Appendix 10.

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

Matrix elements, which give rise to the best-observed correlation with logVP, are presented in Table A10. Their values at particular octane isomers are presented in Figure A10.

Due to the sign of k_{ij}, the contribution of matrix elements $u_{63}(a, b, c)\times k_{63}$, $u_{72}(a, b, c)\times k_{72}$, and $u_{32}(a, b, c)\times k_{32}$ is positive in value, wheres the contribution of matrix elements $u_{64}(a, b, c)\times k_{64}$, $u_{62}(a, b, c)\times k_{62}$, and $u_{75}(a, b, c)\times k_{75}$ is negative in value. The "numerical volume" of the combined index is contributed mainly by the matrix element $u_{75}(a, b, c)\times k_{75}$, although it contributes little information content about logVP. In fact, each of the six matrix elements, which contribute to the best-observed combined index, has a low individual correlation with logVP of octanes. Let us see what contribute these matrix elements.

Table A10. Best correlation to logVP of octanes of the combination of six matrix elements and the contributions of individual matrix elements.

$u_{ij}\times k_{ij}$	*R*	*IC* (%)
$u_{63}(-\infty, -5.3, 1.05) \times 0.3558$	0.589	29.8
$u_{72}(-0.32, -2.1, -2.0) \times 0.5250$	0.573	28.1
$u_{64}(-1.08, 1.91, -1.05) \times -0.0046$	–0.368	10.9
$u_{62}(3.2, 1.10, -2.2) \times -0.0020$	–0.269	5.7
$u_{75}(0.039, 0.30, 0.36) \times -0.0899$	–0.253	5.1
$u_{32}(2.3, -5.8, 1^c) \times 0.0227$	–0.217	3.7
$\sum u_{ij}\times k_{ij}$	0.986	83.3

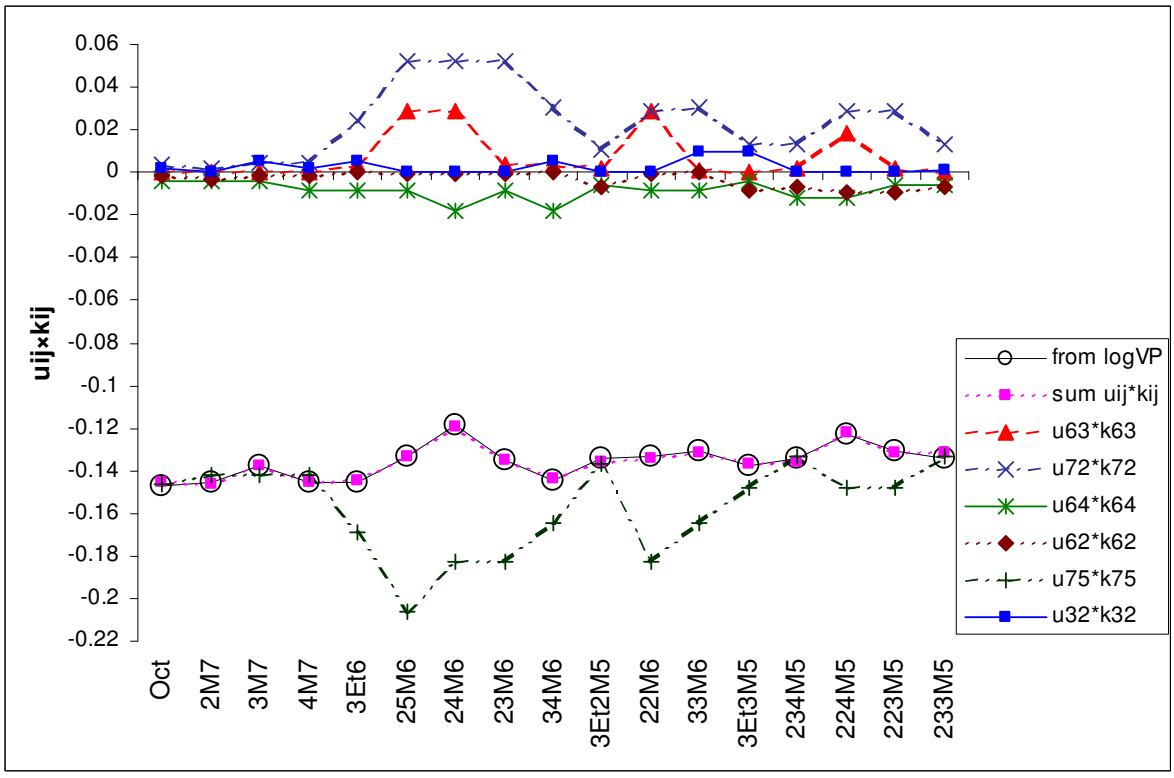

Figure A10. Contribution of particular matrix elements (u_{63}, u_{72}, u_{64}, u_{62}, u_{75}, and u_{32}) to the optimized combined topological index derived from them in the case of logVP of octanes.

$u_{63}(-\infty, -5.3, 1.05)$

The matrix element $u_{63}(-\infty, -5.3, 1.05)$ contributes the most at 25M6, 24M6, 22M6 > 224M5 > 3Et6, 23M6, 34M6 > 3Et2M5, 234M5, 223M5 > 33M6 > 233M5 > Oct, 2M7, 4M7, 3M7, 3Et3M5 = 0.

The exponent on the degree of vertex No. 6 puts the octane isomers into two different groups: 1 = other ones > Oct, 2M7, 4M7, 3M7, 3Et3M5 = 0.

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 vertex No. 6 and No. 3 puts the octane isomers into three different groups as well: Oct, 2M7, 4M7, 3M7, 22M6, 24M6, 25M6, 34M6, 23M6, 3Et6, 33M6 > 224M5, 223M5, 234M5, 3Et2M5, 233M5 > 3Et3M5.

$u_{72}(-0.32, -2.1, -2.0)$

The matrix element $u_{72}(-0.32, -2.1, -2.0)$ contributes the most at 25M6, 24M6, 23M6 > 34M6, 33M6 > 22M6, 224M5, 223M5 > 3Et6 > 3Et3M5 > 234M5, 233M5 > 3Et2M5 > 3M7, 4M7 > Oct > 2M7.

The exponent on the degree of vertex No. 7 contributes to other octane isomers more than to Oct, 3Et6, and 3Et2M6.

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

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

$u_{64}(-1.08, 1.91, -1.05)$

The matrix element $u_{64}(-1.08, 1.91, -1.05)$ contributes the most at 24M6, 34M6 > 234M5, 224M5 > 4M7 > 22M6, 33M6 > 3Et6, 25M6, 23M6 > 3Et2M5, 223M5, 233M5 > Oct, 2M7, 3M7, 3Et3M5.

The exponent on the degree of vertex No. 6 contributes to other octane isomers more than to Oct, 3Et6, and 3Et2M6.

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

The exponent on the distance between vertex No. 6 and No. 4 puts the octane isomers into two groups: Oct, 2M7, 3M7, 4M7, 3Et6, 24M7, 34M6, 25M6, 23M6, 33M6, 22M6, 3Et3M5 > 3Et2M5, 224M5, 234M5, 233M5, 223M5, 2233M4.

$u_{62}(3.2, 1.1, -2.2)$

The matrix element $u_{62}(3.2, 1.1, -2.2)$ contributes the most at 224M5, 223M5 > 3Et3M5 > 3Et2M5, 234M5, 233M5 > 2M7 > Oct, 3M7, 4M7 > 22M6 > 25M6, 24M6, 23M6 > 3Et6, 34M6, 33M6.

The exponent on the degree of vertex No. 6 contributes to Oct, 3Et6, and 3Et2M6 more than to other octane isomers.

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

The exponent on the distance between vertex No. 6 and No. 2 puts the octane isomers into three groups: 3Et2M5, 234M5, 233M5, 224M5, 223M5, 2233M4 > 3Et3M5 > Oct, 3M7, 4M7, 2M7, 3Et6, 25M6, 24M6, 23M6, 34M6, 22M6, 33M6.

$u_{75}(0.039, 0.30, 0.36)$

The matrix element $u_{75}(0.039, 0.30, 0.36)$ contributes the most at 25M6 > 24M6, 23M6, 22M6 > 3Et6 > 34M6, 33M6 > 3Et3M5, 224M5, 223M5 > Oct > 2M7, 3M7, 4M7 > 3Et2M5 > 234M5, 233M5.

The exponent on the degree of vertex No. 7 contributes to Oct, 3Et6, and 3Et2M6 more than to other octane isomers.

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

The exponent on the distance between vertex No. 7 and No. 5 puts the octane isomers into three groups: 223M5, 224M5, 3Et3M5, 22M6 , 23M6, 24M6, 25M6 > 3Et2M5, 2233M4, 233M5, 234M5, 3Et6, 34M6, 33M6 > Oct, 2M7, 3M7, 4M7.

$u_{32}(2.3, -5.8, 1^c)$

The matrix element $u_{32}(2.3, -5.8, 1^c)$ contributes the most at 33M6, 3Et3M5 > 3M7, 3Et6, 34M6 > Oct, 4M7 > 233M5 > 23M6, 3Et2M5, 234M5 > 2M7, 25M6, 24M6 > 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 vertex No. 3 and No. 2 is equal to one at all octanes.