Appendix 9.

Structural interpretation of contribution of matrix elements to the best observed combined topological index for critical density (dc) of octanes.

Matrix elements, which give rise to the best-observed correlation with critical density (dc), are presented in Table A9. Their values at particular octane isomers are presented in Figure A9. Due to the sign of k_{ij}, the contribution of matrix elements $u_{54}(a, b, c)\times k_{54}$, $u_{53}(a, b, c)\times k_{53}$, and $u_{32}(a, b, c)\times k_{32}$ is positive in value, wheres the contribution of matrix elements $u_{83}(a, b, c)\times k_{83}$, $u_{76}(a, b, c)\times k_{76}$, and $u_{65}(a, b, c)\times k_{65}$ is negative in value. The "numerical volume" of the combined index is contributed mainly by the matrix element $u_{53}(a, b, c)\times k_{53}$. It contributes less information about dc than four other matrix elements but anyway more than 10% of it. Each of the six matrix elements, which contribute to the best-observed combined index, has a low correlation with dc of octanes; only $u_{83}(1^a, -2.7, -0.134)$ correlates with $0.7 < R < 0.8$.

Table A9. Best correlation to dc of the combination of six matrix elements and the contributions of individual matrix elements.

$u_{ij}\times k_{ij}$	*R*	*IC* (%)
$u_{83}(1^a, -2.7, -0.134) \times -0.3545$	0.758	27.5
$u_{54}(-2.9, -2.6, -1.39) \times 0.1933$	0.593	15.4
$u_{76}(0.65, 2.7, 0.88) \times -0.0052$	0.550	13.0
$u_{65}(-0.075, -3.1, -0.37) \times -0.0654$	–0.547	12.9
$u_{53}(-0.13, -0.38, 2^c) \times 0.3177$	–0.539	12.5
$u_{32}(0.67, -2.4, 1^c) \times 0.0639$	0.210	1.8
$\sum u_{ij}\times k_{ij}$	0.986	83.1

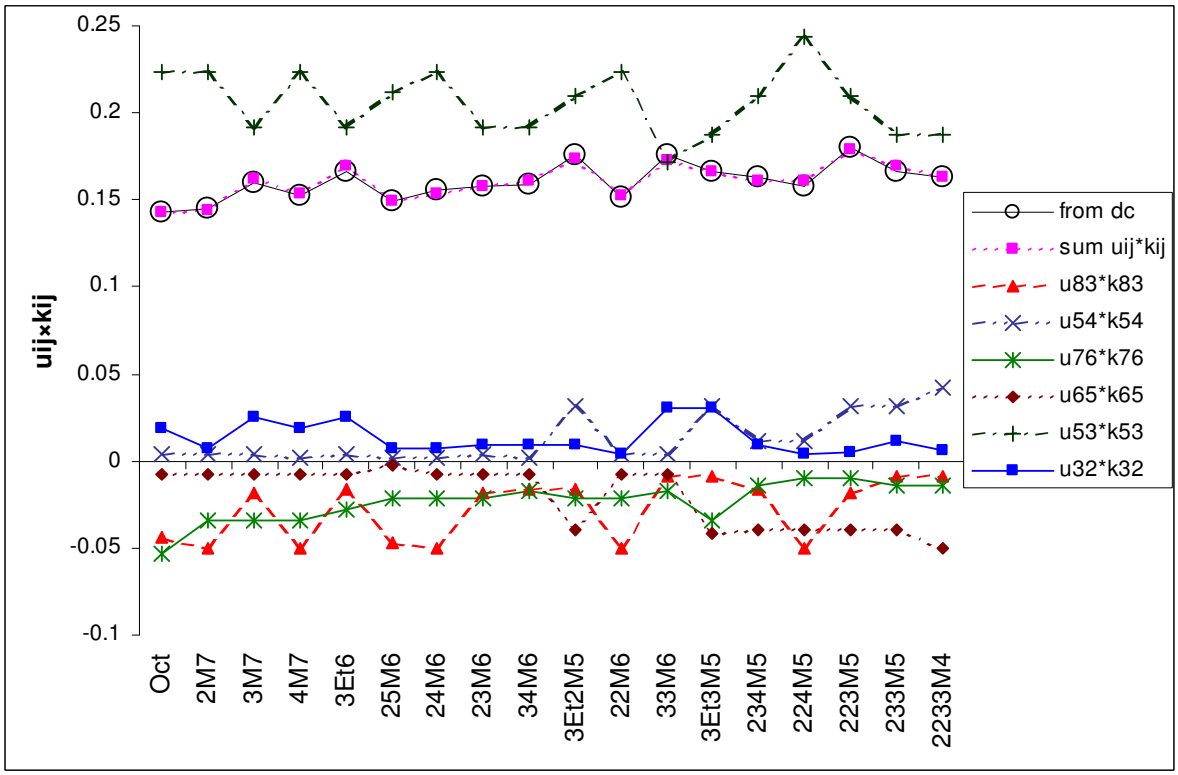

Figure A9. Contribution of particular matrix elements (u_{83}, u_{54}, u_{76}, u_{65}, u_{53}, and u_{32}) to the optimized combined topological index derived from them in the case of dc.

$u_{83}(1^a, -2.7, -0.134)$

The matrix element $u_{83}(1^a, -2.7, -0.134)$ contributes the most at 2M7, 4M7, 24M6, 22M6, 224M5 > 25M6 > Oct > 3M7, 23M6, 223M5 > 3Et6, 34M6, 3Et2M5, 234M5 > 33M6, 3Et3M5, 233M5, 2233M4.

The exponent on the degree of vertex No. 8 has no influence. The exponent on the degree of vertex No. 3 puts the octane isomers into three different groups: Oct, 2M7, 4M7, 24M6, 25M6, 22M6, 224M5 > 3M7, 3Et6, 34M6, 23M6, 223M5, 234M5, 3Et2M5 > 33M6, 233M5, 3Et3M5.

The exponent on the distance between vertices No. 8 and No. 3 puts the octane isomers into four different groups: 3M7, 23M6, 33M6, 3Et3M5, 233M5, 2233M4, 223M5 > 2M7, 4M7, 3Et6, 24M6, 34M6, 3Et2M5, 22M6, 234M5, 224M5 > 25M6 > Oct.

$u_{54}(-2.9, -2.6, -1.39)$

The matrix element $u_{54}(-2.9, -2.6, -1.39)$ contributes the most at 2233M4 > 3Et2M5, 3Et3M5, 223M5, 233M5 > 234M5, 224M5 > Oct > 2M7 > 3M7 > 3Et6 > 22M6 > 33M6 > 23M6 > 4M7, 24M6, 34M6 > 25M6.

The exponent on the degree of vertex No. 5 puts the octane isomers into three different groups: 3Et2M5, 3Et3M5, 223M5, 224M5, 233M5, 234M5, 2233M4 > Oct, 2M7, 3M7, 4M7, 3Et6, 23M6, 24M6, 34M6, 22M6, 33M6 > 25M6

The exponent on the degree of vertex No. 4 puts the octane isomers into three different groups: 2233M4 > Oct, 2M7, 3M7, 3Et3M5, 3Et6, 25M6, 23M6, 33M6, 22M6, 233M5, 223M5, 3Et2M5 > 4M7, 24M7, 34M6, 224M5, 234M5.

The exponent on the distance between vertices No. 5 and No. 4 puts the octane isomers into two groups: 234M5, 224M, 3Et2M5, 3Et3M5, 223M5, 233M5, 4M7, 24M6, 34M6, Oct, 2M7, 3M7, 3Et6, 22M6, 33M6, 23M6, 25M6 > 2233M4, i.e. it distinguishes only 2233M4 from the other octane isomers.

$u_{76}(0.65, 2.7, 0.88)$

The matrix element $u_{76}(0.65, 2.7, 0.88)$ contributes the most at Oct > 2M7, 3M7, 4M7, 3Et3M5 > 3Et2M5, 3Et6 > 25M6, 24M6, 23M6, 22M6 > 234M5, 233M5, 2233M4 > 34M6, 33M6 > 224M5, 223M5.

Vertex No. 7 as well as vertex No. 6 contribute to Oct, 3Et6, and 3Et2M6 more than to other octane isomers.

The distance between these vertices contributes to 22M6, 23M6, 24M6, 25M6 > 3Et6, 34M6, 33M6 > 3Et2M5, 234M5, 233M5 > 224M5, 223M5 > Oct, 2M7, 3M7, 4M7, 3Et3M5

$u_{65}(-0.075, -3.1, -0.37)$

The matrix element $u_{65}(-0.075, -3.1, -0.37)$ contributes the most at 2233M4 > 3Et3M5 > 3Et2M5, 234M5, 224M5, 223M5, 233M5 > 3Et6, 24M6, 23M6, 34M6, 22M6, 33M6 > Oct, 2M7, 3M7, 4M7 > 25M6.

The exponent on the value of vertex No. 6 puts the octane isomers in two groups: other ones > Oct, 2M7, 4M7, 3M7, 3Et3M5.

The exponent on the value of vertex No. 5 puts the octane isomers into three different groups: 3Et2M5, 3Et3M5, 223M5, 224M5, 233M5, 234M5, 2233M4 > Oct, 2M7, 3M7, 4M7, 3Et6, 23M6, 24M6, 34M6, 22M6, 33M6 > 25M6.

The distance from vertex No. 6 to the vertex No. 5 puts the octane isomers into four different groups: Oct, 2M7, 3M7, 4M7, 3Et6, 24M7, 34M6, 25M6, 23M6, 33M6, 22M6 > 2233M4 > 3Et3M5 > 3Et2M5, 224M5, 234M5, 233M5, 223M5.

$u_{53}(-0.13, -0.38, 2^c)$

The matrix element $u_{53}(-0.13, -0.38, 2^c)$ contributes the most at 224M5 > Oct, 2M7, 4M7, 24M6, 22M6 > 25M6 > 3Et2M5, 234M5, 223M5 > 3M7, 3Et6, 23M6, 34M6 > 3Et3M5, 233M5, 2233M4 > 33M6.

The exponent on the value of vertex No. 5 puts the octane isomers in three different groups: 1 = 3Et2M5, 3Et3M5, 223M5, 224M5, 233M5, 234M5, 2233M4 > 0.72 = Oct, 2M7, 3M7, 4M7, 3Et6, 23M6, 24M6, 34M6, 22M6, 33M6 > 0.59 = 25M6.

The exponent on the value of vertex No. 3 puts the octane isomers in three different groups as well: 0.91 = Oct, 2M7, 4M7, 24M6, 25M6, 22M6, 224M5 > 0.87= 3M7, 3Et6, 34M6, 23M6, 223M5, 234M5, 3Et2M5 > 0.84 = 33M6, 233M5, 3Et3M5.

The distance between vertices No. 5 and No. 3 is equal among all octane isomers and does not contribute any separation into groups.

$u_{32}(0.67, -2.4, 1^c)$

The matrix element $u_{32}(0.67, -2.4, 1^c)$ contributes the most at 33M6, 3Et3M5 > 3M7, 3Et6 > Oct, 4M7 > 233M5 > 23M6, 34M6, 3Et2M5, 234M5 > 2M7, 25M6, 24M6 > 2233M4 > 223M5 > 22M6, 224M5.

The exponent on the degree of vertex No. 3 puts the octane isomers into three different groups: 33M6, 233M5, 3Et3M5 > 3M7, 3Et6, 34M6, 23M6, 223M5, 234M5, 3Et2M5 > Oct, 2M7, 4M7, 24M6, 25M6, 22M6, 224M5.

The exponent on the degree of vertex No. 2 puts the octane isomers into three different groups: Oct, 3M7, 4M7, 3Et6, 34M6, 33M6, 3Et3M6 > 2M7, 25M6, 24M6, 23M6, 3Et2M5, 234M5, 233M5 > 22M6, 224M6, 223M6, 2233M4.

The distance between vertices No. 3 and No. 2 is equal among all octane isomers and does not contribute any separation into groups.