Structure-Acidity-IR Spectra Correlations for *p*-Substituted *N*-Phenylsulfonylbenzamides[†]

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[†] This paper is dedicated *in memoriam* to our colleague Prof. Dr. Alexander Perjessy, who passed away on February 13, 2003, and who made so many invaluable contributions in the fields of IR spectroscopy and correlation analysis, especially spectra-structure-property relationships.

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Abstract: The wavenumbers of the IR absorption bands of the C=O, S=O and N-H stretching vibrations for a series of p-substituted *N*-phenylsulfonylbenzamides were measured in trichloromethane. The bond orders, Mulliken charges, charge densities and heats of formation were calculated using the PM3 method. Fifty significant mutual mono parameter (MP) and six dual parameter (DP) correlations were found for the IR spectral, theoretical structural data, substituent constants and previously reported dissociation constants in five polar organic solvents. The transmission of the substituent effects has been discussed and the solvent effect on the slopes of some linear correlations was evaluated using different solvent parameters. The results showed that the factors describing the electronic structure and controlling the dissociation equilibrium and the IR spectra properties of p-substituted *N*-phenylsulfonylbenzamides must be the same.
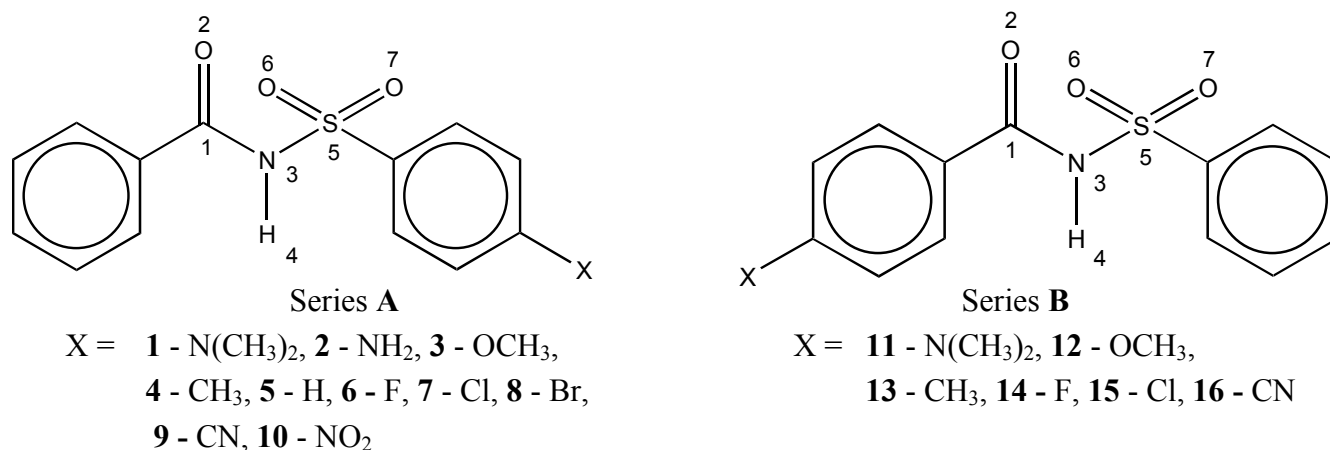
Introduction

N-Phenylsulfonylbenzamides have shown a wide range of practical properties. The compounds of this class exhibit often remarkable fungicidal [1], herbicidal [2] and antibacterial [3-5] activities and effects. Moreover, several *N*-phenylsulfonylbenzamide derivatives are efficient glitter forming agents and are used in electrolytic metallizations [6-8]. The pK_{HA} values of substituted *N*-phenyl-sulfonylbenzamides were determined in five polar organic solvent and the substituent and solvent effects on the dissociation equilibria were investigated [9,10]. To the best of our knowledge, the IR spectral and theoretical data for substituted *N*-phenylsulfonylbenzamides were not studied systematically and have not been reported so far.

The biological importance and practical applications of *N*-phenylsulfonylbenzamides led us to continue the study of these compounds, namely in the fields of IR spectroscopy, structural calculations and correlation analysis. Therefore, the aim of this work was to measure the IR spectra, to calculate the PM3 structural data and to study the MP and DP correlations for *p*-substituted *N*-phenylsulfonylbenz-amides of series **A** and **B**, compounds **1 – 16** (Scheme 1).

Scheme 1

Series **A**

X = **1** - N(CH₃)₂, **2** - NH₂, **3** - OCH₃,
4 - CH₃, **5** - H, **6** - F, **7** - Cl, **8** - Br,
9 - CN, **10** - NO₂

Series **B**

X = **11** - N(CH₃)₂, **12** - OCH₃,
13 - CH₃, **14** - F, **15** - Cl, **16** - CN

Results and Discussion

The infrared spectral data of compounds **1 – 16** as measured in trichloromethane are listed in Table 1. All three characteristic structural fragments of *p*-substituted *N*-phenylsulfonylbenzamides, the C=O, SO₂ and N-H groups, are described by their stretching vibrational wavenumbers. The absorption bands of both the symmetric and asymmetric stretching vibrations of the SO₂ group are observed nearly in the same regions as the $v_s(SO_2)$ and $v_{as}(SO_2)$ bands for the recently reported substituted

benzenesulfonamides [11]. The absorption bands of ν (C=O) and ν (N-H) vibrations appear in the expected regions of the wavenumbers characteristic for *N*-substituted benzamide derivatives [12]. The calculated PM3 bond orders and Mulliken charges for all bonds and atoms on the three characteristic structural fragments of compounds **1-16** are given in the Table 2. The PM3 optimized structure of the unsubstituted parent compound **5** is shown in Figure 1.

Table 1. Characteristic infrared spectral data for substituted *N*-phenylsulfonylbenzamides **1 – 16** in trichloromethane

Compound	$\tilde{\nu}$ / cm^{-1}			
	ν_s(SO$_2$)	ν_{as}(SO$_2$)	ν (C=O)	ν (N-H)
1	1156.4	1344.4	1697.2	-[a]
2	1161.2	1346.0	1699.2	-[a]
3	1162.4	1350.4	1700.0	3278.4
4	1168.0	1350.8	1701.6	3280.0
5	1171.2	1351.5	1702.4	3279.2
6	1171.6	1353.6	1702.4	3281.6
7	1169.2	1354.0	1702.4	3273.6
8	1170.8	1354.4	1702.4	3274.0
9	1172.0	1357.6	1704.4	-[a]
10	1173.2	1357.8	1704.8	-[a]
11	1165.2	1345.6	1686.4	3288.2
12	1168.0	1347.6	1698.8	3281.6
13	1170.4	1348.8	1702.4	3280.0
14	1171.2	1349.6	1705.6	3276.8
15	1171.2	1350.4	1706.0	3273.5
16	1173.0	1352.8	1710.4	3267.2

[a]Insoluble.

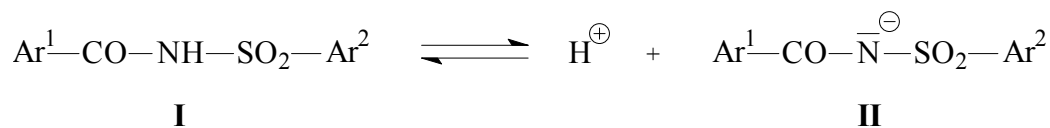**Figure 1.** PM3 optimized structure of compound **5**.
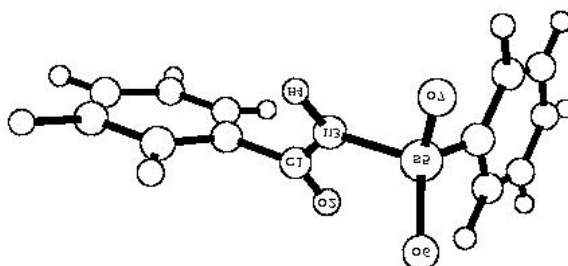
Table 2.   Calculated PM3 Mulliken charges and bond orders for substituted *N*-phenyl-sulfonylbenzamides **1 – 16**[a]

Comp.	$q_M(C_1)$	$-q_M(O_2)$	$-q_M(N_3)$	$q_M(H_4)$	$q_M(S_5)$	$-q_M(O_6)$	$-q_M(O_7)$	$p(S_5=O_6)$	$p(S_5=O_7)$	$p(N_3-H_4)$	$p(C_1=O_2)$
1	0.421	0.385	0.635	0.197	2.400	0.819	0.841	1.2023	1.2298	0.9311	1.8024
2	0.421	0.385	0.636	0.197	2.400	0.818	0.841	1.2025	1.2303	0.9309	1.8020
3	0.422	0.387	0.637	0.198	2.402	0.819	0.839	1.2051	1.2307	0.9308	1.8009
4	0.421	0.385	0.638	0.198	2.397	0.817	0.839	1.2049	1.2320	0.9307	1.8035
5	0.422	0.384	0.639	0.199	2.396	0.817	0.838	1.2057	1.2325	0.9306	1.8043
6	0.423	0.386	0.640	0.200	2.402	0.815	0.837	1.2077	1.2348	0.9302	1.8037
7	0.423	0.385	0.640	0.199	2.399	0.815	0.837	1.2061	1.2342	0.9307	1.8039
8	0.422	0.385	0.639	0.199	2.399	0.815	0.837	1.2074	1.2345	0.9308	1.8045
9	0.425	0.384	0.644	0.202	2.402	0.813	0.835	1.2103	1.2370	0.9298	1.8067
10	0.427	0.383	0.648	0.204	2.403	0.811	0.832	1.214	1.2405	0.9293	1.8093
11	0.433	0.390	0.641	0.199	2.394	0.817	0.840	1.2038	1.2318	0.9345	1.7997
12	0.433	0.389	0.640	0.198	2.396	0.817	0.8390	1.2050	1.2318	0.9304	1.8000
13	0.425	0.386	0.641	0.199	2.397	0.816	0.839	1.2054	1.2327	0.9304	1.8037
14	0.423	0.383	0.637	0.197	2.399	0.815	0.837	1.2075	1.2346	0.9309	1.8036
15	0.421	0.383	0.637	0.198	2.398	0.816	0.837	1.2069	1.2341	0.9307	1.8037
16	0.416	0.377	0.636	0.197	2.402	0.815	0.836	1.2096	1.2359	0.9313	1.8070

[a]For numbering of atoms see Scheme 1.

Tables 2-3 also shows the calculated PM3 charge densities for the hydrogen atom of the N-H group in the undissociated molecules and the heats of the formation for both the undissociated (**I**) and dissociated (**II**) molecules, which play a crucial role in the determination of the pK_{HA} values, used later in the correlations with spectral and theoretical data (see Scheme 2).

Scheme 2.

$$Ar^1\text{—}CO\text{—}NH\text{—}SO_2\text{—}Ar^2 \;\rightleftharpoons\; H^{\oplus} \;+\; Ar^1\text{—}CO\text{—}\overset{\ominus}{N}\text{—}SO_2\text{—}Ar^2$$

I   **II**

Table 3. Calculated PM3 heats of formation for substituted *N*-phenyl-sulfonylbenzamides **1 – 16**

Compound	$-\Delta H_f(\mathbf{I})^a$/kJ.mol^{-1}	$-\Delta H_f(\mathbf{II})^b$/kJ.mol^{-1}
1	243.61	424.92
2	237.80	421.18
3	383.98	572.48
4	263.21	449.88
5	222.47	411.31
6	403.44	604.03
7	248.79	446.70
8	186.55	388.34
9	68.93	282.88
10	245.96	476.03
11	200.01	386.47
12	381.25	574.27
13	261.86	449.48
14	401.22	602.18
15	248.10	445.87
16	70.72	283.07

[a]For undissociated molecule **I**; [b]for dissociated anion **II**.

Fifty mono parameter (MP) correlations of the IR spectral data, theoretical data, substituent constants and the pK_{HA} values measured in five organic solvents (MeOH, CH$_3$CN, DMF, DMSO and Py; taken from our previous publications [9, 10]) are compared in Table 4.

In a few cases some points were omitted from the correlations as outliers, mainly for compounds containing extremely polar substituents in *p*-position, as N(CH$_3$)$_2$, NH$_2$ and NO$_2$. For the two differently substituted series **A** and **B** in most cases also different correlation results were obtained. However, some correlations concerning bond orders and pK_{HA} values create significant common regression lines for both series **A** and **B**. This is in a good agreement with the previous conclusion, that due to the extensive delocalization of the negative charge in the conjugated base the overall transmission effects of the C=O and SO$_2$ groups on the transmission of substituent effects are roughly equal [9]. In the case of the correlations of IR spectral data for the SO$_2$ group the most significant correlations are obtained using the arithmetic means ($\overline{v}(SO_2)$) of the wavenumbers of both $v_s(SO_2)$ and $v_{as}(SO_2)$ vibrations. In the correlations of IR spectral data with substituent constants for the extensively conjugated C=O and SO$_2$ groups the best results are obtained when the electrophilic Brown-Okamato´s σ^+ values are used. However, in the case of the N-H group which is cross-

conjugated with the C=O and SO$_2$ groups the best results are obtained using original Hammett σ constants. Both series of substituent constants were taken from [13].

Table 4.   Mono parameter correlations of IR spectral data[a], substituent constants, dissociation constants and theoretical parameters for substituted *N*-phenyl-sulfonylbenzamides **1 - 16**

$$y = \rho x + q$$

No.[b]	y	x	Series	n[c]	r[d]	s[e]	F[f]	ρ	q
1	ν(C=O)	σ⁺	**A**	10	0.992	0.31	493	2.86±0.13	1702.4
2			**B**	7	0.979	1.71	116	9.94±0.92	1704.7
3	$\bar{\nu}$(SO$_2$)	σ⁺	**A**	9[g]	0.995	0.52	742	5.89±0.22	1261.0
4			**B**	7	0.991	0.35	287	3.24±0.19	1260.7
5	ν(N-H)	σ	**A**	poor	correlation				
6			**B**	7	0.989	1.05	231	-14.19±0.93	3277.4
7	ν(C=O)	p(C=O)	**A**	8[h]	0.967	0.42	85	590.45±64.00	637.0
8			**B**	6[i]	0.883	2.09	14	1578.91±418.81	-1143.6
9	$\bar{\nu}$(SO$_2$)	$\bar{p}$(S＝O)	**A + B**	15[g]	0.887	1.99	48	1253.49±180.70	-269.7
10	ν(N-H)	p(N-H)	**A + B**	11[j]	0.841	2.53	22	-12558.56±2697.25	14965.1
11	ν(C=O)	pK$_{HA}$(MeOH)	**A**	10	0.964	0.65	105	-2.82±0.27	1724.8
12			**B**	6[k]	0.966	2.12	55	-12.72±1.71	1807.6
13	ν(C=O)	pK$_{HA}$(CH$_3$CN)	**A**	10	0.962	0.67	99	-1.95±0.20	1735.7
14			**B**	6[k]	0.968	2.03	60	-8.62±1.11	1853.8
15	ν(C=O)	pK$_{HA}$(DMF)	**A**	10	0.950	0.77	74	-2.04±0.24	1718.5
16			**B**	6[k]	0.970	1.98	64	-9.85±1.23	1784.4
17	ν(C=O)	pK$_{HA}$(DMSO)	**A**	10	0.923	0.95	46	-1.42±0.21	1710.7
18			**B**	6[k]	0.941	2.75	31	-8.22±1.47	1755.6
19	ν(C=O)	pK$_{HA}$(Py)	**A**	10	0.931	0.90	52	-2.09±0.29	1711.9
20			**B**	6[k]	0.956	2.38	43	-9.13±1.40	1746.7
21	$\bar{\nu}$(SO$_2$)	pK$_{HA}$(MeOH)	**A**	10	0.962	1.43	99	-5.97±0.60	1308.8
22			**B**	7	0.962	0.74	61	-3.66±0.47	1290.1
23	$\bar{\nu}$(SO$_2$)	pK$_{HA}$(CH$_3$CN)	**A**	10	0.958	1.49	90	-4.12±0.43	1331.8
24			**B**	7	0.941	0.91	39	-2.41±0.39	1302.2
25	$\bar{\nu}$(SO$_2$)	pK$_{HA}$(DMF)	**A**	10	0.954	1.56	82	-4.35±0.48	1295.8
26			**B**	7	0.944	0.90	41	-2.76±0.43	1282.8
27	$\bar{\nu}$(SO$_2$)	pK$_{HA}$(DMSO)	**A**	10	0.922	2.02	45	-3.01±0.45	1278.9
28			**B**	7	0.956	0.80	53	-2.40±0.33	1275.3
29	$\bar{\nu}$(SO$_2$)	pK$_{HA}$(Py)	**A**	10	0.957	1.52	86	-4.55±0.49	1282.1
30			**B**	7	0.951	0.84	47	-2.63±0.38	1272.6

Table 4. Continued

No.[b]	y	x	Series	n[c]	r[d]	s[e]	F[f]	ρ	q
31	ν(N-H)	pK$_{HA}$(MeOH)	**A + B**	11[l]	0.962	1.57	111	9.33±0.89	3200.5
32	ν(N-H)	pK$_{HA}$(CH$_3$CN)	**A + B**	11[l]	0.976	1.26	179	6.43±0.48	3164.9
33	ν(N-H)	pK$_{HA}$(DMF)	**A + B**	11[l]	0.970	1.41	141	7.27±0.61	3217.1
34	ν(N-H)	pK$_{HA}$(DMSO)	**A + B**	11[l]	0.938	1.99	66	5.75±0.71	3240.6
35	ν(N-H)	pK$_{HA}$(Py)	**A + B**	11[l]	0.963	1.56	114	6.77±0.64	3244.8
36	pK$_{HA}$(MeOH)	ΔE[m]	**A + B**	15[m]	0.904	0.31	58	0.0631±0.0083	20.61
37	pK$_{HA}$(CH$_3$CN)	ΔE[m]	**A + B**	15[n]	0.912	0.43	64	0.0914±0.0114	35.61
38	pK$_{HA}$(DMF)	ΔE[m]	**A + B**	15[n]	0.913	0.39	65	0.0852±0.0105	24.99
39	pK$_{HA}$(DMSO)	ΔE[m]	**A + B**	15[n]	0.878	0.61	44	0.1083±0.0169	27.64
40	pK$_{HA}$(Py)	ΔE[m]	**A + B**	15[n]	0.894	0.45	52	0.0868±0.0121	21.86
41	pK$_{HA}$(MeOH)	q$_M$(H$_4$)	**A**	8[o]	0.950	0.25	56	-447.59±59.81	97.31
42			**B**	5[p]	0.883	0.45	11	1017.23±312.46	-192.75
43	pK$_{HA}$(CH$_3$CN)	q$_M$(H$_4$)	**A**	8[o]	0.948	0.36	53	-624.68±85.87	141.83
44			**B**	5[p]	0.880	0.65	10	1443.32±449.37	-267.68
45	pK$_{HA}$(DMF)	q$_M$(H$_4$)	**A**	8[o]	0.945	0.36	50	-601.61±85.18	128.03
46			**B**	5[p]	0.898	0.55	13	1333.49±376.78	-255.22
47	pK$_{HA}$(DMSO)	q$_M$ (H$_4$)	**A**	8[o]	0.927	0.58	36	-827.36±136.77	171.06
48			**B**	5[p]	0.850	0.87	8	1676.08±599.21	-324.82
49	pK$_{HA}$(Py)	q$_M$(H$_4$)	**A**	8[o]	0.910	0.47	29	-595.98±110.61	123.50
50			**B**	5[p]	0.912	0.50	15	1314.15±342.19	-254.81

[a]Measured in CHCl$_3$. [b]Ordinal number of the correlation. [c]Number of compounds used in correlation. [d]Correlation coefficient. [e]Standard deviation. [f]Fisher-Snedecor test for parameters significant at the 95 % level. [g]Compound **6** omitted. [h]Compounds **1** and **2** omitted. [i]Compound **11** omitted. [j]Compounds **1, 2, 9, 10** and **11** omitted. [k]Compound **16** omitted. [l]Compounds **1, 2, 6, 9** and **10** omitted. [m]See Eq(1). [n]Compound **10** omitted. [o]Compounds **8, 10** omitted. [p]Compounds **5, 13** omitted.

For pK$_{HA}$ vs. ΔE correlations the energy ΔE, proportional to the dissociation equilibrium, was defined as the difference between the heats of formation of the dissociated anion (**II**) and the undissociated molecule (**I**) (see Scheme 2): ΔE = ΔH$_f$(**II**) - ΔH$_f$(**I**) (1)

In the series of correlations with pK$_{HA}$ values determined in five different solvents the effect of the solvent on the ρ values can be evaluated using a variety of solvent parameters [14]. In this study we tried to use the following solvent parameters: E$_T$(30), π*, basicity (B*) and the parameter β. From all possible attempts only the correlations using solvent basicity parameters (B*) [14] were satisfactory for the IR properties of the C=O and N-H groups. The results are given in Table 5.

Table 5. Correlation between the slopes of dependencies of IR spectral wavenumbers vs. pK_{HA} values in different solvents (ρ) and basicity of solvents (B^*) for the series **1 – 16** of substituted *N*-phenylsulfonylbenzamides. $\rho = aB^* + b$

Dependence	Series	n^a	R^b	s^c	F^d	a	b
ν(C=O) vs. $pK_{HA}{}^e$	**A**	5	0.940	0.20	23	2.14±.0.45	-3.92
ν(C=O) vs. $pK_{HA}{}^f$	**B**	5	0.928	0.77	19	7.57±1.75	-16.27
ν(N-H) vs. $pK_{HA}{}^g$	**A + B**	5	0.940	0.54	23	-5.82±1.22	12.15

[a] Number of solvents used in correlation. [b] Correlation coefficient. [c] Standard deviation. [d] Fisher-Snedecor test for parameters significant at the 95 % level. [e] See correlations No. 11, 13, 15, 17 and 19 in Table 4. [f] See correlations No. 12, 14, 16, 18 and 20 in Table 4. [g] See correlations No. 31, 32, 33, 34 and 35 in Table 4.

The results show that mainly the C=O and N-H groups in *N*-phenylsulfonylbenzamides contribute to the change of the dissociation equilibria upon the solvent basicity variation. It is also evident from the Table 5, that the series of compounds **B** are more sensitive to the solvent effects as the compounds of series **A**. The negative slope of the correlation for the N-H group indicates that this structural fragment exhibits an opposite solvent effect than the C=O group.

Table 6 contains six dual parameter (DP) correlation for IR spectral data and Mulliken charges of atoms representing the three characteristic groups (C=O, N-H and SO_2) of the investigated compounds **1 - 16**. A similar approach has been reported for $\nu(SO_2)$ values by Castan and Dagnac [15] and recently for the $\nu(SO_2)$ and $\nu(NH_2)$ values by us [11]. However, as it follows from the statistical parameters in the Table 6, such a DP correlation does not bring further significant improvement in the quantitative study of the substituent effects of *N*-phenylsulfonylbenzamides.

Table 6. Dual parameter correlations of IR spectral data[a], and theoretical parameters for the substituted *N*-phenylsulfonylbenzamides **1 – 16**; $y = \rho_1 x_1 + \rho_2 x_2 + q$

No.[b]	y	x_1	x_2	Series	n^c	R^d	s^e	F^f	ρ_1	ρ_2	q
51	ν(C=O)	$q_M(C_1)$	$q_M(O_2)$	**A**	10	0.836	1.4	8	819.8	417.5	1515.9
52				**B**	7	0.883	4.4	7	-664.3	760.6	2275.9
53	ν(N-H)	$q_M(N_3)$	$q_M(H_4)$	**A**	poor correlation						
54				**B**	7	0.931	3.0	13	-4174.0	-3082.4	1222.6
55	$\bar{\nu}(SO_2)$	$q_M(S_5)$	$\bar{q}_M(O_6,O_7)$	**A**	10	0.925	2.1	24	-576.5	2008.0	4303.5
56				**B**	7	0.830	1.8	4	727.3	179.5	-425.1

[a] Measured in $CHCl_3$. [b] Ordinal number of the correlations. [c] Number of compounds used in correlation. [d] Correlation coefficient. [e] Standard deviation. [f] Fisher-Snedecor test for parameters significant at the 95 % level.

Finally, the previously discussed MP correlation suggest a conclusion that the factors controlling dissociation equilibria as well as the IR spectral and structural properties in p-substituted *N*-phenyl-sulfonylbenzamides must be the same.

Acknowledgements

Experimental

General

The preparation and the pK_{HA} values of the studied compounds **1-16** have been reported previously [9]. The IR spectra were measured at room temperature in the regions of 1400-1000 cm^{-1} and 3300-3200 cm^{-1} using a Zeiss Specord M 80 spectrometer. The measurements were carried out in CHCl$_3$ of spectral purity (Uvasol, Merck) employing NaCl cells of 0.1 and 1.0 mm thickness. The concentrations of the solutions were set up in such a way that a maximum of the absorption of 75-80 % was obtained. Peak positions were determined with an accuracy of ±0.1 cm^{-1} relative to polystyrene standard spectra.

Computational Details

All computations were performed using the semiempirical PM3 Hamiltonian [16] with program packages VAMP [17] and AMPAC [18]. Geometries were completely optimized (keyword PRECISE) with the eigenvectors following routine [19]. Charges were obtained from Mulliken population analysis. Starting structures were created by the SYBYL molecular modeling package [20].

References and Notes

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Sample Availability: The samples of compounds **1 - 16** investigated in this work are available from Dr. Patrik Parik, Department of Organic Chemistry, Faculty of Chemical Technology, University of Pardubice, nam. Cs. legii 565, CZ - 532 10 Pardubice, Czech Republic, Phone: +420 466 037 075, Fax: +420 466 037 067, E-mail: Patrik.Parik@upce.cz.