

Appendix 6.

Structural interpretation of contribution of matrix elements to the best observed combined topological index for BP.

The best observed topological index for BP of octanes composed of a combination of the six elements of the Universal matrix is presented in Table A6 and Figure A6.

Table A6. Best correlation to BP of octanes of the combination of six matrix elements and the contributions of individual matrix elements.

$u_{ij} \times k_{ij}$	R	IC (%)
$u_{72}(-\infty, 3.2, -0.44) \times 0.000205$	-0.834	25.0
$u_{42}(0.21, 4.2, -5.9) \times -0.005451$	0.819	23.8
$u_{32}(-1.39, 2.5, 1^\circ) \times 0.001426$	-0.775	20.5
$u_{63}(-0.98, -4.2, -0.94) \times -0.95898$	0.583	10.5
$u_{74}(1.21, -0.73, 1.20) \times 0.002541$	0.499	7.4
$u_{53}(-0.26, -0.64, 0.80) \times 0.031397$	-0.341	3.3
$\sum u_{ij} \times k_{ij}$	0.995	90.5

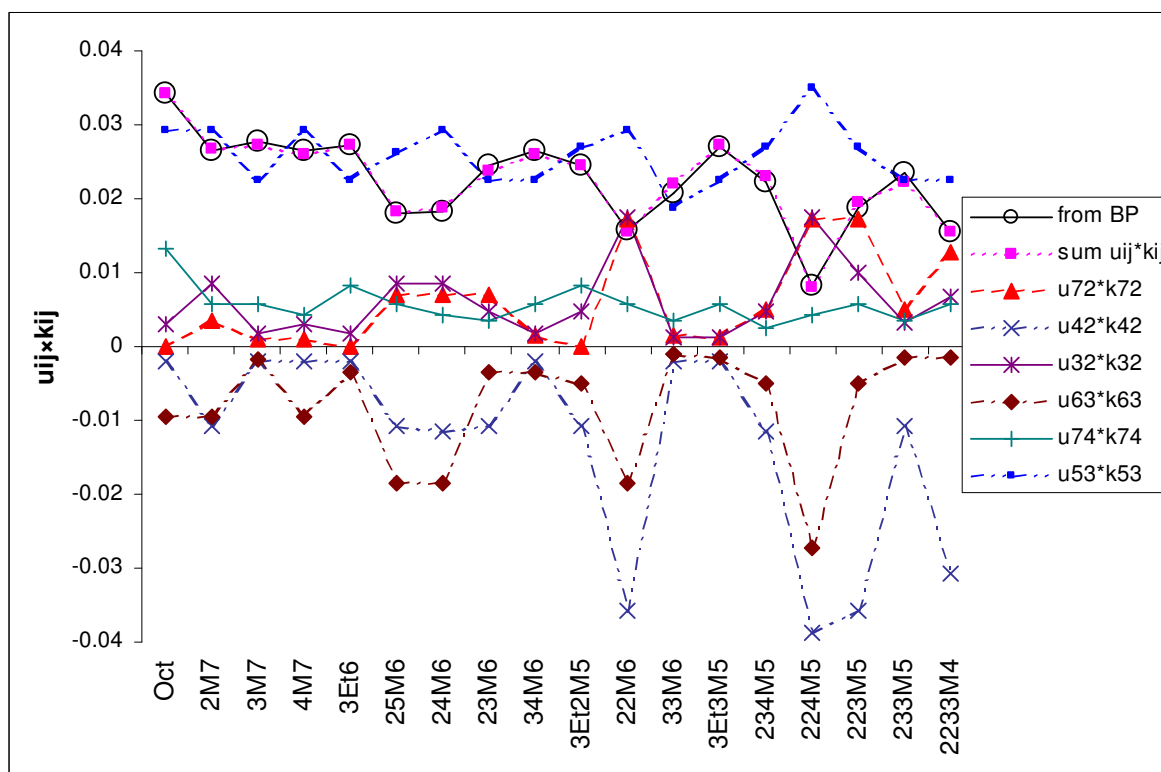


Figure A6. Contribution of particular matrix elements (u_{72} , u_{42} , u_{32} , u_{63} , u_{74} , and u_{53}) to the optimized combined topological index derived from them in the case of BP of octanes.

Positive in value are the contributions of $u_{72}(-\infty, 3.2, -0.44) \times k_{72}$, $u_{32}(-1.39, 2.5, 1^\circ) \times k_{32}$, $u_{74}(1.21, -0.73, 1.20) \times k_{74}$, and $u_{53}(-0.26, -0.64, 0.80) \times k_{53}$, whereas negative in value are the contributions of $u_{42}(0.21, 4.2, -5.9) \times k_{42}$ and $u_{63}(-0.98, -4.2, -0.94) \times k_{63}$.

According to Table A6 and Figure A6, at BP of octanes are of high importance the vertices No. 2, 3, and 4, i.e. the branching bearing vertices in the structure of octanes. They are involved in the contribution to IC : vertex No. 2 together with vertices No. 3, 4, and 7 to 69.3%, vertex No. 3 together with vertices No. 2, 5, and 6 to 34.3%, vertex No. 4 together with vertices No. 2 and 7 to 31.2%, whereas the vertices No. 5, 6, and 7 are involved in only

3.3, 10.5, and 7.4%, respectively. The mutual contribution of only the branches bearing vertices No. 2, 3, and 4 is 44.3%, i.e. almost one half of the total information content contained in this combination of elements of the Universal matrix.

The matrix element $u_{72}(-\infty, 3.2, -0.44)$ contributes to $22M6, 224M5, 223M5 > 2233M4 > 25M6, 24M6, 23M6 > 234M5, 233M5 > 2M7 > 34M6, 33M6 > 3Et3M5 > 3M7, 4M7 > 3Et2M5, 3Et6, Oct = 0$. It stresses thus the importance of the substitution pattern 2,2- over 2- and over 3- and 4-.

The matrix element $u_{42}(0.21, 4.2, -5.9)$ subtracts at $Oct, 3M7, 3Et6, 33M6, 3Et3M5 < 4M7, 34M6 < 2M7, 25M6, 23M6, 3Et2M5, 233M5 < 234M5, 24M6 < 2233M4 < 22M6, 223M5 < 224M5$ i.e. counter the contribution of the matrix element $u_{72}(-\infty, 3.2, -0.44)$ but in different extents.

The matrix element $u_{32}(-1.39, 2.5, 1^\circ)$ contributes to $22M6, 224M5 > 223M5 > 2M7, 25M6, 24M6 > 2233M4 > 23M6, 3Et2M5, 234M5 > 233M5 > Oct, 4M7 > 3M7, 3Et6, 34M6 > 33M6, 3Et3M5$, stressing the importance of the substitution pattern 2,2- over 2- and over 3- and 4- but in a different way than the matrix element $u_{72}(-\infty, 3.2, -0.44)$.

The matrix element $u_{63}(-0.98, -4.2, -0.94)$ subtracts at $33M6 < 3Et3M5 < 233M5, 2233M4 < 3M7 < 3Et6, 23M6, 34M6 < 3Et2M5, 234M5, 223M5 < Oct, 2M7, 4M7 < 25M6, 24M6, 22M6 < 224M5$ i.e. counter the contribution of the matrix elements $u_{72}(-\infty, 3.2, -0.44)$ and $u_{32}(-1.39, 2.5, 1^\circ)$ but in different extents than the matrix element $u_{42}(0.21, 4.2, -5.9)$.

The matrix element $u_{74}(1.21, -0.73, 1.20)$ adds little to $Oct > 3Et6, 3Et2M5 > 2233M4 > 2M7, 3M7, 25M6, 34M6, 22M6, 3Et3M5, 223M5 > 4M7, 24M6, 224M5 > 23M6, 33M6, 233M5 > 234M5$ contributing some fine-tuning to the combined descriptor.

The matrix element $u_{53}(-0.26, -0.64, 0.80)$ contributes the main part of the "numerical volume" of the combined descriptor, and especially to $224M5 > Oct, 2M7, 4M7, 24M6, 22M6 > 3Et2M5, 234M5, 223M5 > 25M6 > 3M7, 3Et6, 23M6, 34M6 > 3Et3M5, 233M5, 2233M4 > 33M6$ stressing thus the importance of vertices No. 2 and 4.

The exponent of $-\infty$ in $u_{72}(-\infty, 3.2, -0.44)$ shows that the vertex No. 7 as an interior vertex in *n*-octane does not contribute anything to the value of the combined index of *n*-octane. The values of exponents to which the degree of vertex No. 2 is raised in matrix elements presented in Table BP (3.2, 4.2, resp. 2.5) show the high contribution of this vertex to the value of the combined index for BP of octanes. The values of exponents to which the degree of vertex No. 3 is raised (-1.39, -0.42, resp. -0.64) resp. those at vertex No. 4 (0.21, 1.21) indicate a lower contribution of these vertices than that of vertex No. 2. The values of exponents to which the values of vertices No. 5, and especially 6 and 7 are raised indicate their importance as terminal vertices.

The distances between pairs of vertices in Table BP have the following influences on the value of the combined molecular descriptor:

The exponent on the distance between vertices No. 7 and No. 2 puts the octane isomers into four different groups: $22M6, 25M6, 24M6, 23M6, 224M5, 223M5 > 3Et6, 3Et2M5, 34M6, 33M6, 234M5, 233M5, 2233M4 > 3Et3M5 > 3M7, 4M7, 2M7, Oct$

The distance between vertices No. 3 and No. 2, between vertices No. 4 and No. 2 as well as between vertices No. 5 and No. 3 is constant.

The exponent on the distance between vertices No. 6 and No. 3 puts the octane isomers into four different groups: $3Et3M5 > 224M5, 223M5, 234M5, 3Et2M5, 233M5 > Oct, 2M7, 4M7, 3M7, 22M6, 24M6, 25M6, 34M6, 23M6, 3Et6, 33M6$.

The exponent on the distance between vertices No. 7 and No. 4 puts the octane isomers into two different groups: $Oct, 2M7, 3M7, 4M7, 25M6, 224M6, 23M6, 22M6, 3Et3M5, 234M5, 224M5, 223M5 > 3Et6, 34M6, 3Et2M6, 33M6, 233M5, 2233M4$