

Appendix 8.

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

The best observed topological index for Tc of octanes composed of a combination of six elements of the Universal matrix is presented in Table A8 and Figure A8. Due to the sign of k_{ij} , the contribution of matrix elements $u_{52}(a, b, c) \times k_{52}$, $u_{86}(a, b, c) \times k_{86}$, $u_{62}(a, b, c) \times k_{62}$, and $u_{74}(a, b, c) \times k_{74}$ is positive in value, whereas the contribution of matrix elements $u_{63}(a, b, c) \times k_{63}$ and $u_{54}(a, b, c) \times k_{54}$ is negative in value.

Table A8. Best correlation to Tc of the combination of six matrix elements and the contributions of individual matrix elements.

$u_{ij} \times k_{ij}$	R	$IC (\%)$
$u_{63}(-2.2, -4.3, -2.4) \times -0.96569987$	0.799	46.8
$u_{52}(-0.30, -0.23, -0.35) \times 0.01459994$	0.560	20.1
$u_{86}(1^a, 5.3, -5.5) \times 0.00309998$	0.430	11.4
$u_{62}(-1.49, -1.19, -0.63) \times 0.01149923$	0.259	4.0
$u_{74}(-0.092, -2.4, 7.4) \times 9.8E-07$	-0.131	1.0
$u_{54}(1.56, -4.5, -0.38) \times -0.0051$	-0.045	0.1
$\sum u_{ij} \times k_{ij}$	0.986	83.4

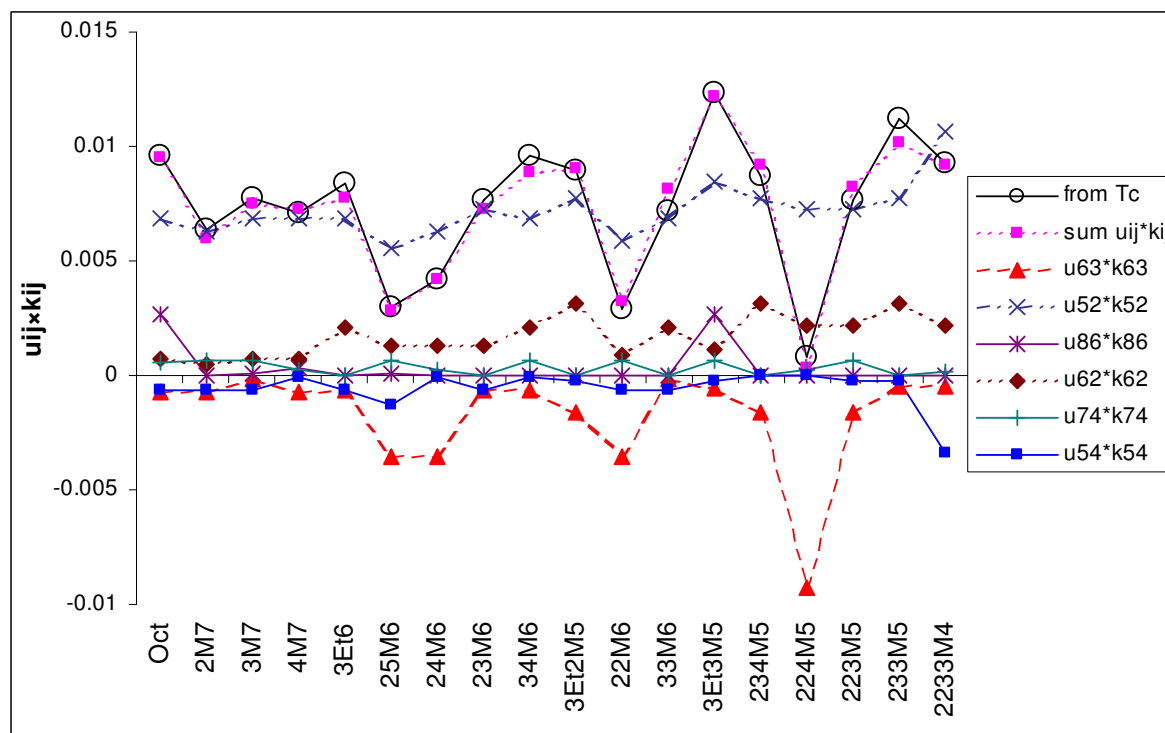


Figure A8. Contribution of particular matrix elements (u_{63} , u_{52} , u_{86} , u_{62} , u_{74} , and u_{54}) to the optimized combined topological index derived from them in the case of Tc.

The contribution of particular elements of the Universal matrix presented in Table Tc and Figure Tc is as follows.

$u_{52}(-0.30, -0.23, -0.35)$

The matrix element $u_{52}(-0.30, -0.23, -0.35)$ contributes the most to the "numerical volume" of the combined index and also the most of information about the contribution of branching to Tc of octanes. It adds the most at $2233M4 > 3Et3M5 > 3Et2M5, 234M5, 233M5 > 23M6 > 224M5, 223M5 > Oct, 3M7, 4M7, 3Et6, 34M6, 33M6 > 2M7, 24M6 > 22M6 > 25M6$.

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. 2 puts the octane isomers into other three groups: $Oct, 3M7, 4M7, 3Et6, 34M6, 33M6, 3Et3M6 > 2M7, 25M6, 24M6, 23M6, 3Et2M5, 234M5, 233M5 > 22M6, 224M6, 223M6, 2233M4$.

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

$u_{63}(-2.2, -4.3, -2.4)$

The matrix element $u_{63}(-2.2, -4.3, -2.4)$ subtracts due to k_{63} the most at $224M5 > 25M6, 24M6, 22M6 > 3Et2M5, 234M5, 223M5 > Oct, 2M7, 4M7 > 3Et6, 23M6, 34M6 > 3Et3M5 > 233M5 > 2233M4 > 33M6 > 3M7$ where it subtracts at least.

Vertex No. 6 contributes to subtraction at Oct, 2M7, 4M7, 3M7, 3Et3M5 less than at other isomers.

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

$u_{86}(1^a, 5.3, -5.5)$

The matrix element $u_{86}(1^a, 5.3, -5.5)$ adds the most at Oct, $3Et3M5 \gg 4M7 \gg 25M6 > 3M7 > 2M7 > 24M6, 34M6, 223M5, 233M5, 2233M4 > 23M6, 3Et2M5, 33M6, 234M5, 224M5$ and very little at 3Et6 and 22M6.

Vertex No. 8 does not contribute anything.

Vertex No. 6 contributes at Oct, 2M7, 4M7, 3M7, 3Et3M5 and nothing at other isomers.

The distance between vertices No. 8 and No. 6 contributes at Oct, $25M6 > 4M7, 24M6, 34M6, 3Et3M5, 223M5, 233M5, 2233M4 > 3M7, 23M6, 3Et2M5, 33M6, 234M5, 224M5 > 2M7, 3Et6, 22M6$.

$u_{62}(-1.49, -1.19, -0.63)$

The matrix element $u_{62}(-1.49, -1.19, -0.63)$ adds the most at $3Et2M5, 234M5, 233M5 > 224M5, 223M5, 2233M4 > 3Et6, 34M6, 33M6 > 25M6, 24M6, 23M6 > 3Et3M5 > 22M6 > Oct, 3M7, 4M7 > 2M7$.

Vertex No. 6 contributes at other isomers more than at Oct, 2M7, 4M7, 3M7, and 3Et3M5.

Vertex No. 2 contributes at Oct, $3M7, 4M7, 3Et6, 34M6, 33M6, 3Et3M5 > 2M7, 25M6, 24M6, 23M6, 3Et2M5, 234M5, 233M5 > 22M6, 224M5, 223M5, 2233M4$.

The distance between vertices No. 6 and No. 2 contributes at $3Et2M5, 234M5, 233M5, 224M5, 223M5, 2233M4 > 3Et3M5 > Oct, 3M7, 4M7, 2M7, 3Et6, 25M6, 24M6, 23M6, 34M6, 22M6, 33M6$.

$u_{74}(-0.092, -2.4, 7.4)$

The matrix element $u_{74}(-0.092, -2.4, 7.4)$ adds very little at 2M7, 3M7, 25M6, 34M6, 22M6, 3Et3M5, 223M5 > Oct > 4M7, 24M6, 224M5 > 2233M4 > 23M6, 33M6, 233M5 > 3Et2M5, 3Et6 > 234M5.

Vertex No. 7 contributes to other octane isomers more than to Oct, 3Et6, and 3Et2M6.

Vertex No. 4 contributes to 2233M4 > Oct, 2M7, 3M7, 3Et3M5, 3Et6, 25M6, 23M6, 33M6, 22M6, 233M5, 223M5, 3Et2M5 > 4M7, 24M7, 34M6, 224M5, 234M5.

The distance between vertices No. 7 and No. 4 contributes at Oct, 2M7, 3M7, 4M7, 25M6, 24M7, 23M6, 22M6, 3Et3M5, 233M5, 223M5, and 224M5 much more than at 3Et6, 34M6, 3Et2M5, 33M6, 234M5, and 2233M4.

$u_{54}(1.56, -4.5, -0.38)$

Due to the sign of k_{54} , the matrix element $u_{54}(1.56, -4.5, -0.38)$ subtracts the most at 2233M5 > 25M6 > 33M6, Oct, 2M7, 3M7, 3Et6, 23M6, 22M6 > 3Et2M5, 3Et3M5, 223M5, 233M5 > 4M7, 24M6, 34M6 > and the least at 234M5 and 224M5.

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

The distance between vertices No. 5 and No. 4 contributes at 2233M4 less than at other octane isomers.