

QSPR ANALYSIS OF A SET OF LIQUID CRYSTALS IN THE BENZYLIDENEANILINE CLASS ACCORDING TO THEIR TRANSITION TEMPERATURE

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ABSTRACT The present paper focuses on the connection amongst the structure of 25 liquid crystals in the benzylideneaniline class and some of their physico-chemical properties. Simple and multiple correlations between transition temperatures and 34 calculated molecular descriptors (25 topological indices and 12 Van der Waals parameters), for each compound, were made. Simple and multiple correlations amongst topological indices and Van der Waals parameters, respectively, observing the variations taking place, are presented.

Keywords: *liquid crystals, benzylideneaniline, topological indices, Van de Waals parameters*

INTRODUCTION

The microstructure of liquid crystals is complex and very variable. Some organic substances pass from crystalline, solid to isotropic, liquid states, not directly, but through a phase [1,2]. The mechanical and symmetrical properties of these phases are intermediate to the properties of liquids and crystals [3,4]. Because of this, these substances are called liquid crystals or liquid anisotropic crystals. Anisotropic liquids are characterized by a molecular order, which can be translational, rotational, or combinations of the two. The translational order is conditioned by the non-spherical or elongated shape of the molecules that make up the mesophase [5]. The molecular structure is a defining criterion in the categorization of mesophases as anisotropic liquids or liquid crystals [6].

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According to Friedel [7,8], three types, or groups of liquid crystals are distinguished: smectic, nematic and cholesteric, as well as discotic liquid crystals called columnar. The liquid crystals belonging to each of these groups are distinguished by their physical properties, primarily optical ones. These differences arise as a result of a difference in structure.

In smectic liquid crystals, molecules, elongated in the form of sticks, are arranged parallel to their length and form layers of equal thickness, close to the length of the molecules [9]. These layers are organized one above the other at equal distances. Molecular layers in typical smectics are mobile, moving slightly parallel to one another. The transition temperature in the mesomorphic state is quite high. This temperature must be of such value as to destroy the bond between the molecules placed at close distances. Distance between layers can be measured by X-ray diffraction [10].

In cholesteric liquid crystals, the molecules have an orientational ordering of the molecules of the long axis and the center of mass unordered formation, similar to the nematic, but in contrast to this the structure of the balance [11]. Cholesterol derivatives are part of this category, hence the name of the group of liquid crystals. In cholesteric liquid crystals molecules are arranged in layers, as in smectics, but the long axes are parallel to the layers' planes. The layers in the cholesteric liquid crystals are thin, monomolecular. The direction of the long axis orientation of the molecules in each layer is terminated with respect to the previous one, which leads to the formation of a spiral molecular structure [9,11]. Most cholesteric fluids are cholesterol derivatives, cholesteryl acetate, cholesteryl nitrate.

The nematic phase is characterized by long-range orientation [12], which means that long axes of molecules tend to move along the preferential axis. The nematic mesomorphic structure is characterized in that the orientation of the axes of the molecules in such crystals is parallel but does not form layers [13].

Liquid column crystals are different from previous shapes, the molecules are not elongated or discoidal in shape and the arrangement involves an overlapping of the discs in the columns [14]. This mesophase is characterized by a packet of columns and molecules. The columns are wrapped together along the two surface crystalline dimensions. Arranging the molecules in columns leads to the formation of new mesophases [15,16].

In technology, thin-film nematic crystals change their transmission properties for natural or polarized light when an electric field is applied [17,18]. It can be used for alphanumeric and analog display, image conversion, and matrix screens for image playback. In medicine, the use of cholesterol-based liquid crystals in skin thermography and diagnosis derives from the special optical properties of thin films of these substances that indicate

rapidly and directly through their color [19]. In chemistry, nematic and cholesteric liquid crystals are very good solvents for organic molecules. They can be incorporated into liquid crystals in concentrations that do not damage the internal order of the liquid crystals. They are used for spectroscopic investigations of the anisotropic properties of molecules. Liquid crystals are used as solvents in ultraviolet-visible spectroscopy, magnetic resonance imaging, electronic spin resonance to obtain information on the length of solute molecule bonds [20,16].

The present paper focuses on the connection amongst the structure of 25 liquid crystals in the benzylideneaniline class, molecules that fall into the nematic liquid crystals, and some of their physico-chemical properties. The polymers and coordination compounds in the benzylideneaniline class (with π conjugate systems) are important optical functional compounds and have been applied extensively in the fields of liquid crystal materials [22]. Thus, we calculated and tested 34 molecular descriptors, of which 25 topological indices and 12 Van der Waals parameters.

RESULTS AND DISCUSSION

The values of the R correlation coefficient that resulted from Pearson's linear correlation test, between the transition temperature and each of the 35 molecular descriptors are shown in Table 1. Relatively low correlations, both in regards to Van der Waals parameters – transition temperatures, and, topological indices – transition temperatures, in the case of liquid crystals in the benzylideneaniline compounds class, are noted.

The obtained coefficients, lower than $R^2=0.4$, lead to weak correlations, almost insignificant when compared to previous studies (column liquid crystals), where correlations higher than 0.8, with the same topological indices or Van der Waals parameters, were obtained.

The tracked Van der Waals parameters were: Van der Waals Molecular Volume (V^W), van der Waals surface (S^W), Van der Waals ratio (V^W/S^W), volume of the sphere (V^{SF}), volume of the ellipsoid (V^{EL}), the ellipsoid semi-axes (EX, EY, EZ), the ratio between the volume of the sphere and the Van der Waals volume (GL_1), the ratio between the volume of the sphere and that of the ellipsoid (GL_2), the degree of volume globularity (GLOB, the ratio between the Van der Waals volume and that of the sphere) [23]. The used topological indices were as follows: Wiener (W), polarity (P), Gordon-Scantlebury Index (N_2), Zagreb (M_1 si M_2), Randić ($^1\chi, ^2\chi, ^3\chi$), Balaban (J_2, J_3), Balaban and Randić index with the covalent radii (J^{rc}, χ^{rc}), Mulliken's electronegativities (J^{el}, χ^{el}) and by Van der Waals radii (J^{Rw}, χ^{Rw}), Kier and

Hall Indices ($\chi^{D^{el}}$, JD^{el} were calculated for Mulliken's electronegativities, the indices $\chi^{D^{rc}}$ and JD^{rc} for the covalent radii, and, respectively, the indices $\chi^{D^{Rw}}$, JD^{Rw} for van der Waals radii) [23].

Table 1. Statistical parameters of the mono-variable regressions equations

Van der Wals parameters			Topological indices		
Independent variable	Statistical parameter		Independent variable	Statistical parameters	
	R ²	F		R ²	F
V ^W	0.442	7.72	W	0.354	6.55
S ^W	0.446	7.89	P	0.402	7.63
V ^W /S ^W	0.205	3.39	N ₂	0.431	7.60
V ^{SF}	0.350	6.03	M ₁	0.446	7.90
S ^{SF}	0.501	9.14	M ₂	0.436	7.70
V ^{EL}	0.415	7.94	¹ χ	0.411	7.92
Ex	0.400	16.94	² χ	0.321	6.09
EY	0.206	4.39	³ χ	0.394	6.64
Ez	0.108	1.20	χ^{rc}	0.407	7.11
GL ₁	0.312	5.22	χ^{el}	0.402	7.65
GL ₂	0.215	4.08	χ^{Rw}	0.401	7.20
GLOB	0.508	12.5	$\chi^{D^{rc}}$	0.391	6.55
			$\chi^{D^{el}}$	0.396	7.23
			$\chi^{D^{Rw}}$	0.386	7.39
			J ₂	0.324	5.47
			J ₃	0.222	4.00
			J ^{rc}	0.055	0.13
			J ^{el}	0.068	0.12
			J ^{Rw}	0.006	0.001
			JD ^{rc}	0.112	1.15
			JD ^{el}	0.009	0.002
			JD ^{Rw}	0.008	0.002

As an example, ,the best' simple linear correlations between temperature and E_x, and, transition temperature and globularity (GLOB), are rendered as a graph, where: R² – coefficient of determination SE – standard error, MSE – Mean Square error.

$$T_z = - 70.06 + 15.05 EX \quad (1)$$

$$R^2 = 0.400 \quad SE = 33.34 \quad F = 16.94 \quad MSE = 146.14$$

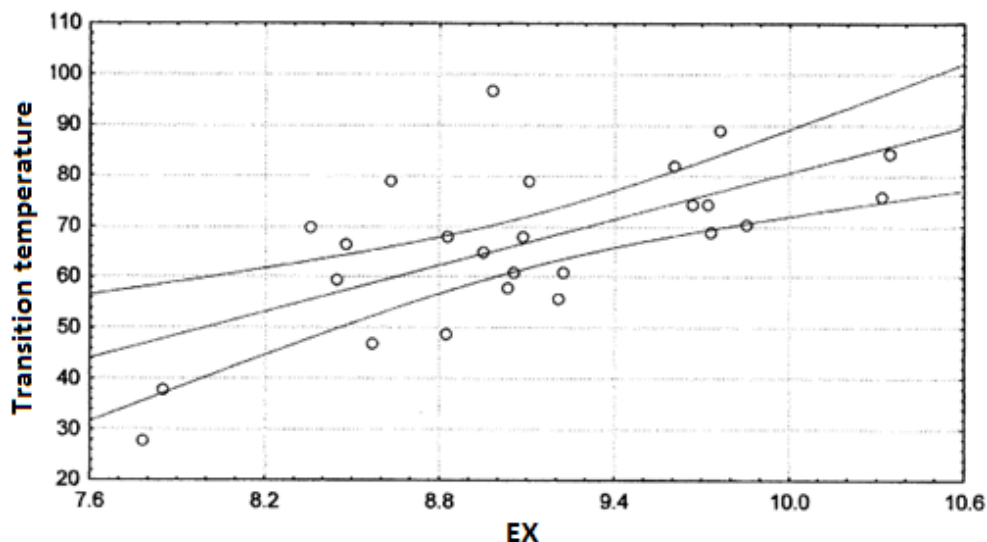


Figure 1. Correlation between the transition temperature and Ex

$$T_z = 167.16 - 384.23 \text{ GLOB} \quad (2)$$

$$R^2 = 0.508 \quad SE = 28.49 \quad F = 12.5 \quad MSE = 164.4$$

Eliminating the values located outside the confidence interval (the two curves), even if, the statistical parameters would improve, is not recommended, as, the application generality of the obtained result would diminish.

As can be seen, the correlation between the transition temperature and the Van der Waals ratio (V^W/S^W) presents very weak correlations, even lower than those between separates of the Van der Waals volume ($R^2=0.442$) and Van der Waals surface ($R^2=0.446$), the vapor dispersion being a lot higher.

$$T_z = 5.45 + 0.17 V^W \quad (3)$$

$$R^2 = 0.442 \quad SE = 22.25 \quad F = 7.73 \quad MSE = 189.9$$

$$T_z = 2.30 + 0.227 S^W \quad (4)$$

$$R^2 = 0.446 \quad SE = 23.13 \quad F = 7.89 \quad MSE = 188.9$$

$$T_z = 872.99 - 1011.61 V^W/S^W \quad (5)$$

$$R^2 = 0.205 \quad SE = 22.1123 \quad F = 3.39 \quad MSE = 221.11$$

In case of correlating the surface of the S^{SF} sferoid, a better correlation can be obtained (R²=0.501), but weaker than in the case of globularity (R²=0.508).

$$T_z = 29.018 - 0.034 S^{SF} \quad (6)$$

$$R^2 = 0.501 \quad SE = 12.82 \quad F = 9.10 \quad MSE = 181.81$$

In these calculations we find the multiple correlation coefficient R² (which for a good correlation should tend to the value of 1, F (the Fisher test value) which, for the statistical significance of correlations, is desired to be as high as possible. S is the explained variance, a statistical indicator commonly used in the study of structure-property relationships as it shows what percentage of the property being analyzed is explained by the variables used in a correlation.

In the case of correlations of transition temperatures with topological indices, low correlation coefficients are also obtained, usually between 0.3-0.45, ²χ, presenting the best correlation of this class of compounds.

$$T_z = 12.776 + 6.872 \text{ } ^2\chi \quad (7)$$

$$R^2 = 0.321 \quad SE = 22.07 \quad F = 6.09 \quad MSE = 200.59$$

Other correlations with over 0.5 were obtained in the case of the correlation between the transition temperature and Gordon (N2), M1, M2 and J3.

$$T_z = -21.420 + 3.420 N2 \quad (8)$$

$$R^2 = 0.431 \quad SE = 32.11 \quad F = 7.60 \quad MSE = 190.69$$

$$T_z = -25.752 + 0.948 M1 \quad (9)$$

$$R^2 = 0.446 \quad SE = 33.05 \quad F = 7.90 \quad MSE = 188.88$$

$$T_z = -33.689 + 0.932 M2 \quad (10)$$

$$R^2 = 0.436 \quad SE = 36.32 \quad F = 7.70 \quad MSE = 190.11$$

$$T_z = 68.023 - 0.119 J3 \quad (11)$$

$$R^2 = 0.222 \quad SE = 3.00 \quad F = 4.00 \quad MSE = 216.14$$

Several multilinear correlations have been made, trying to find those descriptors that are not interleaved and, thus, increase the correlation coefficient. The best result was obtained by the multilinear correlation of the

transition temperature with the topological indices and Van der Waals parameters. Thus, by correlating the transition temperature and ${}^2\chi$, ${}^3\chi$, J^{el} , JD^{rc} , $N2$ (equation 12), a R^2 of 0.720 is obtained, compared to very low coefficients obtained separately.

$$T_z = -782.42 + 144.9 {}^2\chi - 177.8 {}^3\chi + 10185.4 J^{el} - 1119.2 JD^{rc} - 13.37 N2 \quad (12)$$

$$R^2 = 0.720 \quad SE = 15.86 \quad F = 10.49 \quad MSE = 100.31$$

Taking into account the method of calculating the topological indices, we find that the ${}^2\chi$ și J^{el} ones are favorable to the increase of the transition temperature, therefore, there is a flexibility component [Kier and Hall [24]] and a favorable electronic one (J^{el} is the index J calculated for atomic electronegativity). In the case of the above set, the ${}^2\chi$ și ${}^3\chi$ indices are intercorrelated.

Only by correlating the transition temperature with the randic and balaban indices, does the R^2 correlation coefficient decrease.

$$T_z = -1722 + 86.91 \chi^{el} + 407022 J^{Rw} - 225149 J^{rc} - 936228 J^{el} \quad (13)$$

$$R^2 = 0.704 \quad SE = 12.63 \quad F = 6.72 \quad MSE = 108.45$$

As randic indices encode information about the size and branching of molecules, it is interesting to see what happens if the mentioned indices are replaced by the van der Waals report, thus, obtaining function 14.

$$T_z = -7196 + 8997 V^W/S^W - 1270 J2 - 184124 J3 - 225.7 J^{el} \quad (14)$$

$$R^2 = 0.615 \quad SE = 15.34 \quad F = 4.41 \quad MSE = 121.29$$

There is a decrease in the correlation coefficient at 0.615, which denotes an inverse effect from that of the column liquid crystals, where there was an increase in the correlation coefficient following the involvement of the Van der Waals report [23].

A main purpose of QSPR is to detect a mathematical link between the surveyed property and the molecular descriptors derived from the structure of the molecule [25].

Opposed to columnar liquid crystals [23], liquid crystals from the benzylideneaniline group present weaker mathematical models. It can be concluded that the linear chemical structure of these compounds is not that stable when compared to the branched one of columnar liquid crystals.

CONCLUSIONS

The information obtained from the molecules of the benzylideneanilide liquid crystals is insufficient, as the property taken into account also depends on other factors not covered by the considered molecular descriptors. These molecules fall into the nematic liquid crystals, which have the main characteristic of orienting themselves along a straight line called a steering axis, being formed by relatively long molecules without distinct branches. This is also evident from the fact that the best correlation is given by the Ex transition ($R^2 = 0.40$), a ratio that can be assimilated in a first approximation with a length. It is assumed that other parameters such as the average angle of the molecules with the reference axis, the degree of ordering and a series of parameters describing the intermolecular interactions of physical nature (electrostatic) taking into account the polarity of the compounds can be considered. Although the correlation between the transition temperature and Van der Waals parameters, respectively topological indices, give lower correlation coefficients than with column liquid crystals. If multiple correlations are achieved, higher correlation coefficients are obtained. This study is very important as it takes a new, unique approach in regards to the structure of liquid crystals in the benzylideneaniline class and the correlation degree between transition temperature, topological indices and Van der Waals parameters, respectively. An improvement upon mathematical models as a result of multiple regressions between transition temperature – topological indices – Van der Waals parameters can also be observed.

EXPERIMENTAL SECTION

The used method of determining the liquid crystal transition temperature allows a highlight of the type of texture, the type of phase, and the transition temperature of the liquid crystal samples using the polarizing microscope. Study cells contain nematic crystals (4-cyano-phenyl-4-pentylbenzoate). Each cell is made of glass walls on which a transparent conductive layer of In_2O_3 has been deposited. Measurements require the use of a heating device and a one for stabilizing and measuring the temperature. As heating device, an aluminum electric furnace having dimensions of $5 \times 6 \text{ cm}^2$ and 1 cm thickness, was used. Heating of the furnace is made by means of an electrical resistance, the heating current being controlled by the temperature stabilizer. The furnace is provided with a seat for fixing the sample. The temperature transducer that fits through a furnace inlet and has its ends connected to the temperature-determining device is fixed on the cell. The

furnace has outputs for supplying the electrical resistance, allowing the application of an electric field to the samples. Both the furnace and lid are equipped with windows for visualising samples and optical measurements. After the sample has been placed inside, the furnace is connected to the microscope and heated to 70-80°C.

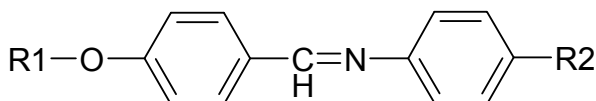


Figure 4. General structure of the benzylideneaniline class

Table 2. The most important representatives of the benzylideneaniline class

Comp.	R1	R2	T _{transition}
t01	CH ₃	CH ₃	38
t02	C ₂ H ₅	CH ₃	79
t03	C ₃ H ₇	CH ₃	49
t04	C ₄ H ₉	CH ₃	68
t05	C ₅ H ₁₁	CH ₃	58
t06	CH ₃	C ₂ H ₅	28
t07	C ₂ H ₅	C ₂ H ₅	70
t08	C ₃ H ₇	C ₂ H ₅	66,5
t09	C ₄ H ₉	C ₂ H ₅	65
t10	C ₅ H ₁₁	C ₂ H ₅	61
t11	CH ₃	C ₃ H ₇	59,5
t12	C ₂ H ₅	C ₃ H ₇	97
t13	C ₃ H ₇	C ₃ H ₇	68
t14	C ₄ H ₉	C ₃ H ₇	82
t15	C ₅ H ₁₁	C ₃ H ₇	74,5
t16	CH ₃	C ₄ H ₉	47
t17	C ₂ H ₅	C ₄ H ₉	79
t18	C ₃ H ₇	C ₄ H ₉	56
t19	C ₄ H ₉	C ₄ H ₉	74,5
t20	C ₅ H ₁₁	C ₄ H ₉	69
t21	CH ₃	C ₅ H ₁₁	61
t22	C ₂ H ₅	C ₅ H ₁₁	89
t23	C ₃ H ₇	C ₅ H ₁₁	70,5
t24	C ₄ H ₉	C ₅ H ₁₁	84,5
t25	C ₅ H ₁₁	C ₅ H ₁₁	76

When this temperature is reached, the heating system is decoupled and monitored during sample cooling: the temperature at which the crystal transitions from the liquid state to the mesophase (transition temperature), the transition temperature F , the solid state and the type of texture that occurs in this phase.

The results of the simple linear correlations of the transition temperatures with the calculated molecular descriptors are presented in the following tables, the first column being the independent variable (topological index or Van der Waals parameter), the second, the R correlation coefficient (which, for good correlation, must tend to the value of 1) and, in the third column, is the Fisher test value for the statistical significance of the correlations, which is desirable to be as high as possible. All formulas were drawn in the Hyperchem program, then optimized by molecular modeling, calculating free energies. In order to refine the calculations, an ab initio calculation was chosen, as, in the ab initio variants, the different energy components of the molecules, including the electron-based component, can be calculated. Topological indices and Van der Waals parameters were calculated using the formulas mentioned above. Linear and multiple correlations were performed with Statistics 7.0 and OriginPro8.

Table 3. Topological indices for benzylideneanilines

Nr	W	P	N2	M1	M2	$^1\chi$	$^2\chi$	$^3\chi$	J	J2	J3
b1	616	40	21	82	91	8.28	6.42	3.85	1.59	0.23	0.0251
b2	733	43	22	86	95	8.78	6.80	4.22	1.57	0.21	0.0227
b3	872	45	23	90	99	9.28	7.15	4.49	1.55	0.20	0.02
b4	1030	46	24	94	103	9.78	7.51	4.58	1.53	0.18	0.017
b5	1208	48	25	98	107	10.28	7.86	4.83	1.50	0.17	0.0149
b6	729	42	23	86	96	8.81	6.59	3.97	1.58	0.22	0.0225
b7	864	44	24	90	100	9.31	6.97	4.18	1.57	0.20	0.0199
b8	1018	46	25	94	104	9.81	7.32	4.45	1.55	0.19	0.0176
b9	1192	48	26	98	108	10.31	7.68	4.70	1.53	0.18	0.0155
b10	1387	50	27	102	112	10.81	8.03	4.95	1.50	0.16	0.0138
b11	864	44	24	90	100	11.31	6.97	4.18	1.57	0.20	0.0201
b12	1014	46	25	94	104	9.81	7.35	4.38	1.55	0.19	0.0179
b13	1184	48	26	98	108	10.31	7.70	4.65	1.54	0.18	0.0159
b14	1375	50	27	102	112	10.81	8.06	4.90	1.52	0.17	0.0142
b15	1588	52	28	106	116	11.31	8.41	5.15	1.50	0.16	0.0127
b16	1018	46	25	94	104	11.81	7.32	4.45	1.55	0.19	0.018
b17	1184	48	26	98	108	10.31	7.70	4.65	1.54	0.18	0.0161
b18	1317	50	27	102	112	10.81	8.06	4.92	1.52	0.17	0.0144
b19	1580	52	28	106	116	11.31	8.41	5.17	1.51	0.16	0.0129
b20	1812	54	29	110	120	11.81	8.76	5.42	1.49	0.15	0.0116
b21	1192	48	26	90	108	10.31	7.68	4.70	1.53	0.18	0.016
b22	1375	50	27	102	112	10.81	8.06	4.90	1.52	0.17	0.0145
b23	1580	52	28	106	116	11.31	8.41	5.17	1.51	0.16	0.013
b24	1808	54	29	110	120	11.81	10.38	5.42	1.49	0.15	0.0118
b25	2060	56	30	114	124	12.31	10.97	5.67	1.48	0.14	0.0106

Table 4. Van der Waals parameters for benzylideneanilines

	S ^W	V ^W	V ^{SF}	S ^{SF}	V ^{EL}	E _x	E _y	E _z	GLOB	GL1	V ^W /S ^W
b1	215.2	266.4	2024.7	774.0	645.1	7.8	6.7	2.9	0.31	0.32	0.81
b2	232.6	289.0	2692.7	936.0	695.1	8.6	6.6	2.9	0.28	0.26	0.81
b3	250.0	310.7	2875.0	977.8	761.2	8.8	7.1	2.9	0.27	0.26	0.80
b4	267.1	333.1	2881.8	979.3	923.0	8.8	8.6	2.9	0.27	0.32	0.80
b5	283.3	355.7	321.7	1053.4	1005.5	9.0	9.1	2.9	0.26	3.13	0.79
b6	233.4	290.9	1973.3	760.8	928.3	7.8	7.3	3.9	0.31	0.47	0.80
b7	249.4	312.8	2443.9	877.4	1055.5	8.4	7.8	3.9	0.29	0.43	0.79
b8	267.0	334.9	2552.9	903.3	1169.1	8.5	8.5	3.9	0.28	0.46	0.79
b9	283.5	356.7	3073.5	1022.3	1266.5	8.9	9.0	3.7	0.26	0.41	0.79
b10	300.5	378.5	3735.6	1164.3	1392.6	9.0	9.6	3.8	0.25	0.37	0.79
b11	250.2	313.0	2522.8	896.2	1069.9	8.4	7.8	3.9	0.28	0.42	0.8
b12	267.4	334.9	3032.3	1013.1	1189.1	8.9	8.4	3.8	0.27	0.39	0.79
b13	283.5	356.8	3138.9	1036.7	1299.9	9.1	8.9	3.8	0.26	0.41	0.79
b14	301.5	378.9	3710.6	1159.1	1459.3	9.6	9.5	3.8	0.25	0.39	0.79
b15	318.1	401.3	4347.2	1288.1	1576.5	9.6	18.1	3.8	0.24	0.36	0.79
b16	266.8	334.9	2633.3	922.1	1269.4	8.6	8.3	4.2	0.28	0.48	0.79
b17	285.7	356.8	3161.2	1841.7	1419.8	9.1	8.8	4.2	0.26	0.45	0.8
b18	300.4	378.9	3478.0	1110.1	1522.4	9.2	9.4	4.2	0.25	0.44	0.79
b19	318.6	400.8	4164.3	1251.7	1705.5	9.7	9.9	4.2	0.24	0.41	0.79
b20	333.9	422.	4925.6	1399.9	1780	9.7	10.5	4.1	0.23	0.36	0.79
b21	282.6	356.9	3281.5	1067.9	1463.4	9.2	8.6	4.4	0.26	0.45	0.79
b22	301.6	379.1	3894.9	1197.1	1631.0	9.7	9.1	4.4	0.24	0.42	0.79
b23	316.6	400.3	4006.2	1219.8	1176.5	9.8	9.8	4.4	0.24	0.29	0.79
b24	334.1	423.6	4696.9	1356.3	1936.2	10.	10.4	4.3	0.23	0.41	0.79
b25	352.6	445.7	5531.3	1512.5	2002.7	10.3	10.9	4.2	0.22	0.36	0.79

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