




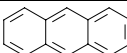
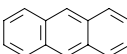
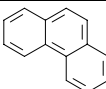
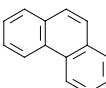
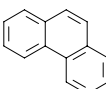
Supporting Material to

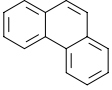
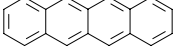
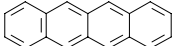
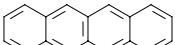
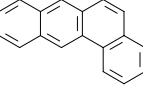
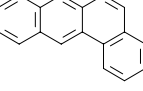
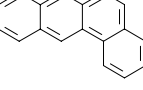
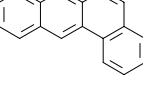
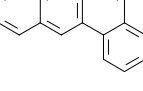
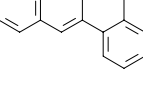
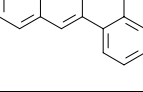
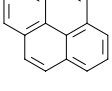
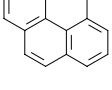
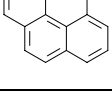
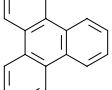
Defining Rules of Aromaticity: A Unified Approach to the Hückel, Clar and Randić Concepts

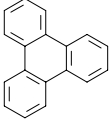
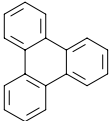
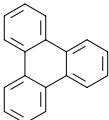
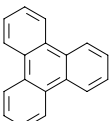
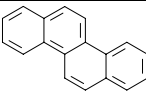
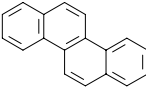
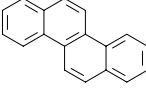
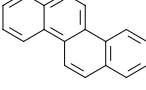
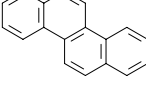
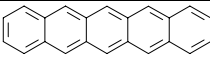
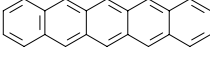
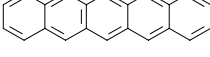
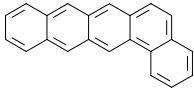
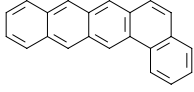
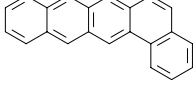
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Arkadiusz Ciesielski, Tadeusz M. Krygowski, Michał K. Cyrański, Alexandru T. Balaban

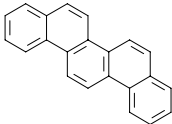
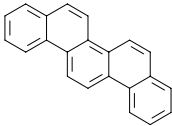
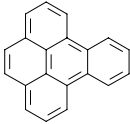
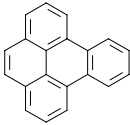
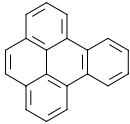
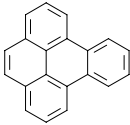
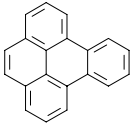
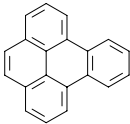
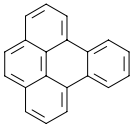
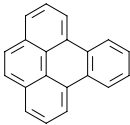
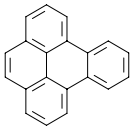
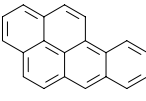
Table 1S. Kekulé polynomials $P_i(\epsilon)=T_i(1-\epsilon)$ for symmetry-independent canonical structures of 18 benzenoid hydrocarbons. For each benzenoid, the number of all possible canonical structures is $K = mM$, where m denotes the multiplicity of symmetry-independent structures. M is the number of symmetrically independent structures. w_i are the weights of canonical structures calculated with use of equation [1]. The $w_i(\text{HOSE})$ calculated following reference **Error! Bookmark not defined.**, based on molecular geometries taken from the reference 37.

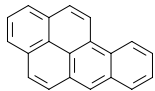
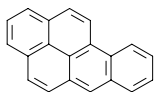
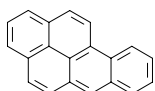
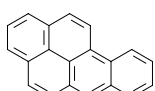
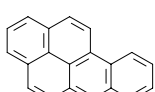
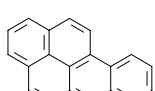
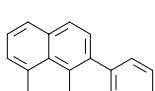
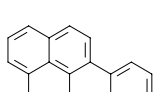




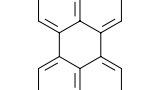
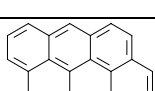
hydrocarbon	$P_i(\epsilon)=T_i(1-\epsilon)$	w_i (HOSE) [%]	w_i [%]	M	K
	$[1+(1-\epsilon)^3]^2$	50.0	50.0	2	2
	$[1+(1-\epsilon)^3+(1-\epsilon)^5]^2$	25.8	26.5	2	3
	$[1+2(1-\epsilon)^3]^2$	48.4	47.1	1	
	$[1+(1-\epsilon)^3+(1-\epsilon)^5+(1-\epsilon)^7]^2$	19.3	17.5	2	4
	$[1+2(1-\epsilon)^3+(1-\epsilon)^5]^2$	30.9	32.5	2	
	$[1+(1-\epsilon)^3+2(1-\epsilon)^5+(1-\epsilon)^7]^2$	15.7	15.0	1	5
	$[1+3(1-\epsilon)^3+(1-\epsilon)^6]^2$	27.6	26.7	1	
	$[1+2(1-\epsilon)^3+(1-\epsilon)^5+(1-\epsilon)^6]^2$	20.3	20.8	2	

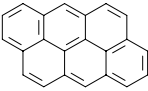
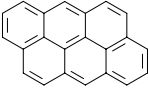
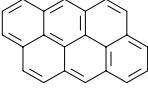
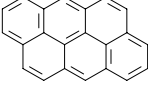
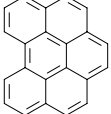
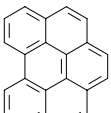
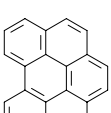
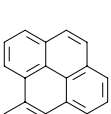
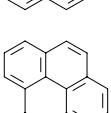
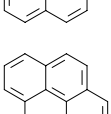
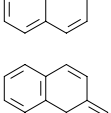
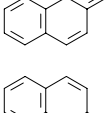
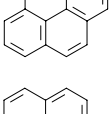
	$[1+2(1-\epsilon)^3+(1-\epsilon)^7+(1-\epsilon)^6]^2$	16.1	16.7	1	
	$[1+(1-\epsilon)^3+(1-\epsilon)^5+(1-\epsilon)^7+(1-\epsilon)^9]^2$	13.0	12.8	2	5
	$[1+2(1-\epsilon)^3+(1-\epsilon)^5+(1-\epsilon)^7]^2$	22.8	22.8	2	
	$[1+2(1-\epsilon)^3+2(1-\epsilon)^5]^2$	28.3	28.8	1	
	$[1+3(1-\epsilon)^3+(1-\epsilon)^5+(1-\epsilon)^6+(1-\epsilon)^8]^2$	16.6	16.5	1	7
	$[1+3(1-\epsilon)^3+(1-\epsilon)^5+2(1-\epsilon)^6]^2$	19.3	19.1	1	
	$[1+(1-\epsilon)^3+2(1-\epsilon)^5+2(1-\epsilon)^7+(1-\epsilon)^9]^2$	10.6	10.0	1	
	$[1+2(1-\epsilon)^3+(1-\epsilon)^5+(1-\epsilon)^6+(1-\epsilon)^7+(1-\epsilon)^8]^2$	12.5	12.6	1	
	$[1+2(1-\epsilon)^3+2(1-\epsilon)^5+(1-\epsilon)^6+(1-\epsilon)^8]^2$	14.1	14.3	1	
	$[1+3(1-\epsilon)^3+(1-\epsilon)^7+2(1-\epsilon)^6]^2$	16.0	16.5	1	
	$[1+2(1-\epsilon)^3+(1-\epsilon)^5+(1-\epsilon)^6+(1-\epsilon)^8+(1-\epsilon)^9]^2$	11.0	11.2	1	
	$[1+2(1-\epsilon)^3+2(1-\epsilon)^5+(1-\epsilon)^6]^2$	18.6	18.8	2	6
	$[1+3(1-\epsilon)^3+(1-\epsilon)^6+(1-\epsilon)^7]^2$	18.6	18.8	2	
	$[1+(1-\epsilon)^3+2(1-\epsilon)^5+2(1-\epsilon)^7]^2$	12.9	12.5	2	
	$[1+4(1-\epsilon)^3+3(1-\epsilon)^6+(1-\epsilon)^9]^2$	14.8	13.2	1	9

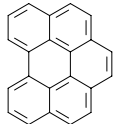
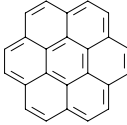
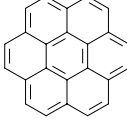
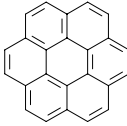
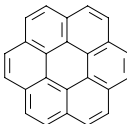
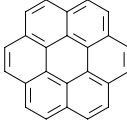
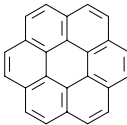
	$[1+3(1-\epsilon)^3+(1-\epsilon)^5+3(1-\epsilon)^6+(1-\epsilon)^9]^2$	12.0	11.9	3	
	$[1+3(1-\epsilon)^3+3(1-\epsilon)^6+(1-\epsilon)^7+(1-\epsilon)^9]^2$	10.2	10.8	3	
	$[1+3(1-\epsilon)^3+3(1-\epsilon)^6+2(1-\epsilon)^9]^2$	8.8	9.9	1	
	$[1+(1-\epsilon)^3+3(1-\epsilon)^5+3(1-\epsilon)^7+(1-\epsilon)^9]^2$	9.8	8.7	1	
	$[1+2(1-\epsilon)^3+(1-\epsilon)^5+(1-\epsilon)^6+(1-\epsilon)^7+(1-\epsilon)^8+(1-\epsilon)^9]^2$	9.6	9.9	2	8
	$[1+3(1-\epsilon)^3+(1-\epsilon)^5+2(1-\epsilon)^6+(1-\epsilon)^8]^2$	13.7	12.9	2	
	$[1+2(1-\epsilon)^3+2(1-\epsilon)^5+(1-\epsilon)^6+2(1-\epsilon)^8]^2$	10.8	11.6	1	
	$[1+2(1-\epsilon)^3+2(1-\epsilon)^5+(1-\epsilon)^6+(1-\epsilon)^7+(1-\epsilon)^8]^2$	11.9	12.2	2	
	$[1+4(1-\epsilon)^3+3(1-\epsilon)^6]^2$	18.7	18.5	1	
	$[1+(1-\epsilon)^3+(1-\epsilon)^5+(1-\epsilon)^7+(1-\epsilon)^9+(1-\epsilon)^{11}]^2$	11.2	10.0	2	6
	$[1+2(1-\epsilon)^3+(1-\epsilon)^5+(1-\epsilon)^7+(1-\epsilon)^9]^2$	17.1	16.8	2	
	$[1+2(1-\epsilon)^3+2(1-\epsilon)^5+(1-\epsilon)^7]^2$	21.7	23.2	2	
	$[1+(1-\epsilon)^3+2(1-\epsilon)^5+2(1-\epsilon)^7+2(1-\epsilon)^9+(1-\epsilon)^{11}]^2$	8.0	7.3	1	9
	$[1+3(1-\epsilon)^3+(1-\epsilon)^5+(1-\epsilon)^6+(1-\epsilon)^7+(1-\epsilon)^8+(1-\epsilon)^{10}]^2$	11.4	11.2	1	
	$[1+3(1-\epsilon)^3+2(1-\epsilon)^5+2(1-\epsilon)^6+(1-\epsilon)^8]^2$	14.9	15.0	1	

	$[1+3(1-\varepsilon)^3+(1-\varepsilon)^5+2(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^8]^2$	13.5	13.5	1	
	$[1+2(1-\varepsilon)^3+(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^8+(1-\varepsilon)^9+(1-\varepsilon)^{10}]^2$	9.0	8.8	1	
	$[1+2(1-\varepsilon)^3+2(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^8+(1-\varepsilon)^{10}]^2$	10.2	10.3	1	
	$[1+3(1-\varepsilon)^3+(1-\varepsilon)^5+2(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^8]^2$	12.9	13.5	1	
	$[1+3(1-\varepsilon)^3+(1-\varepsilon)^5+2(1-\varepsilon)^6+(1-\varepsilon)^8+(1-\varepsilon)^9]^2$	11.9	12.3	1	
	$[1+2(1-\varepsilon)^3+(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^8+(1-\varepsilon)^{10}+(1-\varepsilon)^{11}]^2$	8.2	8.1	1	
	$[1+2(1-\varepsilon)^3+2(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+2(1-\varepsilon)^8+2(1-\varepsilon)^9+(1-\varepsilon)^{10}+(1-\varepsilon)^{11}]^2$	5.9	5.7	1	13
	$[1+3(1-\varepsilon)^3+2(1-\varepsilon)^5+2(1-\varepsilon)^6+(1-\varepsilon)^7+3(1-\varepsilon)^8+(1-\varepsilon)^{10}]^2$	7.8	7.7	2	
	$[1+2(1-\varepsilon)^3+3(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+3(1-\varepsilon)^8+2(1-\varepsilon)^{10}]^2$	6.6	6.6	2	
	$[1+5(1-\varepsilon)^3+6(1-\varepsilon)^6+(1-\varepsilon)^9]^2$	11.8	11.1	1	
	$[1+4(1-\varepsilon)^3+(1-\varepsilon)^5+4(1-\varepsilon)^6+2(1-\varepsilon)^8+(1-\varepsilon)^9]^2$	9.1	9.2	2	
	$[1+3(1-\varepsilon)^3+2(1-\varepsilon)^5+3(1-\varepsilon)^6+(1-\varepsilon)^7+2(1-\varepsilon)^8+(1-\varepsilon)^9]^2$	8.3	8.4	1	
	$[1+3(1-\varepsilon)^3+(1-\varepsilon)^5+3(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^8+2(1-\varepsilon)^9+(1-\varepsilon)^{10}]^2$	6.9	7.1	2	

	$[1+3(1-\varepsilon)^3+2(1-\varepsilon)^5+3(1-\varepsilon)^6+2(1-\varepsilon)^8+(1-\varepsilon)^9+(1-\varepsilon)^{10}]^2$	7.4	7.7	1	
	$[1+3(1-\varepsilon)^3+3(1-\varepsilon)^6+2(1-\varepsilon)^7+(1-\varepsilon)^9+2(1-\varepsilon)^{10}+(1-\varepsilon)^{11}]^2$	5.9	6.1	1	
	$[1+(1-\varepsilon)^3+3(1-\varepsilon)^5+4(1-\varepsilon)^7+2(1-\varepsilon)^9]^2$	7.9	7.2	1	11
	$[1+4(1-\varepsilon)^3+3(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^9+(1-\varepsilon)^{10}]^2$	10.0	9.4	1	
	$[1+3(1-\varepsilon)^3+2(1-\varepsilon)^5+3(1-\varepsilon)^6+(1-\varepsilon)^8+(1-\varepsilon)^9]^2$	10.4	10.1	2	
	$[1+3(1-\varepsilon)^3+(1-\varepsilon)^5+3(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^9+(1-\varepsilon)^{10}]^2$	8.7	8.7	1	
	$[1+3(1-\varepsilon)^3+(1-\varepsilon)^5+3(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^8+(1-\varepsilon)^9]^2$	8.9	9.4	2	
	$[1+4(1-\varepsilon)^3+4(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^9]^2$	10.7	10.9	1	
	$[1+2(1-\varepsilon)^3+2(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+2(1-\varepsilon)^8+(1-\varepsilon)^9+(1-\varepsilon)^{10}]^2$	7.0	7.2	1	
	$[1+2(1-\varepsilon)^3+2(1-\varepsilon)^5+(1-\varepsilon)^6+2(1-\varepsilon)^7+2(1-\varepsilon)^8+(1-\varepsilon)^9]^2$	7.9	7.9	1	
	$[1+4(1-\varepsilon)^3+4(1-\varepsilon)^6+2(1-\varepsilon)^9]^2$	9.2	10.1	1	
	$[1+(1-\varepsilon)^3+2(1-\varepsilon)^5+3(1-\varepsilon)^7+2(1-\varepsilon)^9]$	8.1	7.7	1	9

	$[1+3(1-\varepsilon)^3+(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^8+(1-\varepsilon)^9]^2$	10.7	10.8	1	
	$[1+3(1-\varepsilon)^3+2(1-\varepsilon)^5+2(1-\varepsilon)^6+(1-\varepsilon)^8]^2$	13.5	13.7	1	
	$[1+2(1-\varepsilon)^3+2(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+2(1-\varepsilon)^8]^2$	10.0	10.3	1	
	$[1+2(1-\varepsilon)^3+3(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^8]^2$	11.9	11.8	1	
	$[1+4(1-\varepsilon)^3+3(1-\varepsilon)^6+(1-\varepsilon)^7]^2$	15.3	15.2	1	
	$[1+3(1-\varepsilon)^3+(1-\varepsilon)^5+2(1-\varepsilon)^6+(1-\varepsilon)^8+(1-\varepsilon)^9]^2$	11.0	11.3	1	
	$[1+2(1-\varepsilon)^3+2(1-\varepsilon)^5+(1-\varepsilon)^6+2(1-\varepsilon)^7+(1-\varepsilon)^8]^2$	10.9	10.8	1	
	$[1+2(1-\varepsilon)^3+(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^8+2(1-\varepsilon)^9]$	8.5	8.4	1	
	$[1+2(1-\varepsilon)^3+2(1-\varepsilon)^5+(1-\varepsilon)^6+2(1-\varepsilon)^8+(1-\varepsilon)^{10}]^2$	9.6	9.1	2	9
	$[1+2(1-\varepsilon)^3+2(1-\varepsilon)^5+(1-\varepsilon)^6+2(1-\varepsilon)^8+(1-\varepsilon)^{10}]^2$	9.6	9.1	2	
	$[1+3(1-\varepsilon)^3+(1-\varepsilon)^5+2(1-\varepsilon)^6+2(1-\varepsilon)^8]^2$	11.6	11.9	4	
	$[1+4(1-\varepsilon)^3+4(1-\varepsilon)^6]^2$	14.8	16.2	1	
	$[1+(1-\varepsilon)^3+2(1-\varepsilon)^5+3(1-\varepsilon)^7+3(1-\varepsilon)^9]^2$	7.5	7.0	2	10
	$[1+3(1-\varepsilon)^3+(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+(1-\varepsilon)^8+2(1-\varepsilon)^9]^2$	9.4	9.3	2	

	$[1+3(1-\epsilon)^3+2(1-\epsilon)^5+2(1-\epsilon)^6+(1-\epsilon)^8+(1-\epsilon)^9]^2$	11.0	11.3	2	
	$[1+2(1-\epsilon)^3+2(1-\epsilon)^5+(1-\epsilon)^6+2(1-\epsilon)^7+2(1-\epsilon)^8]^2$	9.5	9.6	1	
	$[1+2(1-\epsilon)^3+3(1-\epsilon)^5+(1-\epsilon)^6+2(1-\epsilon)^7+(1-\epsilon)^8]^2$	10.9	10.9	2	
	$[1+4(1-\epsilon)^3+3(1-\epsilon)^6+2(1-\epsilon)^7]^2$	13.0	13.5	1	
	$[1+(1-\epsilon)^3+3(1-\epsilon)^5+5(1-\epsilon)^7+4(1-\epsilon)^9]^2$	6.1	5.7	1	14
	$[1+4(1-\epsilon)^3+3(1-\epsilon)^6+2(1-\epsilon)^7+(1-\epsilon)^9+2(1-\epsilon)^{10}+(1-\epsilon)^{11}]^2$	6.8	6.4	1	
	$[1+3(1-\epsilon)^3+2(1-\epsilon)^5+3(1-\epsilon)^6+(1-\epsilon)^7+(1-\epsilon)^8+2(1-\epsilon)^9+(1-\epsilon)^{10}]^2$	7.2	7.1	2	
	$[1+3(1-\epsilon)^3+3(1-\epsilon)^5+3(1-\epsilon)^6+2(1-\epsilon)^8+(1-\epsilon)^9+(1-\epsilon)^{10}]^2$	7.9	7.7	1	
	$[1+4(1-\epsilon)^3+(1-\epsilon)^5+4(1-\epsilon)^6+(1-\epsilon)^7+2(1-\epsilon)^8+(1-\epsilon)^9]^2$	8.4	8.5	2	
	$[1+2(1-\epsilon)^3+3(1-\epsilon)^5+(1-\epsilon)^6+2(1-\epsilon)^7+3(1-\epsilon)^8+2(1-\epsilon)^{10}]^2$	6.4	6.3	2	
	$[1+3(1-\epsilon)^3+2(1-\epsilon)^5+3(1-\epsilon)^6+2(1-\epsilon)^7+2(1-\epsilon)^8+(1-\epsilon)^9]^2$	7.6	7.9	1	
	$[1+5(1-\epsilon)^3+6(1-\epsilon)^6+2(1-\epsilon)^9]^2$	9.0	9.5	1	
	$[1+3(1-\epsilon)^3+2(1-\epsilon)^5+2(1-\epsilon)^6+(1-\epsilon)^7+3(1-\epsilon)^8+(1-\epsilon)^9+(1-\epsilon)^{10}]^2$	6.7	6.9	2	

	$[1+2(1-\varepsilon)^3+2(1-\varepsilon)^5+(1-\varepsilon)^6+(1-\varepsilon)^7+2(1-\varepsilon)^8+3(1-\varepsilon)^9+(1-\varepsilon)^{10}+(1-\varepsilon)^{11}]^2$	5.4	5.2	1	
	$[1+(1-\varepsilon)^3+3(1-\varepsilon)^5+6(1-\varepsilon)^7+8(1-\varepsilon)^9+(1-\varepsilon)^{12}]^2$	4.1	4.0	2	20
	$[1+4(1-\varepsilon)^3+3(1-\varepsilon)^6+3(1-\varepsilon)^7+2(1-\varepsilon)^9+3(1-\varepsilon)^{10}+3(1-\varepsilon)^{11}+(1-\varepsilon)^{12}]^2$	4.1	4.0	2	
	$[1+3(1-\varepsilon)^3+3(1-\varepsilon)^5+3(1-\varepsilon)^6+(1-\varepsilon)^7+2(1-\varepsilon)^8+3(1-\varepsilon)^9+2(1-\varepsilon)^{10}+2(1-\varepsilon)^{11}]^2$	4.7	4.6	6	
	$[1+4(1-\varepsilon)^3+2(1-\varepsilon)^5+4(1-\varepsilon)^6+2(1-\varepsilon)^7+4(1-\varepsilon)^8+2(1-\varepsilon)^9+(1-\varepsilon)^{10}]^2$	5.7	5.8	6	
	$[1+2(1-\varepsilon)^3+4(1-\varepsilon)^5+(1-\varepsilon)^6+4(1-\varepsilon)^7+4(1-\varepsilon)^8+4(1-\varepsilon)^{10}]^2$	4.7	4.8	3	
	$[1+6(1-\varepsilon)^3+9(1-\varepsilon)^6+4(1-\varepsilon)^9]^2$	7.0	7.1	1	