

Appendix 7.

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

Matrix elements, which give rise to the best-observed correlation with the refractive index (n_D) of octanes, not considering 2233M4, which is in solid state at room temperature, are presented in Table A7. Their values at particular octane isomers are presented in Figure A7.

In difference to the situation at BP, at n_D all vertex degrees in Table A7 are raised to negative values of exponents meaning that vertices of higher degrees contribute less than those of lower degrees.

Due to the sign of k_{ij} , the contribution of matrix elements $u_{52}(a, b, c) \times k_{52}$, $u_{75}(a, b, c) \times k_{75}$, $u_{74}(a, b, c) \times k_{74}$, and $u_{86}(a, b, c) \times k_{86}$ is positive in value, whereas the contribution of matrix elements $u_{63}(a, b, c) \times k_{63}$ and $u_{83}(a, b, c) \times k_{83}$ is negative in value. The "numerical volume" of the combined index as well as the highest information content about n_D is contributed by the matrix element $u_{52}(a, b, c) \times k_{52}$.

Table A7. Best correlation to n_D of the combination of six matrix elements and the contributions of individual matrix elements.

$u_{ij} \times k_{ij}$	R	IC (%)
$u_{52}(-0.48, -0.37, -0.53) \times 0.08195$	0.803	43.2
$u_{63}(-0.26, -3.5, -2.2) \times -0.9049$	0.642	25.0
$u_{83}(1^a, -0.25, -\infty) \times -0.00398$	-0.516	15.3
$u_{75}(-\infty, -\infty, 1.42) \times 0.00036$	0.330	6.0
$u_{74}(-0.32, -1.11, 0.73) \times 0.00552$	-0.062	0.2
$u_{86}(1^a, -\infty, -0.85) \times 0.00329$	-0.051	0.1
$\sum u_{ij} \times k_{ij}$	0.995	89.9

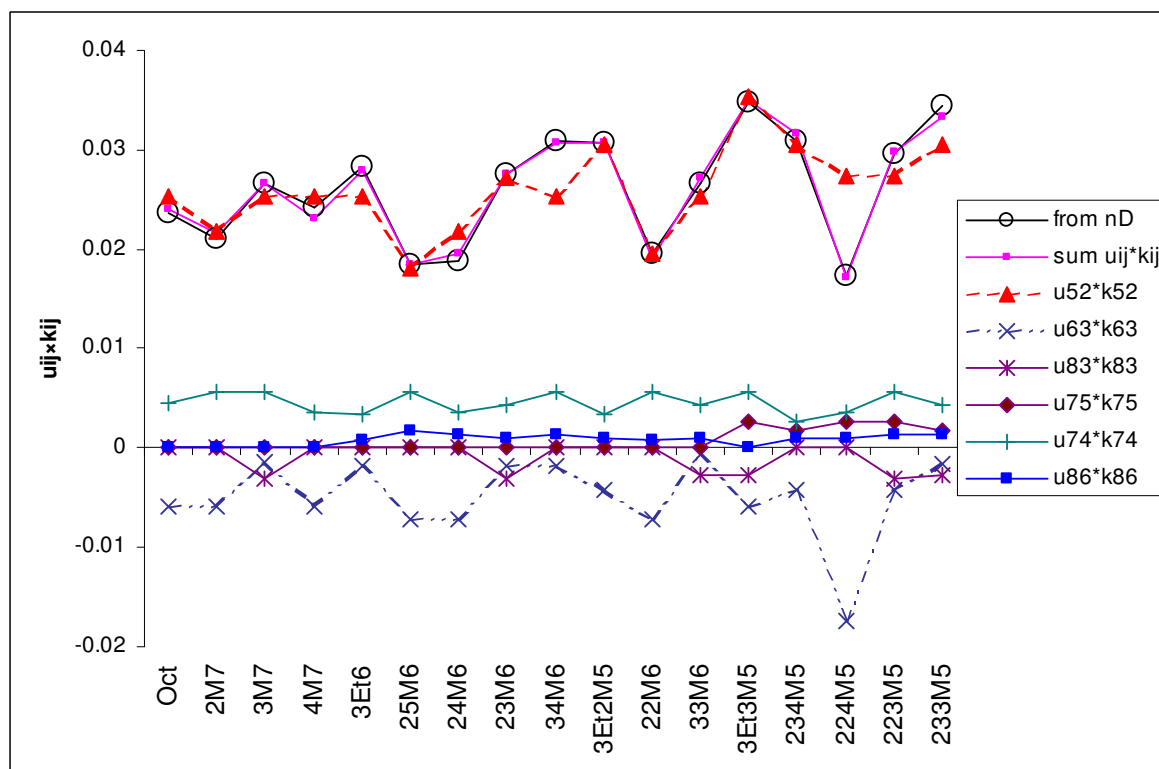


Figure A7. Contribution of particular matrix elements (u_{52} , u_{63} , u_{83} , u_{75} , u_{74} , and u_{86}) to the optimized combined topological index derived from them in the case of n_D .

$u_{52}(-0.48, -0.37, -0.53)$

The matrix element $u_{52}(-0.48, -0.37, -0.53)$ follows the most closely the trend of n_D and it presents the following sequence of n_D values of octanes: 3Et3M5 > 3Et2M5, 234M5, 233M5 > 224M5, 223M5 > 23M6 > Oct > 3M7, 4M7, 3Et6, 34M6, 33M6 > 2M7, 24M6 > 22M6 > 25M6.

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

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.

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

$u_{63}(-0.26, -3.5, -2.2)$

The matrix element $u_{63}(-0.26, -3.5, -2.2)$ contributes to the value of the combined index at 33M6 > 3M7 > 233M5 > 3Et6, 23M6, 34M6 > 3Et2M5, 234M5, 223M5 > 3Et3M5 > Oct, 2M7, 4M7 > 25M6, 24M6, 22M6 > 224M5, i.e. also in this case the vertices in position No. 3 contribute more than those in other positions.

This matrix element subtracts from the values contributed by the matrix element $u_{52}(-0.48, -0.37, -0.53)$ at most at 224M5 followed by 25M6, 24M6, 22M6 > Oct, 2M7, 4M7 > 3Et3M5 > 3Et2M5, 234M5, 223M5 > 3Et6, 23M6, 34M6 > 233M5 > 3M7 and here more than from 33M6.

In this matrix element, vertex No. 6 contributes to Oct, 2M7, 4M7, 3M7, 3Et3M5 less than to other octane isomers.

Vertex No. 3 contributes to Oct, 2M7, 4M7, 24M6, 25M6, 22M6, 224M5 > 3M7, 3Et6, 34M6, 23M6, 223M5, 234M5, 3Et2M5 > 33M6, 233M5, 3Et3M5.

The distance between vertices No. 6 and No. 3 contributes to 3Et3M5 > 224M5, 223M5, 234M5, 3Et2M5, 233M5 > Oct, 2M7, 4M7, 3M7, 22M6, 24M6, 25M6, 34M6, 23M6, 3Et6, 33M6.

$u_{83}(1^a, -0.25, -\infty)$

The matrix element $u_{83}(1^a, -0.25, -\infty)$ subtracts from 3M7, 23M6, 223M5 more than from 33M6, 233M5, and 3Et3M5. From the values at other isomers it does not subtract anything.

Vertex No. 8 does not contribute any information since its degree is equal to one in all tested cases.

Vertex No. 3 contributes to Oct, 2M7, 4M7, 24M6, 25M6, 22M6, 224M5 > 3M7, 3Et6, 34M6, 23M6, 223M5, 234M5, 3Et2M5 > 33M6, 233M5, 3Et3M5.

Due to the exponent of $-\infty$, the distance between vertices No. 8 and No. 3 contributes to 3M7, 23M6, 33M6, 3Et3M5, 223M5, and 233M5 only.

$u_{75}(-\infty, -\infty, 1.42)$

The matrix element $u_{75}(-\infty, -\infty, 1.42)$ adds to 3Et3M5, 224M5, and 223M5 more than to 234M5 and 233M5. To other isomers it does not contribute anything.

Due to the exponent of $-\infty$, vertex No. 7 eliminates the contribution of Oct, 3Et6, and 3Et2M5 to the matrix element $u_{75}(-\infty, -\infty, 1.42)$. Vertex No. 5 eliminates the contribution of Oct, 2M7, 3M7, 4M7, 3Et6, 24M6, 34M6, 23M6, 22M6, 33M6, and 25M6.

The distance between vertices No. 7 and No 5 contributes to Oct, 2M7, 4M7, 3M7 > 3Et6, 34M6, 3Et2M5, 33M6, 234M5, 233M5 > 25M6, 24M6, 23M6, 22M6, 3Et3M5, 224M5, 223M5.

$u_{74}(-0.32, -1.11, 0.73)$

The matrix element $u_{74}(-0.32, -1.11, 0.73)$ adds to 2M7, 3M7, 25M6, 34M6, 22M6, 3Et3M5, 223M5 > Oct > 23M6, 33M6, 233M5 > 4M7, 24M6, 224M5 > 3Et6, 3Et2M5 > 234M5.

In this matrix element, vertex No. 7 contributes to Oct, 2M7, 3M7, 4M7, 3Et3M5 less than to other octane isomers.

Vertex No. 4 contributes to Oct, 2M7, 3M7, 3Et6, 25M6, 23M6, 3Et2M5, 22M6, 33M6, 3Et3M5, 223M5, 233M5 > 4M7, 24M6, 34M6, 234M5, 224M5.

The distance between vertices No. 7 and No. 4 contributes to Oct, 2M7, 3M7, 4M7, 25M6, 24M6, 23M6, 22M6, 3Et3M5, 234M5, 224M5, 223M5 > 3Et6, 34M6, 3Et2M5, 33M6, 233M5.

$u_{86}(1^a, -\infty, -0.85)$

The matrix element $u_{86}(1^a, -\infty, -0.85)$ adds to 25M6 > 24M6 > 34M6 > 223M5 > 233M5 > 23M6 > 3Et2M5 > 33M6 > 234M5 > 224M5 > 3Et6, 22M6 whereas to Oct, 3Et3M5, 4M7, 3M7, 2M7 it does not contribute anything.

Vertex No. 8 does not contribute any information since its degree is equal to one in all tested cases.

Due to the exponent of $-\infty$, vertex No. 6 contributes nothing at Oct, 2M7, 3M7, 4M7, and 3Et3M5, whereas it contributes an equal value of 1 at other isomers.

The distance between vertices No. 8 and No. 6 contributes to Oct, 25M6, 3Et3M5 > 4M7, 24M6, 34M6, 223M5, 233M5 > 3M7, 23M6, 3Et2M5, 33M6, 234M5, 224M5 > 2M7, 3Et6, 22M6.