	4^TM_1*_pc	697	5^TW_ch
539	6^TM_2*	592	TC_c	645	5^TM_1*_pc	698	6^TW_ch
540	TM_2*	593	3^TC*_c	646	6^TM_1*_pc	699	TW_ch
541	1^TW	594	4^TC*_c	647	TM_1*pc		

Notation in text: ${}^{m}TO$, ${}^{m}TO*$, ${}^{m}TO_q$, ${}^{m}TO*_q$, TO, $TO*$, TO_q, $TO*_q$

T is the overall-index sign. For the molecule each connected subgraph up to size m is constructed. O is one of these: M_1 for first Zagreb index M_1, M_2 for second Zagreb index M_2, W for Wiener index W. C represents the sum over vertex degree δ_i of each atom i. C^v represents the sum over valence vertex degree δ_i^v of each atom i.

$$ {}^{m}TO = \sum_{\substack{\text{subgraph } S \\ \text{of size } m}} O(S) $$

$$ {}^{m}TO* = \sum_{\substack{\text{subgraph } S \\ \text{of size } m}} O*(S) $$

$$ {}^{m}TO_q = \sum_{\substack{\text{subgraph } S \\ \text{of size } m \\ \text{of type } q}} O(S) $$

$$ {}^{m}TO*_q = \sum_{\substack{\text{subgraph } S \\ \text{of size } m \\ \text{of type } q}} O*(S) $$

$$ TO = \sum_{\text{subgraph } S} O(S) $$

$$ TO* = \sum_{\text{subgraph } S} O*(S) $$

$$TO_q = \sum_{\substack{\text{subgraph } S \\ \text{of type } q}} O(S)$$

$$TO^*_q = \sum_{\substack{\text{subgraph } S \\ \text{of type } q}} O^*(S)$$

where m is the order (this is also called the "size" or "the number of edges") of the subgraphs of the H-suppressed molecular graph; if q is specified (as path, cluster, path-cluster, chain), only subgraphs of this type are used (see 459-488).

The sums run over the subgraphs (regarding m and q if denoted) and sum up the values of the indices specified (e.g. W for Wiener index) of the subgraphs. In TC, TM_1, TM_2 calculations the δ values of the vertices of the subgraphs are used. If no asterisk appears in the symbol of an index, then these are taken as they are in the parent graph. If an asterisk appears in the symbol of an index, then the δ values are taken as they are in the respective isolated subgraph.
For M_1 see 45, for M_2 see 46, for W see 44, for δ_i see vertex degree, for δ_i^v see valence vertex degree.
Source:

- Bonchev, D.; Trinajstić, N. Overall Molecular Descriptors. 3. Overall Zagreb Indices. *SAR QSAR Environ. Res.* **2001**, *12*, 213-236
- Bonchev, D. The Overall Wiener Index – A New Tool for Characterization of Molecular Topology. *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 582-592
- Bonchev, D. Overall Connectivity – A Next Generation Molecular Connectivity. *J. Mol. Graphics Model.* **2001**, *20*, 65-75
- Bonchev, D. Overall Connectivities/Topological Complexities: A New Powerful Tool for QSPR/QSAR. *J. Chem. Inf. Comput. Sci.* **2000**, *40*, 934-941

701 topological radius

R is a descriptor of the category 'topological'.
Notation in text: R

$$R = \min_{1 \le i \le A} \left(\max_{1 \le j \le A} (D_{ij}) \right)$$

where A is the number of atoms in the H-suppressed molecular graph and D_{ij} is an entry of the distance matrix.
For A see 0 and for D_{ij} see distance matrix.

Source:
TodCon, page 112

702 number of connectivity components

con.comp. is a descriptor of the category 'topological'.
Notation in text: *con.comp.*

$$con.comp. = the\ number\ of\ connected\ components$$

In most cases, this index is equal to 1. If the compund is made of more than one component, the index increases.

703 graph-theoretical planarity

gt planar is a descriptor of the category 'topological'.

Notation in text: *gt planar*

$$gt\ planar = \begin{cases} 1 & if\ the\ molecular\ graph\ is\ planar \\ 0 & else \end{cases}$$

Source:

- Rücker, C.; Meringer, M. How Many Organic Compunds are gt-nonplanar? *MATCH-Commun. Math. Comput. Chem.* **2002**, *45*, 159-172

704 geometrical diameter

D_3D is a descriptor of the category 'geometrical'.
Notation in text: D_{3D}

D_{3D} is the maximum distance of two points on the vdw-surface of the molecule incl. H atoms:

$$D_{3D} = \max(|b-a|: for\ points\ a,b \in vdw-surface)$$

For vdw-surface see 374.

705 enclosing sphere

V_sphere is a descriptor of the category 'geometrical'.
Notation in text: V_{sphere}

V_{sphere} is the volume of the enclosing sphere (incl. vdw-radii) of the molecule incl. H atoms:

$$V_{sphere} = \frac{4}{3}\left(\frac{D_{3D}}{2}\right)^3 \pi = \frac{D_{3d}{}^3}{6}\pi$$

For vdw-radii see 288, for D_{3D} see 704.

706 relative number of rings

rel. N_rings is a descriptor of the category 'topological'.
Notation in text: $rel.\,N_{rings}$

$rel.\,N_{rings}$ is the relative number of rings. It is relative to the number of atoms of an H-suppressed molecule:

$$rel.\,N_{rings} = \frac{rings}{A}$$

where *rings* is the number of rings.
For *rings* see 146-152. For A see 0.

707 relative cyclomatic number

rel. C is a descriptor of the category 'topological'.
Notation in text: $rel.\,C$

$rel.\,C$ is the relative cyclomatic number. It is relative to the number of atoms of an H-suppressed molecule:

$$rel.\,C = \frac{C}{A}$$

where C is the cyclomatic number.
For C see 39. For A see 0.

Some auxiliary structures for calculating descriptors

adjacency matrix

The adjacency matrix A (not to be confused with the descriptor number of atoms A) is defined as:

$$A_{ij} = \begin{cases} 1 & if\ edge\,(i,j)\ exists \\ 0 & else \end{cases}$$

alpha

The modifying term α (in e.g. Kier and Hall shape and flexibility indices, see 65-68) is defined as:

$$\alpha = \sum_{i=1}^{A} \alpha_i = \sum_{i=1}^{A} \left(\frac{R_i}{R_{C_{sp3}}} - 1 \right)$$

where R_i is the covalent radius of the i[th] atom in an H-suppressed molecule and $R_{C_{sp3}}$ is the covalent radius of a sp3 carbon atom:

Atom / Hybrid i	R_i	α_i	Atom / Hybrid i	R_i	α_i
C_{sp3}	0.77	0.00	P_{sp3}	1.10	0.43
C_{sp2}	0.67	-0.13	P_{sp2}	1.00	0.30
C_{sp}	0.60	-0.22	S_{sp3}	1.04	0.35
N_{sp3}	0.74	-0.04	S_{sp2}	0.94	0.22
N_{sp2}	0.62	-0.20	F	0.72	-0.07
N_{sp}	0.55	-0.29	Cl	0.99	0.29
O_{sp3}	0.74	-0.04	Br	1.14	0.48
O_{sp2}	0.62	-0.20	I	1.33	0.73

Source: TodCon, page 250

charge term matrix

CT is a square matrix of dimension $n \times n$, where n is the number of rows (and columns). n is equal to the descriptor A (number of non-H atoms). Entries are the integers …, -1, 0, 1, 2, … . CT is calculated by matrix M and the vertex degree δ:

$$CT_{ij} = \begin{cases} \delta_i & if\ i = j \\ M_{ij} - M_{ji} & if\ i \neq j \end{cases}$$

with M is defined as:

$$M = A \cdot D^{-2}$$

where A is the adjacency matrix, matrix D^{-2} is defined by the entries in the distance matrix D:

$$D^{-2}{}_{ij} = \begin{cases} D_{ij}{}^{-2} & if\ i \neq j \\ 0 & if\ i = j \end{cases}$$

For δ see vertex degree, for A see adjaceny matrix, for D and D_{ij} see distance matrix.

detour matrix

Δ is a square matrix of dimension $n \times n$, where n is the descriptor A (number of non-H atoms). Entries are 0, 1, 2, …
An entry Δ_{ij} represents the length of the longest path from atom (vertex) i to atom (vertex) j in a molecular graph without H atoms. Many authors set $\Delta_{ii} = 0$ for all vertices i:

$$\Delta_{ij} = \begin{cases} 0, if\ i = j \\ l, else; l\ is\ the\ length\ of\ the\ longest\ path\ from\ i\ to\ j \end{cases}$$

There is also a detour matrix Δ^* which includes closed detours (rings of maximal length) from atom i to itself:

$$\Delta^*_{ii} = \begin{cases} 0, if\ atom\ i\ is\ not\ in\ a\ ring \\ l, else; l\ is\ the\ size\ of\ the\ largest\ ring\ containing\ atom\ i \end{cases}$$
$$\Delta^*_{ij} = \Delta_{ij} \quad for\ i \neq j$$

For A see 0.
Source:
Buckley, F.; Harary F. *Distance in Graphs.* Addison-Wesley, Redwood City California, **1990**, page 213
Ivanciuc, O.; Balaban, A. T. Design of Topological Indices. Part 8. Path Matrices and Derived Molecular Graph Invariants. *MATCH - Commun. Math. Comp. Chem.* **1994**, *30*, 141-152
Rücker, G.; Rücker, C. Symmetry-Aided Computation of the Detour Matrix and the Detour Index. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 710-714
TodCon, page 103

distance matrix, distance

D is a square matrix of dimension $n \times n$, where n is the descriptor A (number of non-H atoms). Entries are 0, 1, 2, …
An entry D_{ij} represents the length of the shortest path from atom (vertex) i to atom (vertex) j in an H-supressed molecular graph.
$D_{ij} = d(i, j)$ is also called the distance of atom i to atom j.
For A see 0.

eccentricity

η_i is the maximum entry in the i[th] line of the distance matrix of an H-suppressed graph:

$$\eta_i = \max_{1 \le j \le A} \{D_{ij}\}$$

D_{ij} is the distance of atom i to atom j. A is the number of atoms.
For A see 0. For D_{ij} see distance matrix.
Source:
· TodCon, page 112

modified vertex degree

δ_i^{mod} (or δ_i^m) in e.g. Ren's AI indices (see 377-456) is the modified vertex degree of the atom i in an H-suppressed molecule. It is defined as the number of neighbours of atom i ($=\delta_i$) modified by the value k_i.

$$\delta_i^{\text{mod}} = \delta_i + k_i$$

where k_i is defined as:

$$k_i = \frac{1}{\left(\frac{2}{A}\right)^2 \cdot \frac{Z_i^v - h_i}{Z_i - Z_i^v - 1} + 1}$$

where A is the number of atoms, h_i is the number of H atoms attached to atom i, Z_i^v is the number of valence electrons of atom i and Z_i is the atomic number of atom i.
See also valence vertex degree.
For δ_i see vertex degree, for A see 0.

Szeged matrix

SZ is a square matrix of dimension $n \times n$, where n is equal to the descriptor A (number of non-H atoms). Entries are 0, 1, 2, …
A entry SZ_{ij} is the number of atoms being closer to i than to j:

$$SZ_{ij} = \left|\{a \mid a\ atom; D_{ia} < D_{ja}\}\right|$$

Source:
· TodCon, page 438

unsaturated adjacency matrix

The unsaturated adjacency matrix $\hat{A}$ is defined as:

$$\hat{A}_{ij} = \begin{cases} 1 & if\ there\ is\ a\ single\ bond\ between\ atoms\ i\ and\ j \\ 2 & if\ there\ is\ a\ double\ bond\ between\ atoms\ i\ and\ j \\ 3 & if\ there\ is\ a\ triple\ bond\ between\ atoms\ i\ and\ j \\ 1.5 & if\ there\ is\ an\ aromatic\ bond\ between\ atoms\ i\ and\ j \\ 0 & else \end{cases}$$

unsaturated vertex distance degree

$\hat{\sigma}_i$ is defined as the i[th] row sum of the unsaturated distance matrix $\hat{D}$ of an H-suppressed molecular graph:

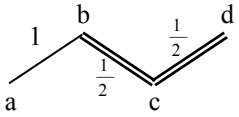
$$\hat{\sigma}_i = \sum_{j=1}^{A} \hat{D}_{ij}$$

For A see 0. For $\hat{D}$ and $\hat{D}_{ij}$ see unsaturated distance matrix.

unsaturated distance matrix

$\hat{D}$ is a square matrix of dimension $n \times n$, where n is equal to the descriptor A (number of non-H atoms).

An entry $\hat{D}_{ij}$ represents the length of the shortest path from atom (vertex) i to atom (vertex) j in a H-supressed molecular graph. Single bonds represent a distance of 1, double bonds represent a distance of $\frac{1}{2}$, triple bonds represent a distance of $\frac{1}{3}$, aromatic bonds represent a distance of $\frac{2}{3}$:



In this example, the distance $\hat{D}_{ac}$ from a to c is $1+\frac{1}{2}=\frac{3}{2}$ and the distance $\hat{D}_{ad}$ is $1+\frac{1}{2}+\frac{1}{2}=2$.
For A see 0.

valence vertex degree

δ_i^v is the valence vertex degree of atom i in an H-suppressed molecule:

$$\delta_i^v = \frac{Z_i^v - h_i}{Z_i - Z_i^v - 1}$$

with Z_i^v is the number of valence electrons of atom i, h_i is the number of H atoms attached to atom i, and Z_i is the total number of electrons (= the atomic number) of atom i.

vertex degree

δ_i is the vertex degree of atom i in an H-suppressed molecule. It is defined as the number of neighbours of atom i, which is the i[th] row sum of the adjacency matrix

$$\delta_i = \sum_{j=1}^{n} A_{ij}$$

where n is equal to the descriptor A (number of non-H atoms).

vertex distance degree

σ_i is defined as the i[th] row sum of the distance matrix D of an H-suppressed molecular graph:

$$\sigma_i = \sum_{j=1}^{A} D_{ij}$$

For A see 0. For D and D_{ij} see distance matrix.