CLUSTER AND PRINCIPAL COMPONENT ANALYSIS OF THE SOLVENT EFFECTS ON THE C=O STRETCHING FREQUENCY OF ACETOPHENONE

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ABSTRACT

The solvatochromic shift of the C=O stretching frequency of acetophenone is studied by cluster (CA) and principal component analysis (PCA) confirming our previous results about the determining contributions to the polarity, polarizability, and electrophilicity of the medium on this effect. It is shown that the used combination of Varimax mode of PCA and multiple regression (apportioning modeling) makes it possible to obtain absolute principal component scores (APCS), which include the solvent parameters describing definite solute–solvent interactions. The adequateness of the suggested chemometric model is checked by "reverse" CA of 25 solvents as objects with respect to the APCS calculated.

Key Words: IR-spectral data of acetophenone; Solvent effects; Cluster and principal component analysis

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INTRODUCTION

The solvatochromic shift of ν(C=O) band of acetophenone has been used repeatedly to provide information about solute–solvent interactions and the factors determining the sensitivity of carbonyl frequencies to the solvent effects. It is selected as the standard by the development of the so-called Bellamy–Hallam–Williams plot (1,2) and the method is successfully applied for identification of X=O group bands (3–5). Likewise, the measurement of the solvent-induced changes of ν(C=O)-acetophenone is used to quantify the electophilicity of the medium (6).

In our previous papers (7–9) we have investigated the applicability of the solvent parameters introduced by Koppel and Palm (10) and by Kamlet, Abboud and Taft (11) to describe the solvatochromic shift of C=O frequency of acetophenone by means of multiple linear regression analysis. Two peculiarities are characteristic of our results.

1. The best-fit regression equation describing the solvatochromic effects of ν(C=O)-acetophenone by Koppel–Palm's parameters (8) includes the cross-term $(\varepsilon - 1)(n^2 - 1)/(2\varepsilon + 1)(2n^2 + 1)$ instead of $(\varepsilon - 1)/(2\varepsilon + 1)$. Thus, confirming the conclusion reported in Ref. (12) that the first one has predominant contribution to the account of the IR-band shift induced by nonspecific solute–solvent interactions.
2. The treatment of the ν(C=O)-acetophenone in various solvents by means of Kamlet–Abboud–Taft's parameters (9) demonstrates the presumed effects of the medium polarity–polarizability (π^*-parameter) and electrophilicity (α-parameter) supporting the results published in Ref. (13). However, the analysis of the data with an extended set of regressors shows that nonspecific solute–solvent interactions can be accurately described by the combination of π^*- and $(n^2 - 1)/(2n^2 + 1)$-terms. This conclusion is in agreement with the correction of the π^*-scale by the so-called δ-term compensating the polarizability of the solvent (14,15).

In this paper the solvatochromic shift of the C=O stretching frequency of acetophenone is characterized by means of cluster (CA) and principal component analysis (PCA). The following scheme of investigation is applied.

CA and PCA are subsequently performed using the parameters describing the effects of the medium as variables. CA has helped to find out groups of similarity among the parameters utilized as solvent characteristics. This approach made it possible to eliminate some closely correlated parameters and to reduce the dimension of the parameter space. PCA was carried out to treat data for ν(C=O)-acetophenone of 25 solvents. The independent regressors (absolute principal components scores, APCS) obtained were applied in a multiple regression (MR) procedure known as apportioning model (PCA/MR) (16) conventionally

used in environmetrical studies. As the dependent regression function $\Delta \nu_{\text{solv}}/\nu$ (C=O) was selected. The adequateness of the suggested model has been checked by comparison between the calculated and the experimentally found responses. Furthermore, CA was applied again, investigating the solvents as objects and APCS values from PCA/MR model as variables.

EXPERIMENTAL

The values of solvent parameters summarized in Refs. (9,17) are used as basic regressors. Their origin and significance are explained in Chap. 7 of Ref. (17). The symbols to follow are coincide to the list of abbreviations in the same paper.

Parameters $Y2$, $P2$ and YP originate from the nonlinear model of Buckingham about the solvatochromic shift of vibrational frequencies (19). The data of ν_{solv}(C=O)-acetophenone from Ref. 9 are interpreted in order to compare and analyze the results obtained by multiple linear regression analysis. In the same study, it is shown that the most adequate response to characterize the solvatochromic shift of IR-characteristic frequencies is

$$\frac{\Delta \nu_s}{\nu_s} = \frac{\nu_g - \nu_s}{\nu_s}$$

where ν_g and ν_s are the corresponding frequencies in gas phase and in the given solvent, respectively.

As already mentioned, three major multivariate statistical approaches were used.

Cluster Analysis

The treatment of the input data was carried out by the Z-transformation with Euclidean distance between the objects as similarity measure. The hierarchical clustering algorithms chosen were single, average, centroid, and Ward's linkage. The cluster significance was checked by the Sneath index (20).

Principal Components Analysis

We have used a variation of the traditional PCA called *Varimax rotation* where a rearrangement of the PC loadings for each variable is observed in such a way that the bigger ones get bigger and the smaller ones get smaller. It helps in distinguishing the content of each orthogonal principal component and its better interpretation (20).

Table 1. Input Data

	ε	Y	Y2	θ	n	P	P2	YP	π*	E	B	α	β	E_T^{30}	Z	S	DN	AN	G	ν_{AcPh}	$(\Delta\nu/\nu)$
Gas phase											0					−0.5560			0	1709	0.000
n-hexane	1.890	0.1862	0.0347	0.1014	1.3751	0.1863	0.035	0.035	−0.081	0.00	0	0.00	0.00	30.9		−0.3370	99.0	0.0	44	1697	0.007
Cyclohexane	2.023	0.2027	0.0411	0.1116	1.4266	0.2042	0.042	0.041	0.000	0.00	0	0.00	0.00	31.2		−0.3240			49	1696	0.008
Benzene	2.284	0.2306	0.0532	0.1297	1.5011	0.2276	0.052	0.052	0.590	2.10	48	0.00	0.10	34.5	54.0	−0.2150	0.1	8.2	80	1690	0.011
Toluene	2.380	0.2396	0.0574	0.1357	1.4961	0.2261	0.051	0.054	0.540	1.30	58	0.00	0.11	33.9		−0.2370			74	1691	0.011
Chlorobenzene	5.708	0.3792	0.1438	0.2536	1.5241	0.2343	0.055	0.089	0.710	0.00	38	0.00	0.07	37.5		−0.1820				1688	0.012
Bromobenzene	5.400	0.3729	0.1390	0.2467	1.5597	0.2443	0.060	0.091	0.790	0.00	40	0.00	0.06	37.5	59.2	−0.1640				1689	0.012
Carbon tetrachloride	2.238	0.2261	0.0511	0.1267	1.4601	0.2150	0.046	0.049	0.294	0.00	0	0.00	0.00	32.5		−0.2450	0.0	8.6	69	1692	0.010
Tetrachloroethylene	2.500	0.2500	0.0625	0.1428	1.5053	0.2288	0.052	0.057	0.280	0.00	0	0.00	0.00	31.9		−0.2630				1693	0.009
Trichloroethylene	3.409	0.3081	0.0949	0.1865	1.4773	0.2204	0.049	0.068	0.530	0.00	0	0.00	0.00	35.9						1688	0.012
Chloroform	4.806	0.3587	0.1286	0.2320	1.4459	0.2105	0.044	0.075	0.760	3.28	14	0.34	0.00	39.1	63.2	−0.2000		23.1	106	1683	0.015
1,2-Dichloroethane	10.360	0.4309	0.1857	0.3231	1.4448	0.2101	0.044	0.091	0.807	0.00	40	0.00	0.00	41.9	63.4	−0.1510	0.0	16.7	95		
Dichloromethane	9.080	0.4217	0.1778	0.3085	1.4242	0.2034	0.041	0.086	0.800	2.70	23	0.22	0.00	41.1	64.7	−0.1890		20.4	100	1685	0.014
Carbon disulfide	2.641	0.2612	0.0682	0.1507	1.6319	0.2629	0.069	0.069	0.514	0.00	0	0.00	0.00	32.6		−0.2400			74		
Diethyl ether	4.335	0.3449	0.1189	0.2186	1.3526	0.1780	0.032	0.061	0.270	0.00	280	0.00	0.47	34.6		−0.2770	19.2	3.9	64	1694	0.009
Di-i-propyl ether	3.970	0.3322	0.1104	0.2070	1.3679	0.1837	0.034	0.061	0.270	0.00	293	0.00	0.49	34.0						1694	0.009

Di-n-buthyl ether	3.060	0.2893	0.0837	0.1715	1.3992	0.1948	0.038	0.056	0.240	0.00	285	0.00	0.46	33.4	60.1	−0.2860			61	1694 0.009
Tetrahydrofuran	7.320	0.4041	0.1633	0.2837	1.4214	0.2024	0.041	0.082	0.580	0.00	287	0.00	0.55	37.4	58.8		20.0	8.0		1690 0.011
1,4-Dioxane	2.209	0.2231	0.0498	0.1247	1.4224	0.2028	0.041	0.045	0.550	4.20	237	0.00	0.37	36.0		−0.1790	14.8	10.8	86	1688 0.012
Ethoxybenzene											0			36.4	58.9				89	
Anisole	4.330	0.3447	0.1188	0.2185	1.5179	0.2325	0.054	0.080	0.730	1.40	155	0.00	0.22	37.2		−0.2140				1689 0.012
Acetone	20.070	0.4635	0.2149	0.3906	1.3588	0.1804	0.033	0.084	0.720	2.10	224	0.07	0.48	42.2	65.5	−0.1748	17.0	12.5		
Butanone	18.500	0.4605	0.2121	0.3828	1.3788	0.1876	0.035	0.086	0.670	2.00	209	0.05	0.48							
Acetonitrile	36.200	0.4796	0.2300	0.4431	1.3442	0.1749	0.031	0.084	0.850	5.20	160	0.15	0.31	46.0	71.3	−0.1039	14.1	18.9	93	1687 0.013
Benzonitrile	25.200	0.4708	0.2217	0.4117	1.5289	0.2357	0.056	0.111	0.900	0.00	155	0.00	0.41	42.0	65.0		11.9	15.5		1686 0.014
Pyiridine	12.300	0.4414	0.1948	0.3416	1.5095	0.2301	0.053	0.102	0.870	0.00	472	0.00	0.64	40.2	64.0	−0.1970	33.1	14.2	94	1687 0.013
Triethylamine	2.420	0.2432	0.0591	0.1381	1.4010	0.1955	0.038	0.048	0.140	0.00	650	0.00	0.71	33.3		−0.2850	61.0		62	1693 0.009
Nitromethane	38.600	0.4808	0.2312	0.4484					0.848	5.10	65			46.3	71.2	−0.1340	2.7	20.5	99	
Nitrobenzene	35.740	0.4793	0.2297	0.4420	1.5562	0.2433	0.059	0.117	1.010	0.00	67	0.00	0.39	42.0		−0.2180	4.4	14.8	100	1681 0.017
Dimethylsulfoxide	49.000	0.4848	0.2351	0.4674	1.4770	0.2203	0.049	0.107	1.000	3.20	362	0.00	0.76	45.0	71.1		29.8	19.3		1682 0.016
Methanol	33.620	0.4780	0.2285	0.4369	1.3288	0.1690	0.029	0.081	0.600	14.90	218	0.98	0.62	55.5	83.6	0.0499	19.0	41.3		1680 0.017
Ethanol	24.300	0.4698	0.2207	0.4084	1.3611	0.1812	0.033	0.085	0.540	11.60	235	0.86	0.77	51.9	79.6	0.0000	31.5	37.1		1680 0.017
Water	80.100	0.4907	0.2408	0.5036	1.3330	0.1706	0.029	0.084	1.090			0.18	1.13	63.1	94.6	0.1540	18.0	54.8		

Apportioning Model by PCA/MR

The Thurston and Spengler approach (16) (combination of PCA and MR) has been used to model the response function $\Delta\nu_S/\nu_S$ with respect to the identified independent regressors, APCS being in fact groups of correlated solvent parameters. Finally, clustering of the objects of interest (solvent systems) was performed but the APCS values were involved as variables.

RESULTS AND DISCUSSION

CA of the input data set (Tab. 1) is presented in Figure 1 as a dendogram plot. The results obtained suggest the following interpretation.

The first and the second clusters (1,2) reflect the expected levels of similarity between the parameters characterizing the polarizability and polarity of the medium, respectively, according to the Onzager's reaction field theory (18,19). The other two subsets (3,4) are connected with the polarity of the solvent: the first one (3) includes π^*- and G-scales; the second one (4) contains E_T^{30}- and S empirical-parameters. The cluster of the solvent Lewis acidity (5) combines α- and AN-parameters. The corresponding subsets for Lewis basicity contain B- and β-parameters (6) and the donor number (DN) as a separate cluster.

The obtained classification could not be characterized as quite successful. Along with the polarity parameters, the fourth cluster includes the E-term of Koppel–Palm. In the same way the Z- and YP-parameters describing the nonspecific ability of the solvent fall into subsets of the specific solute–solvent interactions (Fig. 1). Two basic reasons could explain these defects.
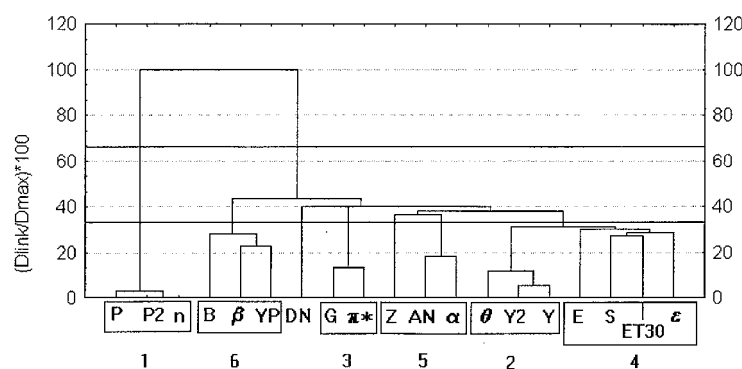

Figure 1. Dendrogram plot of the solvent parameters as objects (levels of significance 33.3 and 66.6% of D_{max}).

1. The investigated data set is limited to the solvents with well-known values of ν(C=O)-acetophenone.
2. The various solvent property scales correlate with each other when the considerations are restricted to a set of selected (mainly non-hydrogen bonding or hydrogen bonding) solvents (see, e.g. (21)). Otherwise, any parameter can be examined as a linear combination of corresponding parameters describing the universal and specific solvent effects of the medium. For example, Gutmann's AN of nonprotonic solvents correlates well with π^* and of protonic solvents with a linear combination of π^* and α (21,22). This could explain the combination of parameter(s) reflecting opposite solute–solvent interactions and, in particular, the appearance of the solvent polarity depending Z- and YP-scales in the fifth and sixth clusters, respectively (Fig. 1).

Taking into account the results stated above, we treated only definite parameters from the variety of groups of similarity. The parameters DN, AN, Z, S, E_T^{30} and G are not considered anymore. Due to the limited number of input data their application could lead to unreliable classification results. In view of this, the next level of interpretation includes the following parameters: $(P, P2, n)$, (π^*), $(\theta, Y, Y2)$, (B, β, YP), (ε, E), (α). A correlation analysis within each group of variables was additionally carried out and parameters with high correlation coefficients were excluded from the CA. Finally, only seven variables remained: P, θ, π^*, E, α, B, and β. The θ-parameter of the dielectric saturation (18) was preferred to Y for reasons pointed out in Ref. (23). Additionally, a next cluster analysis was performed in order to check the independence of the chosen parameters (Fig. 2).
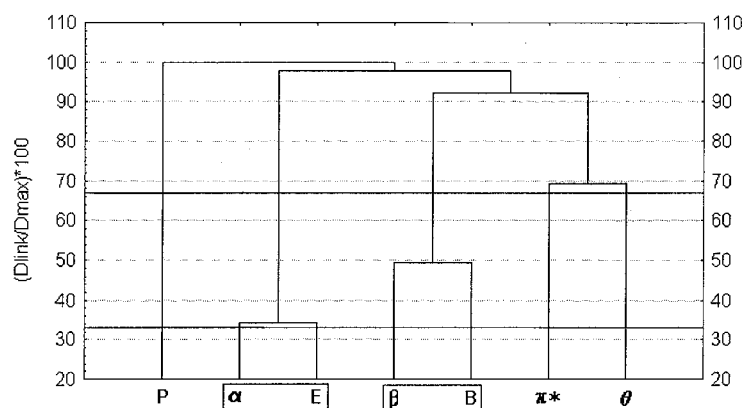

Figure 2. Dendrogram plot of solvent parameters selected by correlation analysis.

Table 1. Normalized Factor Scores of the Investigated Solvents

Solvent	PC 1	PC 2	PC 3	PC 4
n-hexane	−0.450	−1.305	−1.051	1.561
Cyclohexane	−0.284	−1.310	−0.947	0.612
Benzene	0.200	0.662	−0.530	−1.189
Toluene	0.051	−0.665	−0.489	−1.001
Chlorobenzene	−0.349	0.340	−0.744	−.786
Bromobenzene	−0.237	0.314	−0.689	−1.400
Carbon tetrachloride	−0.239	−0.859	−0.937	−0.062
Tetrachloroethylene	−0.117	−0.937	−0.852	−0.711
Trichloroethylene	−0.343	0.163	−1.007	−0.184
Chloroform	0.764	0.161	−1.101	−0.305
Dichloromethane	0.130	0.896	−1.215	0.627
Diethyl ether	−0.792	−0.284	0.585	1.737
Di-*i*-propyl ether	−0.701	−0.436	0.723	1.348
Di-*n*-butyl ether	−0.500	−0.820	0.765	0.618
Tetrahydrofuran	−0.694	0.338	0.805	0.536
1,4-Dioxane	0.306	−0.825	0.503	−0.463
Anisole	−0.056	−0.044	−0.008	−1.250
Acetonitrile	−0.214	1.888	−0.496	2.314
Benzonitrile	−0.657	1.453	0.105	−0.513
Pyridine	−0.546	0.627	1.740	−1.150
Triethylamine	−0.386	−1.663	2.631	−0.213
Nitrobenzene	−0.652	1.845	−0.255	−0.683
Dimethylsulfoxide	−0.408	1.712	1.334	−0.228
Methanol	3.384	0.296	0.342	0.597
Ethanol	2.791	0.104	0.789	0.183

Table 2. Varimax Normalized Loadings of Four Principal Components. Significant Loadings > 0.70 (Marked Cells)

Solvent Parameter	PC 1	PC 2	PC 3	PC 4
θ	0.298	0.902	0.238	0.094
P	−0.395	0.208	−0.233	−0.854
π^*	0.071	0.883	0.016	−0.402
E	0.943	0.201	0.104	0.172
B	−0.035	0.002	0.982	0.092
α	0.956	0.146	0.048	0.180
β	0.225	0.263	0.910	0.141
% Total variance	30.1	27.4	25.2	14.1

Table 3. Results of the Multiple Regression Analysis: ($\Delta\nu/\nu = \sum_{i=1}^{4} b_i \cdot APCS_i$); $r = 0.998$

APCS	b_i	Statistical Error of b_i	Significance of b_i
APCS 1	0.0017	0.0002	Sign.
APCS 2	0.0021	0.0002	Sign.
APCS 4	−0.0009	0.0000	Sign.

Using the Varimax rotation mode, principal components analysis of the solvents is carried out with respect to seven variables (solvent parameters in Fig. 2). The factor scores of the data set are presented in Table 2. Table 3 shows the factor loading values of four principal components explaining over 95% of the total variance.

From the factor loadings in Table 3 it could be seen that the PC 1 is formed dominantly by E and α variables, PC 2 – by θ- and π^*-variables, PC 3 – by B- and β-variables, and PC 4 – by P-variable. The results obtained are remarkable by the fact that each PC includes solvent parameters describing a definite solvent effect. As a rule, the factors obtained by the use of PCA include linear combination of solvent parameters reflecting various solute–solvent interactions. Thus, it is accepted that they do not possess a precise physical meaning (24). Our multivariate statistical approach overcomes this contradiction.

The next step of the multivariate statistical treatment is multiple regression, using the results from PCA. The APCS are calculated as independent variables (16). The dependent variable is the response function $\Delta\nu_s/\nu_s$-(acetophenone) of all 25 solvents in consideration. The regression results are presented in Table 4.

The regression model obtained is of the type:

$$\Delta\nu_S/\nu_S = (0.0017 \pm 0.0002)\,\text{APCS-1} + (0.0021 \pm 0.0002)\,\text{APCS-2}$$
$$- (0.0009 \pm 0.0000)\,\text{APCS-4} \tag{1}$$

The independent variable APCS 3 is statistically insignificant, therefore, it is excluded from Equation (1). This result confirms the conclusion obtained on the basis of the multiple regression analysis data that acetophenone does not possess an effective electrophilic center (8,9). In Figure 3a the calculated responses from the regression model are compared with the experimentally obtained ones. As seen, there is a good correlation between two sets of results that is a proof about the adequateness of the model. The comparison of the correlation with our previous results (Fig. 3b) obtained by multiple linear regression analysis (8) demonstrates relatively better fitness of the APCS regression model. Finally, a clustering of the solvents is performed to compare the links of similarity, using empirical solvent parameters (Tab. 1) with the alternative results obtained by means of APCS. This
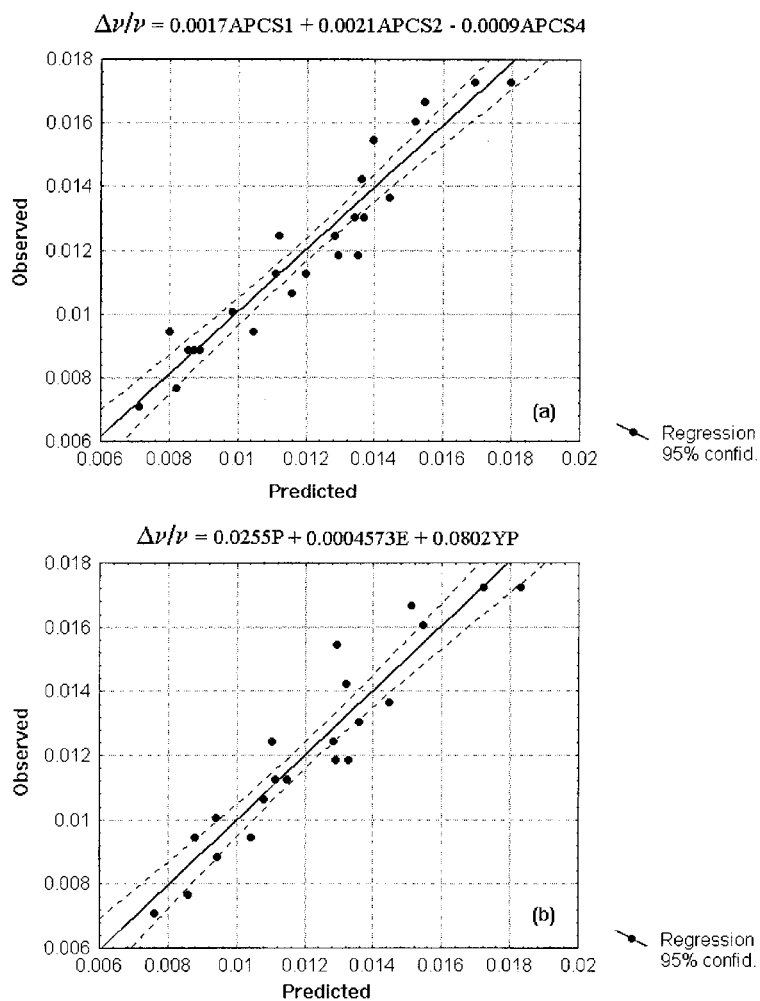
$$\Delta\nu/\nu = 0.0017\text{APCS1} + 0.0021\text{APCS2} - 0.0009\text{APCS4}$$

$$\Delta\nu/\nu = 0.0255\text{P} + 0.0004573\text{E} + 0.0802\text{YP}$$

Figure 3. The comparison of the calculated and experimental obtained results of the $\Delta\nu_{solv}$ (C=O)-acetophenone according to: PCA/MR- (a) and MR-analysis (8) (b).

conditionally named "reverse" clustering also enables to verify the reliability and the adequateness of the suggested chemometric methods. The dendrograms of both types of clustering are presented in Figures 4 and 5.

The analysis on the empirical parameters forms the following groups of similarity (Fig. 4).

Subclass (1) contains solvents with typical nonspecific solvent effect; sub-classes (2) and (3) comprise aromatic hydrocarbons that are weak π-bases. The
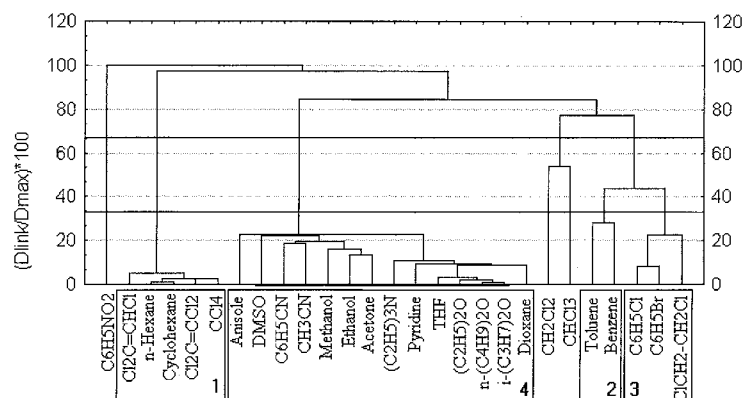
Figure 4. Dendrogram plot of solvents as objects with respect to the solvent parameters shown in Figure 2.

electron-acceptor (-I) effect of the halogeno-substituents reduces their nucleophilic ability, thus determining the observed splitting into two subgroups.

The largest class (4) includes the electron-pair donors. Two independent units form chloroform and dichloromethane that should be explained by the weak hydrogen-bond donor effect of the first one and by the relatively high polarity of the second compound.

As a defect of this classification we can point out the separation of nitrobenzene as a self-dependent solvent and the inclusion of 1,2-dichloroethane in cluster (3).
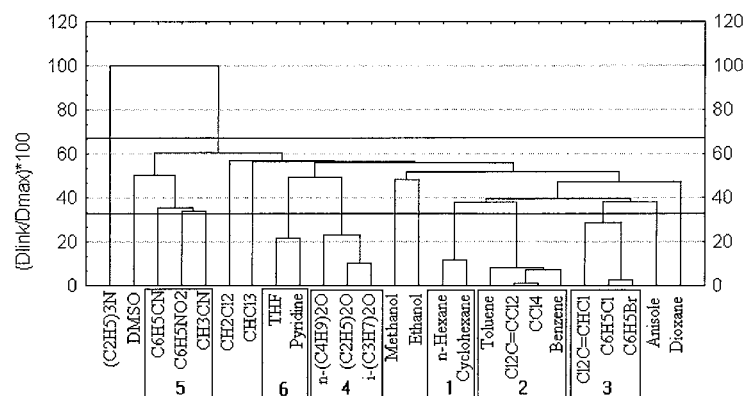

Figure 5. Same objects clustering as in Figure 4 with respect to APCS calculated.

The clustering on APCS leads to the following re-arrangements (Fig. 5).

1. The hydrocarbons and their halo-derivatives are located in three sub-classes differentiated in accordance with the polarity effect: subset (1) includes typical nonspecifically acting alkanes; subset (2) also contains nonpolar compounds with zero (or close to zero) dipole moment (μ); and subset (3) contains solvents described by $2.5 < \mu < 5.5^*$.

2. Subclasses (4) and (5) divide the oxygen- and nitrogen containing electron-pair donors, respectively. Belonging to (5) N-bases are characterized by high polarity (i.e., $11.5 \leq \mu \leq 15.5$) which explains the incorporation of nitrobenzene in this subgroup. The stronger Luis basicity and the intermediate μ-values of tetrahydrofuran ($\mu = 5.8$) and pyridine ($\mu = 7.9$) are the reasons for their limitation in subgroup (6). In the same way dimethylsulfoxide is eliminated from (4) because of its higher polarity ($\mu = 13$). Triethylamine is also an independent representative being both a strong electron-donor and a low polarity solvent ($\mu = 2.9$). However, the assumptions stated in the following text do not explain the removal of 1,4-dioxane and anisole from subclass (4).

3. The clustering on APCS isolates the hydrogen bonding solvents as methanol and ethanol without integrating them on a level of significance 33.3% of D_{max} (Fig. 5). In accordance with the alternative results (Fig. 4) chloroform and dichloromethane form single subsets.

The confrontation of both approaches discussed previously makes clear their specificity. The clustering on the empirical parameters differentiates more commonly the nonspecific and specific effects whereas the grouping by PCA underlines and grades the polarity of the solvents. In this sense the arrangement obtained by means of APCS is close to the classification received by Chastrette et al. (25). In this comprehensive work a combination of PCA and nonhierarchical cluster analysis is used but the clustering is carried out by means of principal components defined by physicochemical constants and HOMO and LUMO calculated energies. The empirical scales discussed previously are not utilized. According to our results their inclusion should provoke a supplementary distinction of the solvent effects.

CONCLUSIONS

1. By the use of PCA/MR multivariate statistical approach the solvatochromic shift of ν(C=O)-acetophenone is studied and our previous

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$^*\mu \cdot 10^{30}$ C.m. According to data presented in Ref. (17; Tab. A-1, p. 408) and Ref. (25; Tab. 1).

conclusion about the determining contributions to the polarity, polariz-ability, and electrophilicity of the medium on this effect are confirmed. The comparison of the applied approach with the results obtained by multiple linear regression analysis demonstrates relatively better fitness of the APCS regression model.

2. The combination of Varimax mode and multiple regression (apportion-ing modeling) applied to this study makes it possible to reveal fac-tors (APCS), which include the solvent parameters describing definite solute–solvent interactions. In this way APCS regressors are loaded with a certain physical meaning.

3. The adequateness of the suggested chemometric model is checked by "reverse" cluster analysis of 25 solvents as objects with respect to the calculated APCS. A more precise linkage of the solvents is obtained as compared to the clustering, using empirical solvent parameters.

ABBREVIATIONS

ε dielectric constant

Y $\left(\frac{\varepsilon-1}{2\varepsilon+1}\right)$; Koppel–Palm's parameter of solvent polarity

$Y2$ $\left(\frac{\varepsilon-1}{2\varepsilon+1}\right)^2$

θ $\frac{3\varepsilon \log \varepsilon}{\varepsilon \log \varepsilon - \varepsilon + 1} - \frac{6}{\log \varepsilon - 2} - 2$; reaction field parameter of Block and Walker (18)

n refractive index

P $\left(\frac{n^2-1}{2n^2+1}\right)$; Kopel–Palm's parameter of solvent polarizability

$P2$ $\left(\frac{n^2-1}{2n^2+1}\right)^2$

YP $\left(\frac{\varepsilon-1}{2\varepsilon+1}\right)\left(\frac{n^2-1}{2n^2+1}\right)$

π^* empirical scale of solvent polarity/polarizibility (Kamlet–Taft)

E empirical parameter of solvent acidity (Koppel–Palm)

B B_{PhOH}; empirical parameter of solvent basicity of Koppel and Paju

α empirical parameter of hydrogen bond donor acidity (Kamlet–Taft)

β empirical parameter of hydrogen bond acceptor basicity (Kamlet–Taft)

E_{T}^{30} empirical parameter of Dimroth and Reichardt

Z empirical parameter of solvent polarity (Kosower)

S empirical parameter of solvent polarity (Browstein)

DN donor number (Gutmann)

AN acceptor number (Gutmann)

G empirical parameter of solvent polarity (Allerhand–Schleyer)

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