K

- **Kaliszan shape parameter** → shape descriptors
- **Kamlet descriptors** → Linear Solvation Energy Relationships
- **Kamlet's general equation** → Linear Solvation Energy Relationships
- **Kantola–Villar–Loew hydrophobic models** → lipophilicity descriptors
- **K correlation analysis** → variable reduction
- **K correlation index** ≡ *multivariate K correlation index* → statistical indices (⊙ correlation measures)

Kekulé number (K) (≡ *Kekulé structure count, SC*)

This is the number of Kekulé structures in an aromatic system [Trinajstić, 1992]. It can be calculated by extensive enumeration of the structures or by using appropriate algorithms.

For benzenoid systems, the Kekulé number K is obtained from the positive eigenvalues λ_i of the → *adjacency matrix* as

$$K = \prod_{i=1}^{A/2} \lambda_i$$

where A is the number of atoms. The logarithm of the Kekulé number is related to the resonance energy of the compound and used as a → *resonance index*.

The Kekulé number of alternant hydrocarbons is equal to the sum of "even" K^+ and "odd" K^- Kekulé structures:

$$K = K^+ + K^-$$

The even or odd parity is determined in the Dewar–Longuet-Higgins scheme [Dewar and Longuet-Higgins, 1952] according to whether the number of transpositions of double bonds required to transform one Kekulé structure into another one is even or odd.

The difference between the numbers of even and odd Kekulé structures is called **algebraic structure count** ASC [Wilcox Jr, 1968, 1969] or **corrected structure count** CSC [Herndon, 1973a, 1974b]:

$$ASC = K^+ - K^- \qquad K^+ \geq K^-$$

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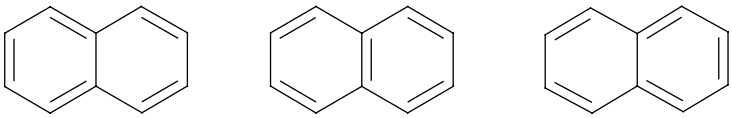


Figure K1 The three Kekulé resonance structures of the naphthalene.

ASC represents a structure count excluding structures that do not contribute to stabilizing resonance interactions. However, the concept of parity and the derived ASC descriptor do not work in nonalternant systems with three odd-membered rings [Randić and Trinajstić, 1993a].

📖 [Kekulé, 1865; Gutman and Trinajstić, 1973b; Herndon, 1973b; Balaban and Tomescu, 1985; Dias, 1992; Ivanciuc and Balaban, 1992b; Balaban, Liu *et al.*, 1993; Guo and Zhang, 1993; Guo, Randie *et al.*, 1996 Mishra and Patra, 1998; Cash, 1998]

- **Kekulé structure count** ≡ *Kekulé number*
- **Kellog and Abraham interaction field** → molecular interaction fields (⊙ hydrophobic fields)
- **Kendall rank correlation coefficient** → statistical indices (⊙ correlation measures)
- **Kier alpha-modified shape descriptors** → Kier shape descriptors
- **Kier bond rigidity index** → flexibility indices
- **Kier–Hall connectivity indices** ≡ *Molecular Connectivity Indices* → connectivity indices
- **Kier–Hall electronegativity** → vertex degree
- **Kier–Hall solvent polarity index** → electric polarization descriptors
- **Kier molecular flexibility index** → flexibility indices
- **Kier steric descriptor** → steric descriptors

Kier shape descriptors (κ)

These are topological shape descriptors ${}^m\kappa$ defined in terms of the number of graph vertices A and the number of paths ${}^mP$ with length m ($m = 1, 2, 3$) in the → *H-depleted molecular graph*, according to the following [Kier, 1985; Kier, 1986b]:

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

$$ {}^3\kappa = 4 \cdot \frac{{}^3P_{\max} \cdot {}^3P_{\min}}{({}^3P)^3} = \begin{cases} \dfrac{(A-3) \cdot (A-2)^2}{({}^3P)^2} & \text{for even } A\,(A>3) \\[2ex] \dfrac{(A-1) \cdot (A-3)^2}{({}^3P)^2} & \text{for odd } A\,(A>3) \end{cases} $$

where ${}^mP_{\min}$ and ${}^mP_{\max}$ are the minimum and maximum mth order → *path count* in the molecular graphs of molecules with the same number A of graph vertices. These extremes are obtained from two reference structures chosen in an isomeric series and, for the ith molecule, is therefore

$$ {}^mP_{\min} \leq {}^mP_i \leq {}^mP_{\max} $$

The reference structure for ${}^1P_{\min}$ is the → *linear graph* while for ${}^1P_{\max}$ it is the → *complete graph* in which all vertices are bonded to each other; their numerical values are calculated as follows:

$$ {}^1P_{\min} = A-1 \qquad {}^1P_{\max} = \frac{A \cdot (A-1)}{2} $$

The scaling factor of 2 in the numerator of ${}^1\kappa$ index formula makes the value ${}^1\kappa = A$ when there are no cycles in the graph of the molecule. Monocyclic molecules have a lower value and bicyclic structures have an even lower value. The structural information encoded in ${}^1\kappa$ is related to the complexity, or, more precisely, to the number of cycles of a molecule.

The reference structure for ${}^2P_{\min}$ is the linear graph while for ${}^2P_{\max}$ it is the → *star graph* in which all vertices but one are adjacent to a central vertex; their numerical values are calculated as follows:

$$ {}^2P_{\min} = A-2 \qquad {}^2P_{\max} = \frac{(A-1) \cdot (A-2)}{2} $$

where A is the total number of vertices in the graph. The scaling factor of 2 in the numerator of ${}^2\kappa$index formula makes the value ${}^2\kappa = A-1$ for all linear graphs. The information encoded by ${}^2\kappa$ index is related to the degree of star graph-likeness and linear graph-likeness, that is, ${}^2\kappa$ encodes information about the spatial density of atoms in a molecule.

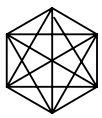
The reference structure for ${}^3P_{\min}$ is the linear graph while for ${}^3P_{\max}$ it is the *twin star graph*; their numerical values are calculated as follows:

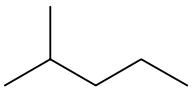
$$ {}^3P_{\min} = A-3 \qquad {}^3P_{\max} = \begin{cases} \dfrac{(A-2)^2}{4} & \text{for even} \quad A \\ \dfrac{(A-1) \cdot (A-3)}{4} & \text{for odd} \quad A \end{cases} $$

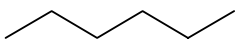
The scaling factor of 4 is used in the numerator of ${}^3\kappa$ index to bring ${}^3\kappa$ onto approximately the same numerical scale as the other kappa indices. The ${}^3\kappa$ values are larger when → *molecular branching* is nonexistent or when it is located at the extremities of a graph; ${}^3\kappa$ encodes information about the centrality of branching.

Example K1

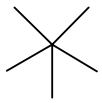
Path counts and Kier shape descriptors for 2-methylpentane (central column).

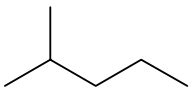


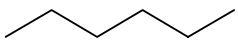




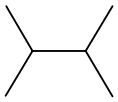
${}^1P_{\max} = 15$ ${}^1P = 5$ ${}^1\kappa = 6.000$ ${}^1P_{\min} = 5$



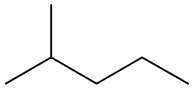




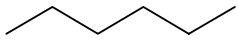
${}^2P_{\max} = 10$ ${}^2P = 5$ ${}^2\kappa = 3.200$ ${}^2P_{\min} = 4$



$^3P_{max} = 4$



$^3P = 3$ $^3\kappa = 5.333$



$^3P_{min} = 3$

To take into account the different shape contribution of heteroatoms and hybridization states, **Kier alpha-modified shape descriptors**, denoted as $^m\kappa_\alpha$ ($m = 1,2,3$), were proposed by the following [Kier, 1986a]:

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

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

where α is a parameter derived from the ratio of the → *covalent radius* R_i of the ith atom relative to the sp^3 carbon atom ($R_{C_{sp^3}}$):

$$\alpha = \sum_{i=1}^{A}\left(\frac{R_i}{R_{C_{sp^3}}} - 1\right)$$

The only nonvanishing contributions to α are given by heteroatoms or carbon atoms with a valence state different from sp^3 (Table K1).

Table K1 Covalent radius R and α parameter values for some atom types.

Atom/hybrid	R (Å)	α	Atom/hybrid	R (Å)	α
C_{sp^3}	0.77	0	P_{sp^3}	1.10	0.43
C_{sp^2}	0.67	−0.13	P_{sp^2}	1.00	0.30
C_{sp}	0.60	−0.22	S_{sp^3}	1.04	0.35
N_{sp^3}	0.74	−0.04	S_{sp^2}	0.94	0.22
N_{sp^2}	0.62	−0.20	F	0.72	−0.07
N_{sp}	0.55	−0.29	Cl	0.99	0.29
O_{sp^3}	0.74	−0.04	Br	1.14	0.48
O_{sp^2}	0.62	−0.20	I	1.33	0.73

Kappa indices can also be calculated for molecular fragments and functional groups X. The calculation of these indices for groups was performed using a "pseudomolecule" X–X: two fragments X of the same kind are linked together, kappa values are calculated for the pseudomolecule, and these are then divided by two.

To quantify the shape of the whole molecule, Kier proposed a linear combination of the above-defined κ indices, each representing a particular shape attribute of the molecule:

$$shape = b_0 \cdot {}^0\kappa + b_1 \cdot {}^1\kappa + b_2 \cdot {}^2\kappa + b_3 \cdot {}^3\kappa$$

where ${}^0\kappa$ is the → *Kier symmetry index* used to encode the shape contribution due to symmetry.

Specific combinations of κ indices were also proposed as indices of molecular flexibility (→ *Kier molecular flexibility index*) and steric effects (→ *Kier steric descriptor*).

📖 [Kier, 1986c, Kier, 1987a, 1987b, 1987c, 1990, 1997; Gombar and Jain, 1987; Mokrosz, 1989; Hall and Kier, 1991; Skvortsova, Baskin *et al.*, 1993; Hall and Vaughn, 1997]

- **Kier symmetry index** → symmetry descriptors
- **K_Z index** → Hosoya Z matrix
- ***K* inflation factor** → variable reduction (⊙ *K* correlation analysis)
- **Kirchhoff matrix** ≡ *Laplacian matrix*
- **Kirchhoff number** → resistance matrix
- **Kirchhoff sum index** ≡ *Ω/D index* → resistance matrix
- **Kirkwood function** → physico-chemical properties (⊙ dielectric constant)
- **KLOGP** → lipophilicity descriptors (⊙ Klopman hydrophobic models)
- **Klopman–Henderson cumulative substructure count** → scoring functions
- **Klopman hydrophobic atomic constants** → lipophilicity descriptors (⊙ Klopman hydrophobic models)
- **Klopman hydrophobic models** → lipophilicity descriptors
- **Klopman LOG *P*** ≡ *KLOG P* → lipophilicity descriptors (⊙ Klopman hydrophobic models)
- **k-matching** → graph
- **Kohonen artificial neural networks** ≡ *Self-Organizing Maps*
- **Kohonen maps** ≡ *Self-Organizing Maps*
- **KOKOS descriptors** → biodescriptors (⊙ amino acid descriptors)
- **Koppel–Paju B scale** → Linear Solvation Energy Relationships (⊙ hydrogen-bond parameters)
- **Kovats retention index** → chromatographic descriptors
- **KOWWIN®** → lipophilicity descriptors
- **Krygowski bond energy** → delocalization degree indices
- **Kubinyi fitness function** → regression parameters
- **Kuhn length** → size descriptors
- **Kulczynski similarity coefficients** → similarity/diversity (⊙ Table S9)
- **Kullback–Leibler divergence** → information content
- **Kupchik modified connectivity indices** → connectivity indices
- **Kupchik vertex degree** → vertex degree
- **kurtosis** → statistical indices (⊙ moment statistical functions)