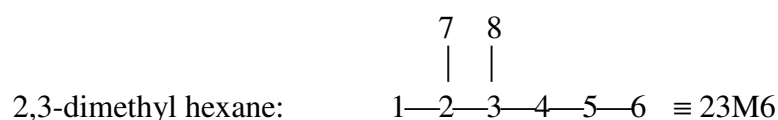


Appendix 1

2,3-Dimethyl hexane: its formula, its label, its simple distance matrix composed of distances d_{ij} , its vectors of degrees of vertices, v_i and v_j , as well as the $U(a, b, c)$ matrix derived from them. The matrix elements belonging to the vertex-degree-weighted path one index $P_1(a, b)$ are presented on the right side of the matrix in bold underlined, whereas on the left side in italics. The relation between them is: $P_{\text{right}}(a, b) = P_{\text{left}}(b, a)$.



v_i	distance matrix							
1	0	1	2	3	4	5	2	3
3	1	0	1	2	3	4	1	2
3	2	1	0	1	2	3	2	1
2	3	2	1	0	1	2	3	2
2	4	3	2	1	0	1	4	3
1	5	4	3	2	1	0	5	4
1	2	1	2	3	4	5	0	3
1	3	2	1	2	3	4	3	0

v_j	1	3	3	2	2	1	1	1
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$U(a, b, c)$ matrix of 2,3-dimethyl hexane

0	<u>1^a3^b1^c</u>	1 ^a 3 ^b 2 ^c	1 ^a 2 ^b 3 ^c	1 ^a 2 ^b 4 ^c	1 ^a 1 ^b 5 ^c	1 ^a 1 ^b 2 ^c	1 ^a 1 ^b 3 ^c
3 ^a 1 ^b 1 ^c	0	<u>3^a3^b1^c</u>	3 ^a 2 ^b 2 ^c	3 ^a 2 ^b 3 ^c	3 ^a 1 ^b 4 ^c	<u>3^a1^b1^c</u>	3 ^a 1 ^b 2 ^c
3 ^a 1 ^b 2 ^c	3 ^a 3 ^b 1 ^c	0	<u>3^a2^b1^c</u>	3 ^a 2 ^b 2 ^c	3 ^a 1 ^b 3 ^c	3 ^a 1 ^b 2 ^c	<u>3^a1^b1^c</u>
2 ^a 1 ^b 3 ^c	2 ^a 3 ^b 2 ^c	2 ^a 3 ^b 1 ^c	0	<u>2^a2^b1^c</u>	2 ^a 1 ^b 2 ^c	2 ^a 1 ^b 3 ^c	2 ^a 1 ^b 2 ^c
2 ^a 1 ^b 4 ^c	2 ^a 3 ^b 3 ^c	2 ^a 3 ^b 2 ^c	2 ^a 2 ^b 1 ^c	0	<u>2^a1^b1^c</u>	2 ^a 1 ^b 4 ^c	2 ^a 1 ^b 3 ^c
1 ^a 1 ^b 5 ^c	1 ^a 3 ^b 4 ^c	1 ^a 3 ^b 3 ^c	1 ^a 2 ^b 2 ^c	1 ^a 2 ^b 1 ^c	0	1 ^a 1 ^b 5 ^c	1 ^a 1 ^b 4 ^c
1 ^a 1 ^b 2 ^c	1 ^a 3 ^b 1 ^c	1 ^a 3 ^b 2 ^c	1 ^a 2 ^b 3 ^c	1 ^a 2 ^b 4 ^c	1 ^a 1 ^b 5 ^c	0	1 ^a 1 ^b 3 ^c
1 ^a 1 ^b 3 ^c	1 ^a 3 ^b 2 ^c	1 ^a 3 ^b 1 ^c	1 ^a 2 ^b 2 ^c	1 ^a 2 ^b 3 ^c	1 ^a 1 ^b 4 ^c	1 ^a 1 ^b 3 ^c	0