

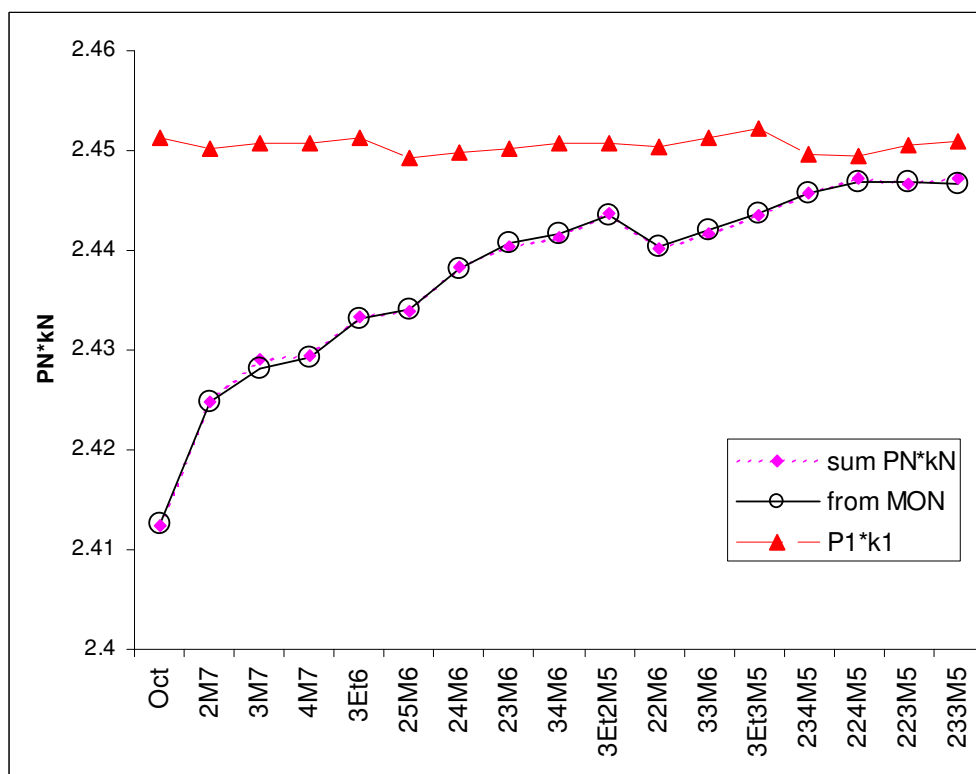
Appendix 2.

The best observed correlations between values of physicochemical properties (PCP) and mutually optimized combinations of vertex degree weighted path indices using two-digit values of exponents and factors k_N in $\sum P_N(a, b, \dots) \times k_N$ for physicochemical properties MON, Tc^2/Pc , n_D , BP, Tc, dc and logVP.

MON

Table MON. The best-observed mutually optimized combinations of vertex degree weighted path indices using two-digit values of exponents and factors k_N in the case of MON.

$P_N(a, b, \dots)$	k_N	R	$IC (\%)$
$P_4(0.71, -1.08, 0.22, -3.4, 2.2)$	-0.021	0.983	36.8
$P_3(-1.12, -2.7, -3.2, -0.030)$	-0.459	0.961	32.5
$P_2(-1.33, -6.0, -0.83)$	0.204	-0.909	26.3
$P_1(0.040, 0.132)$	0.316	-0.158	0.5
$\sum P_N(a, b, \dots) \times k_N$		0.9993	96.2



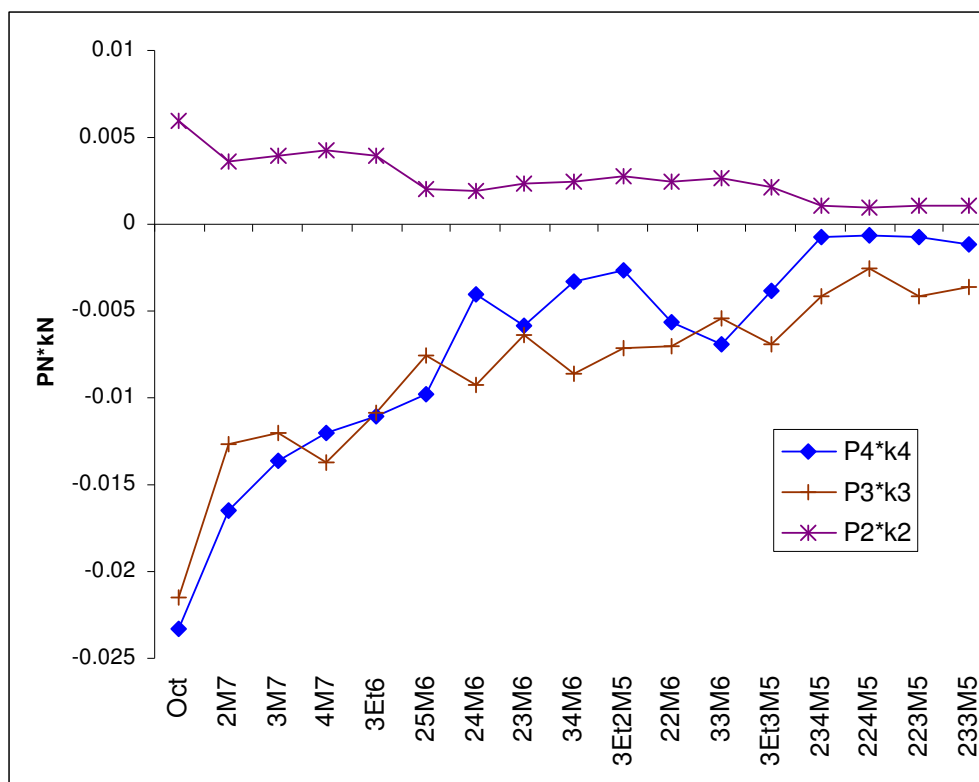


Figure MON. Contribution of particular vertex degree weighted path indices to the optimized combined topological index derived from them in the case of MON of octanes using two-digit values of exponents and factors k_N .

$$Tc^2/Pc$$

Table Tc^2/Pc . The best-observed mutually optimized combinations of vertex degree weighted path indices using two-digit values of exponents and factors k_N in the case of Tc^2/Pc .

$P_N(a, b, \dots)$	k_N	R	IC (%)
$P_4(1.01, -0.62, 0.28, -2.3, 2.0)$	0.025	0.963	41.8
$P_1(-0.165, -0.047)$	0.138	0.961	41.4
$P_2(-0.92, -2.7, -1.64)$	0.152	0.555	9.6
$P_3(-\infty, -1.53, -3.1, -1.38)$	0.685	-0.209	1.3
$\sum P_N(a, b, \dots) \times k_N$		0.998	94.1

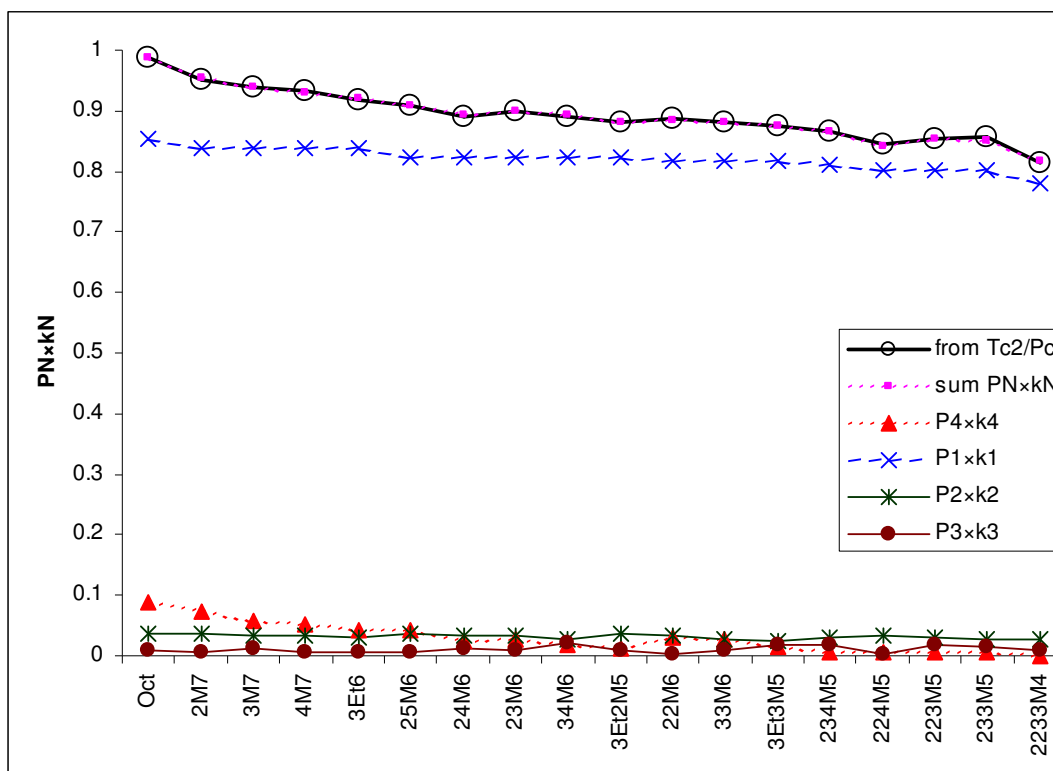


Figure Tc^2/Pc . Contribution of particular vertex degree weighted path indices to the optimized combined topological index derived from them in the case of Tc^2/Pc of octanes using two-digit values of exponents and factors k_N .

BP

Table BP. The best-observed mutually optimized combinations of vertex degree weighted path indices using two-digit values of exponents and factors k_N in the case of BP.

$P_N(a, b, \dots)$	k_N	R	$IC (\%)$
$P_1(-0.40, 1.68)$	-0.0911	0.906	49.8
$P_4(1.04, -2.3, 0.44, -4.1, 2.7)$	0.4223	0.648	20.6
$P_3(-2.0, -1.43, -0.82, 0.020)$	0.4816	0.592	16.8
$P_2(0.63, -0.71, 2.9)$	-0.0050	-0.163	1.1
$\sum P_N(a, b, \dots) \times k_N$		0.993	88.3

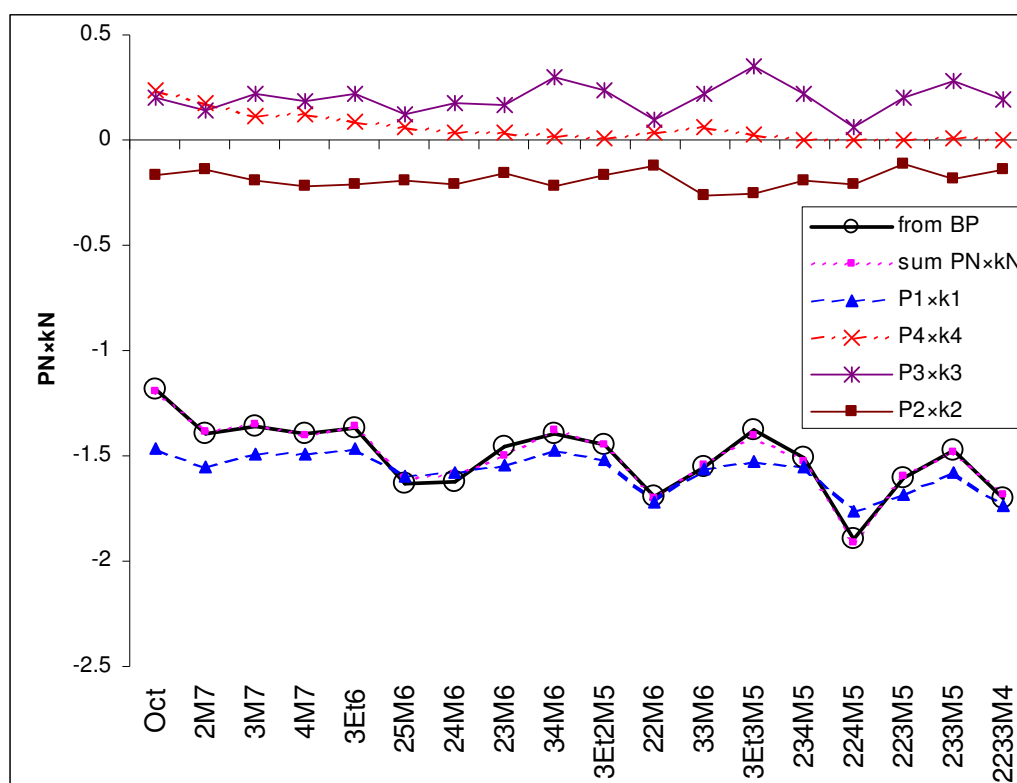


Figure BP. Contribution of particular vertex degree weighted path indices to the optimized combined topological index derived from them in the case of BP of octanes using two-digit values of exponents and factors k_N .

n_D

Table n_D . The best-observed mutually optimized combinations of vertex degree weighted path indices using two-digit values of exponents and factors k_N in the case of n_D .

$P_N(a, b, \dots)$	k_N	R	IC (%)
$P_4(0.63, 0.69, -4.0, 2.6, 2.0)$	-0.052	0.965	44.9
$P_3(-0.174, -0.13, -0.63, 0.091)$	0.400	0.923	37.5
$P_1(-\infty, 0.86)$	-0.414	0.358	4.0
$P_2(-4.2, 0.24, 0.65)$	0.134	-0.168	0.9
$\sum P_N(a, b, \dots) \times k_N$		0.992	87.4

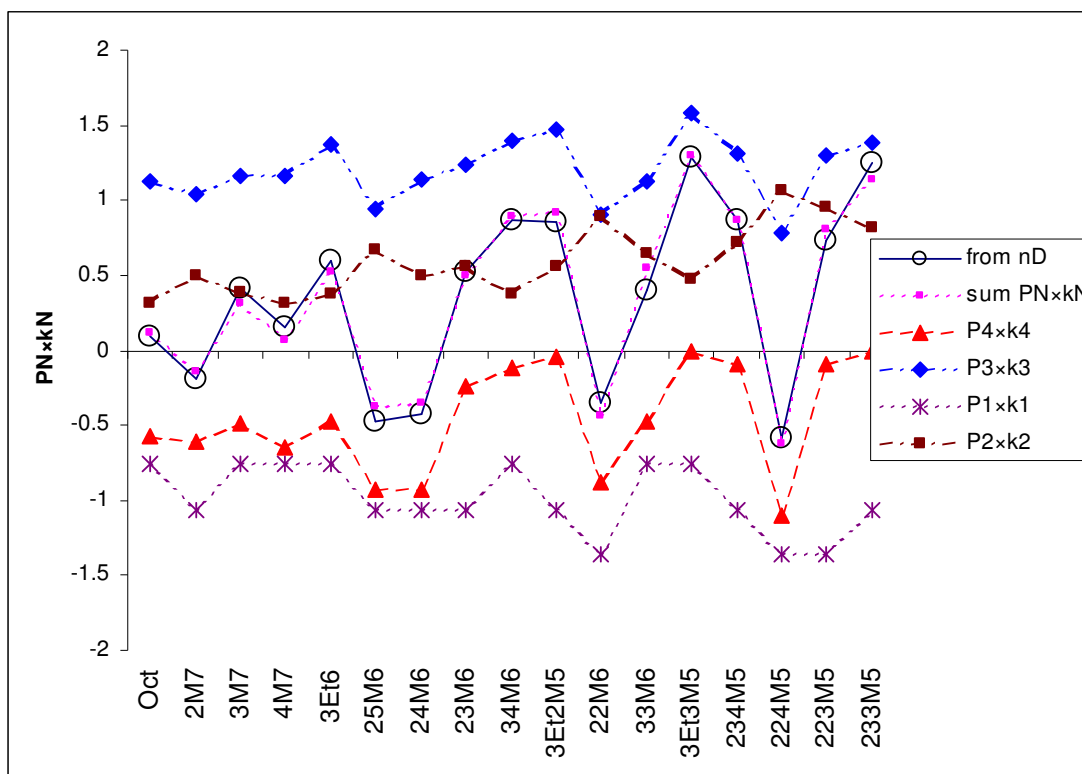


Figure n_D . Contribution of particular vertex degree weighted path indices to the optimized combined topological index derived from them in the case of n_D of octanes using two-digit values of exponents and factors k_N .

Tc

Table Tc. The best-observed mutually optimized combinations of vertex degree weighted path indices using two-digit values of exponents and factors k_N in the case of Tc.

$P_N(a, b, \dots)$	k_N	R	IC (%)
$P_4(0.65, 1.06, 0.063, 0.97, -0.154)$	-0.018751	0.851	31.0
$P_2(3.5, -6.1, 3.0)$	0.004864	-0.773	23.9
$P_3(3.8, 1.34, 1.79, 1.51)$	7.6E-05	-0.729	20.7
$P_1(-0.115, 1.23)$	-0.976309	0.628	14.5
$\sum P_N(a, b, \dots) \times k_N$		0.995	90.1

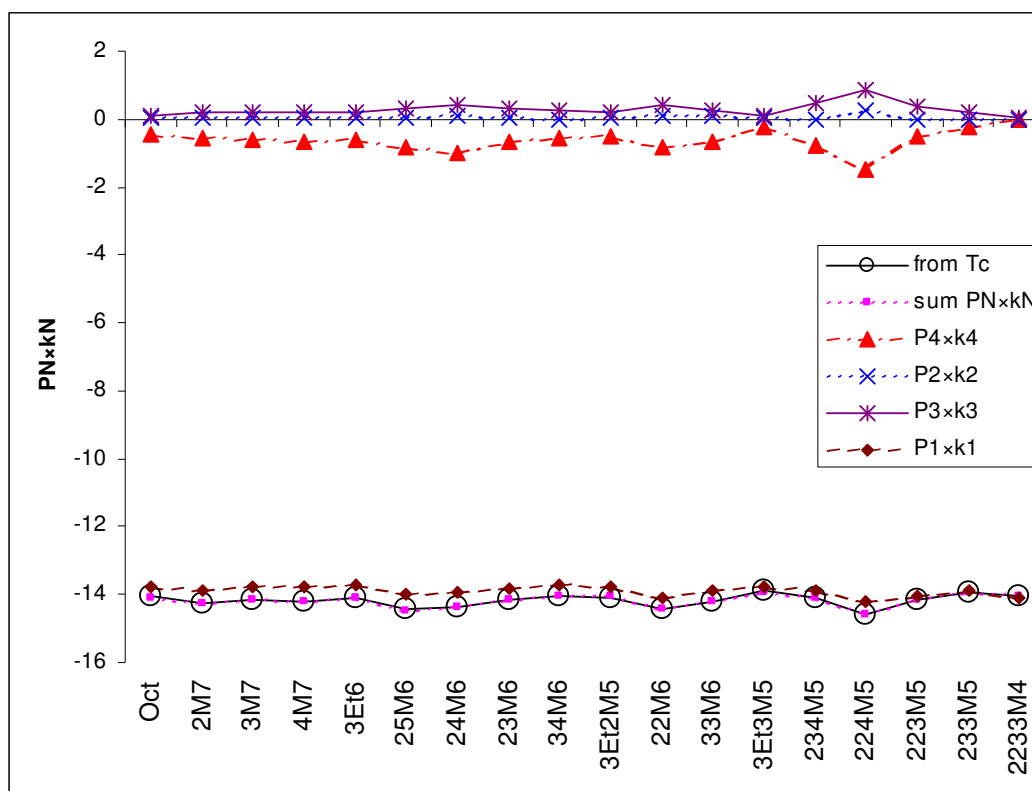


Figure Tc. Contribution of particular vertex degree weighted path indices to the optimized combined topological index derived from them in the case of Tc of octanes using two-digit values of exponents and factors k_N .

dc

Table dc. The best-observed mutually optimized combinations of vertex degree weighted path indices using two-digit values of exponents and factors k_N in the case of dc.

$P_N(a, b, \dots)$	k_N	R	IC (%)
$P_3(1.16, 2.4, 0.072, 1.47)$	0.00363	0.840	31.5
$P_1(-0.55, -2.1)$	-0.49733	-0.689	19.0
$P_4(4.1, -3.9, 3.9, -2.1, 0.14)$	0.00113	-0.430	6.7
$P_2(-0.19, -0.78, 0.30)$	0.49791	0.029	0.028
$\sum P_N(a, b, \dots) \times k_N$		0.904	57.2

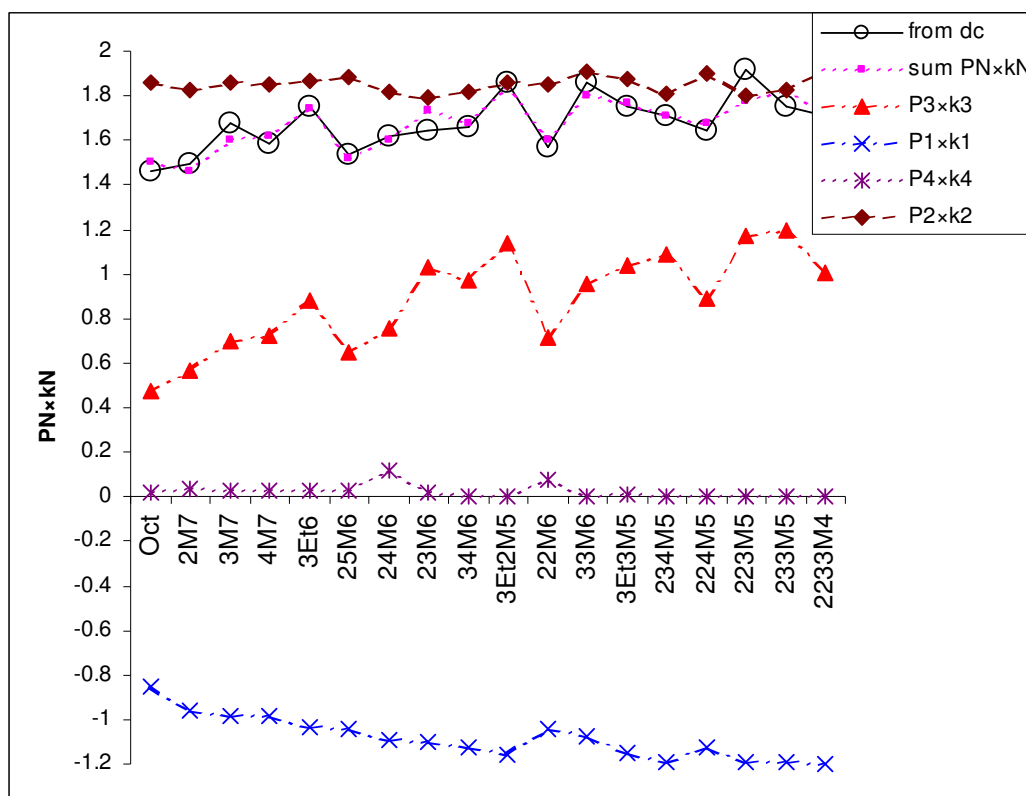


Figure dc. Contribution of particular vertex degree weighted path indices to the optimized combined topological index derived from them in the case of dc of octanes using two-digit values of exponents and factors k_N .

logVP

Table logVP. The best-observed mutually optimized combinations of vertex degree weighted path indices using two-digit values of exponents and factors k_N in the case of logVP.

$P_N(a, b, \dots)$	k_N	R	IC (%)
$P_1(-3.6, -1.24)$	0.603	-0.682	31.2
$P_2(0.50, -1.31, -\infty)$	0.352	0.462	13.2
$P_3(-\infty, -8.6, 1.62, 6.0)$	-0.021	0.449	12.4
$P_4(0.98, 2.3, -3.5, 0.71, 1.29)$	0.024	0.364	8.0
$\sum P_N(a, b, \dots) \times k_N$		0.936	64.8

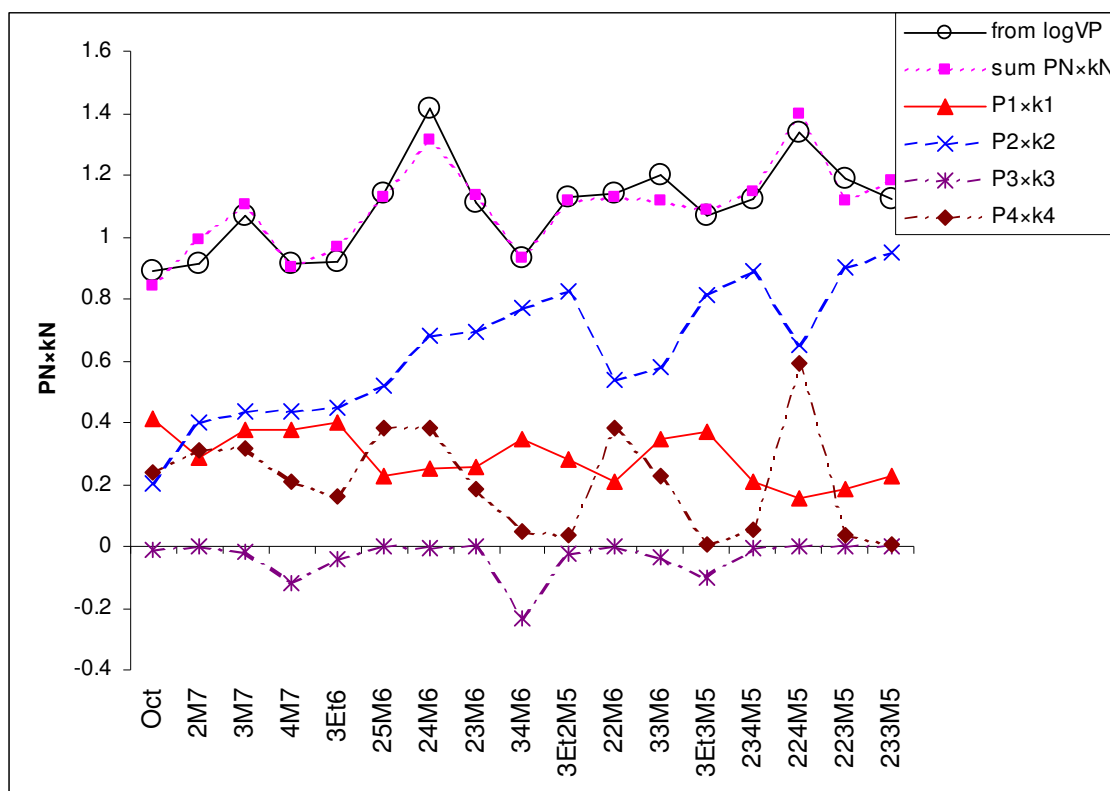


Figure logVP. Contribution of particular vertex degree weighted path indices to the optimized combined topological index derived from them in the case of logVP of octanes using two-digit values of exponents and factors k_N .