Monatshefte für Chemie 128, 541–551 (1997)

Monatshefte für Chemie
Chemical Monthly

Printed in Austria

Infrared Spectra of *ortho*-Substituted Acetanilides: Vicinal Effects and Conformation

A. Perjéssy[1,*], **D. Rasała**[2], **D. Loos**[1], and **D. Piorun**[2]

[1] Department of Organic Chemistry and Institute of Chemistry, Faculty of Natural Sciences, Comenius University, SL-84215 Bratislava, Slovak Republic
[2] Institute of Chemistry, Pedagogical University, PL-52020 Kielce, Poland

Summary. The infrared spectra of twenty-two *ortho*-substituted acetanilides (**1a**–**1v**) in CCl_4 and $CHCl_3$ were measured in the region of the C=O and NH stretching vibrations and compared with those of *para*-substituted acetanilides (**2a**–**2i**). The wave numbers of the C=O stretching vibrations were analyzed using empirical substituent constants and single- and multiparametric correlations. On the basis of the above approaches, the separation of the polar effects into inductive, field, resonance, and steric components has been assessed for the *ortho*-substituted series. For compounds containing polar substituents with double bonds, specific vicinal effects caused by intramolecular hydrogen bonding have been observed. The conformations of *ortho*-substituted acetanilides **1a**–**1v** were studied by both infrared spectroscopy and AM1 calculations.

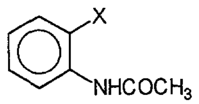
Keywords. *ortho-* and *para*-Substituted acetanilides; Carbonyl stretching vibration wave numbers; Correlations with substituent effects; Theoretical MMPI and AM1 calculations.

Infrarotspektren von *ortho*-substituierten Acetaniliden: Nachbargruppeneffekte und Konformation

Zusammenfassung. Die Infrarotspektren von 22 *ortho*-substituierten Acetaniliden (**1a**–**1v**) in CCl_4 und $CHCl_3$ wurden im Bereich der C=O- und NH-Streckschwingungen gemessen und mit jenen von *para*-substituierten Acetaniliden (**2a**–**2i**) verglichen. Die Wellenzahlen der C=O-Streckschwingungen wurden mit Hilfe empirischer Substituentenkonstanten und ein- und mehrparametriger Korrelationen untersucht. Auf dieser Grundlage konnte für die *ortho*-substituierte Reihe eine Zerlegung der polaren Effekte in induktive, feldbedingte, resonanzabhängige und sterische Komponenten erzielt werden. In Verbindungen mit Doppelbindungen enthaltenden polaren Substituenten wurden durch intramolekulare Wasserstoffbrückenbindungen hervorgerufene spezifische Nachbargruppeneffekte beobachtet. Die Konformationen der *ortho*-substituierten Acetanilide **1a**–**1v** wurden sowohl infrarotspektroskopisch als auch mittels AM1-Rechnungen untersucht.

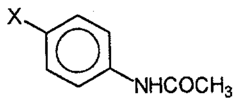
Introduction

Acetanilides represent an interesting model system for biologically and biochemically important molecules containing a conformationally and tautomerically flexible peptidic fragment. The structures of some acetanilide derivatives have been investigated previously [1–6]. The substituent effects in a series of *para*-substituted acetanilides have been studied using ^{1}H NMR chemical shifts and wave numbers of carbonyl stretching vibrations [7]. Recently, *Kolehmainen et al.* [8] have investigated in detail the substituent effects and conformation of *ortho*-substituted acetanilides using multinuclear NMR data and molecular mechanististic calculations. However, the above mentioned methods were not able to provide enough informations and evidences about the patterns of vicinal interactions arising from intramolecular hydrogen bonding in the *ortho*-substituted parts of the molecules. Therefore, we have measured the infrared spectra of a series of twenty-two *ortho*-substituted acetanilides (**1a**–**1v**) in diluted solutions of $CHCl_3$ and CCl_4 in the regions of 1730–1630 and 3470–3290 cm^{-1}.



	X		*X*
1a	$N(CH_3)_2$	**1l**	Cl
1b	OCH_3	**1m**	I
1c	NHC_6H_5	**1n**	Br
1d	SCH_3	**1o**	CF_3
1e	CH_3	**1p**	CN
1f	C_2H_5	**1q**	$NHCOCH_3$
1g	$CH(CH_3)_2$	**1r**	$CONH_2$
1h	$C(CH_3)_3$	**1s**	$COOCH_3$
1i	C_6H_5	**1t**	COC_6H_5
1j	F	**1u**	$COCH_3$
1k	H	**1v**	NO_2

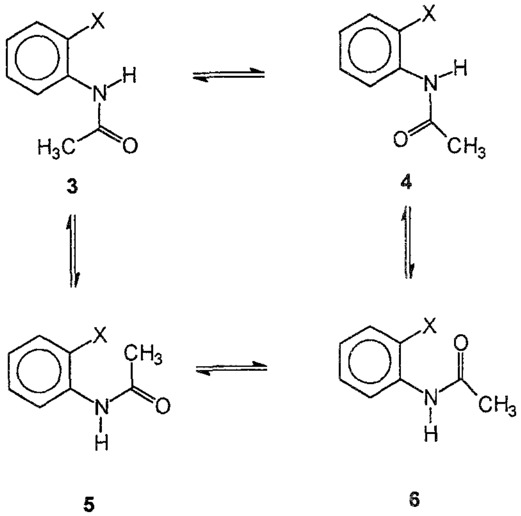
The spectroscopic properties of the above compounds were compared with those reported previously [7] for a series of *para*-substituted acetanilides (**2a**–**2i**).



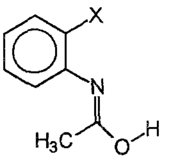
	X		*X*
2a	OCH_3	**2f**	Br
2b	CH_3	**2g**	CF_3
2c	F	**2h**	CN
2d	Cl	**2i**	NO_2
2e	I		

Results and Discussion

Due to their conformational flexibility, *ortho*-substituted acetanilides can theoretically exist in four isomeric forms (**3**–**6**) which result from restricted rotation around the CH-NH and NH-CO bonds.



Moreover, a ketoamino-enolimino tautomeric equilibrium can occur resulting in two further possible (**7** and **8**).



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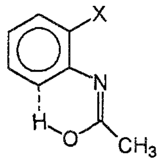

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The existence of structures **7** and **8** is, however, can most probably be excluded because all investigated *ortho*-substituted acetanilides (**1a**–**1v**) exhibit strong absorption bands belonging to the C=O stretching vibration of the amide group (Table 1). The solvent effect on the wave numbers of these bands (passing from CCl_4 to $CHCl_3$) is rather strong; in most cases, a shift of 22–14 cm^{-1} is observed. The ν(C=O) absorption band for unsubstituted acetanilde **1k** is observed at 1706.4 cm^{-1} in CCl_4 and can be assigned to molecules without hydrogen bonding interaction. At increased concentrations of the compound in CCl_4, a shoulder at 1691.8 cm^{-1} appears, and its intensity continuously increases with increasing concentration (Fig. 1). This effect can be assigned to the C=O stretching vibration of hydrogen bonded 'cyclic dimers' (**9**) which are in the equilibrium with 'monomeric' molecules in one of the possible conformations **3**–**6** and are rather common in the case of secondary amides [9–10].

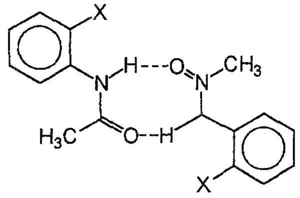

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Table 1. Infrared spectroscopic data of *ortho*-substituted acetanilides

Compound	ν(C=O) (cm^{-1})		ν(C=O) (cm^{-1})
	CCl_4	$CHCl_3$	CCl_4
1a	1694.0	1677.2	3359.6
1b	1701.2	1684.8	3438.0
1c	1702.4	1681.6	3433.2
1d	1706.8	1691.2	3359.2
1e	1705.6	1685.6	3459.6
1f	1704.4	1684.8	3462.4
1g	1705.2	1684.0	3464.0
1h	1704.4	1684.5	3495.8
1i	1706.0	1686.4	3430.4
1j	1711.6	1692.0	3449.6
1k	1706.4	1687.6	3446.0
1l	1712.4	1609.2	3428.8
1m	1712.0	1696.8	3420.0
1n	1712.4	1698.0	3416.8
1o	1716.8	1701.2	3400.0
1p	1721.6	1702.8	3420.8
1q	[a]	1673.6[b]	[a]
1r	[a]	1684.8[b]	[a]
1s	1692.8[c]	1687.2[d]	3324.8
1t	1706.8[e]	1694.0[f]	3320.0
1u	1706.0[g]	1690.4[h]	3298.0
1v	1716.8	1709.2	3368.0

[a] Insoluble; [b] ν(C=O) for $CONH_2$ group: 1665.2 cm^{-1}; [c] ν(C=O) for $COOCH_3$ group: 1692.8 cm^{-1}; [d] ν(C=O) for $COOCH_3$ group: 1700.0 cm^{-1} [e] ν(C=O) for COC_6H_5 group: 1639.2 cm^{-1}; [f] ν(C=O) for COC_6H_5 group: 1636.4 cm^{-1}; [g] ν(C=O) for $COCH_3$ group: 1657.2 cm^{-1}; [h] ν(C=O) for $COCH_3$ group: 1654.0 cm^{-1}

The occurrence of hydrogen bonds suggests that the investigated *ortho*-substituted acetanilides must exist preferably in conformation **3** or **5**.

The sharp medium intensity absorption bands of *ortho*-substituted acetanilides in the region of 3455–3298 cm^{-1} can be assigned to the NH stretching vibration of the 'monomeric' molecules, whereas the broad absorption bands of very litle intensity at *ca.* 3100 cm^{-1} (observed in concentrated solutions) belong to the NH stretching vibrations of the intermolecularly hydrogen bonded 'dimeric' species **9**.

The correlation of the empirical infrared spectroscopic data, *i.e.* the ν(C=O) and ν(N-H) values, with substituent constants for series **1** and **2** are listed in Table 2. Applying a single parametric approach to the wave numbers of the carbonyl stretching vibration, it is evident that the statistically most significant ones are the correlations with *Hammett's* σp constants in both series. For the *ortho*-substituted acetanilides, only the first sixteen compounds (**1a**–**1p**) from Table 1 have been used in the correlations. Compounds **1q**–**1v** do not follow the correlation for ν(C=O) values, since they always exhibit absorption bands lower by 7–26 cm^{-1} in CCl_4 and 3–18 cm^{-1} in $CHCl_3$ than expected from correlation equations. This can be

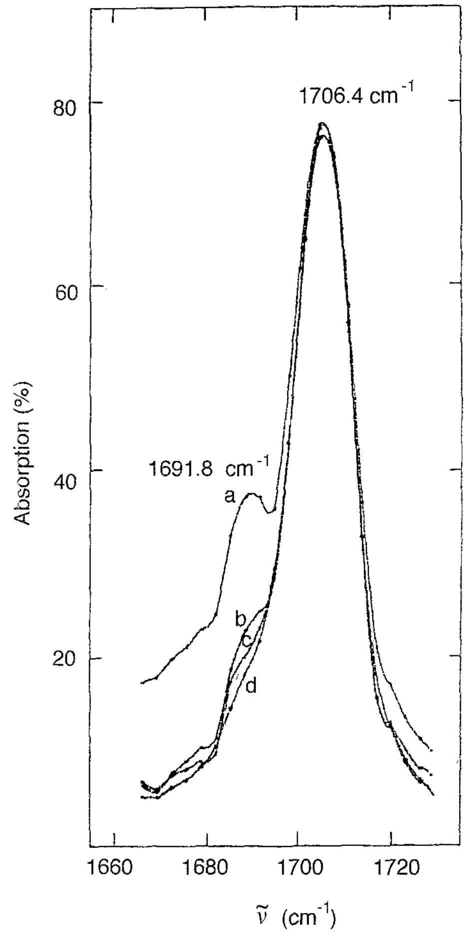
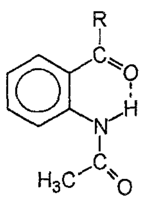


Fig. 1. Infrared spectra of **1k** in CCl$_4$ measured in the concentrations region of $10^{-5} - 10^{-2}$ mol·dm^3, cell thickness: a: 10 mm, b: 5 mm, c: 2.5 mm, d: 1 mm

reasonably explained by the existence of specific vicinal effects between the *ortho*-substituents and the acetylamino moiety. In the case of compounds **1q**–**1u**, an intramolecular hydrogen bond is formed between the C=O group of the *ortho*-substituent and the NH group of the acetylamino function, shaping a six- or a seven-membered ring (**10** and **11**).



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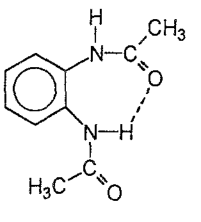

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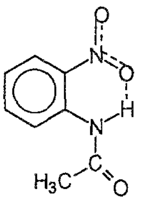

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R = NH$_2$, OCH$_3$, C$_6$H$_5$, CH$_3$

In *ortho*-nitroacetanilide (**1v**), most probably an intramolecular hydrogen bonding occurs (**12**) between the nitro group oxygen and the acetylamino hydrogen atom.

Table 2. Correlation of infrared spectroscopic data with substituent constants of *ortho*-substituted acetanilides **1a–1p** in comparison with *para*-substituted acetanilides **2a–2i**[a]

$$y = a^1x^1 + a^2x^2 + a^3x^3 + b$$

Series	y	Solvent	x^1	x^2	x^3	n	r	s	F	a^1	a^2	a^3	b
1	ν(C=O)	CCl_4	σ_p	–	–	16	0.979	1.38	328	18.11±1.00	–	–	1708.9
1	ν(C=O)	CCl_4	σ_p^+	–	–	15[d]	0.943	2.30	104	11.19 ± 1.10	–	–	1709.9
1	ν(C=O)	CCl_4	$\mathscr{F}$	$\mathscr{R}$	--	16	0.982	1.33	177	18.82 ± 1.62	16.76±1.31[c]	--	1707.3
1	ν(C=O)	CCl_4	σ_l	σ_d	–	16	0.968	1.76	98	22.20±2.14	19.14±1.38	–	1706.9
1	ν(C=O)	CCl_4	σ_l	σ_d	ν_{ef}	16	0.968	1.38	61	22.19±2.24	19.14±1.97	−0.02±1.74	1706.9
1	ν(C=O)	CCl_4	σ_I^*	σ_R^*	–	16	0.979	1.45	148	18.74±1.79	17.09±1.12	–	1707.3
1	ν(C=O)	CCl_4	σ_I^*	σ_R^*	ν_{ef}	16	0.979	1.51	91	18.76±1.89	17.09±1.89	0.07±1.44	1707.3
1	ν(C=O)	CCl_4	σ_p	$\sigma_p^+ - \sigma_p$	–	15[d]	0.969	1.78	91	16.27±1.84	−12.74±4.07	–	1708.4
1	ν(C=O)	$CHCl_3$	σ_p	–	–	16	0.945	2.59	118	20.38±1.88	–	–	1690.2
1	ν(C=O)	$CHCl_3$	σ_p^+	–	–	15[d]	0.859	4.04	36	11.66±1.93	–	–	1692.4
2	ν(C=O)	CCl_4	σ_p	–	–	10	0.964	2.15	106	21.20±2.07	–	–	1703.8
2	ν(C=O)	CCl_4	σ_p^+	–	–	10	0.962	2.21	98	15.41±1.55	–	–	1706.6
2	ν(C=O)	CCl_4	$\mathscr{F}$	$\mathscr{R}$	--	10	0.969	2.13	54	16.89±3.36	23.38±3.16[e]	--	1705.0
2	ν(C=O)	CCl_4	σ_l	σ_d	–	10	0.959	2.44	40	17.99±3.60	22.28±3.21	–	1705.0
2	ν(C=O)	CCl_4	σ_l	σ_d	ν_{ef}	10	0.960	2.60	24	17.58±3.92	22.16±3.42	1.57±3.48	1704.4
2	ν(C=O)	CCl_4	σ_I^*	σ_R^*	–	10	0.976	1.89	69	17.08±2.98	23.03±2.70	–	1705.0
2	ν(C=O)	CCl_4	σ_p	$\sigma_p^+ - \sigma_p$	–	10	0.970	2.10	56	18.81±2.88	7.19±6.17	–	1705.1
2	ν(N–H)	CCl_4	σ_p	–	–	12[f]	0.963	8.60	129	−97.50 ± 8.57	–	–	3445.6

[a] The substituent constants σ_p and σ_p^+ were taken from Ref. [11], the constants for the *Swain-Lupton* equation ($\mathscr{F}$, $\mathscr{R}$) were taken from Ref. [12], the constants for the *Charton* equations (σ_l, σ_d, and ν_{ef}) were taken from Ref. [13] and for its *Tomasik* modification (σ_I^*, σ_R^*) from Ref. [14]; n is the number of compounds used in the correlation, r is correlation coefficient, s is the standard deviation, and F is the F-ratio of the correlations; [b] compound **1c** omitted; [c] $\%\mathscr{R} = 44.8$; [d] compound **1d** omitted; [e] $\%\mathscr{R} = 61.1$; [f] compounds **1a–1d, 1p, 1s–1u** omitted

Table 3. Separation of the overall substituent effect

Substituent constants	Slope of the correlation			Equation
	Series 1		Series 2	
$\mathscr{F}$	18.8	$>$	16.9	*Swain-Lupton*
$\mathscr{R}$	16.8	$<$	23.6	
$\%\mathscr{R}$	44.8	$<$	61.1	
σ_I	22.2	$>$	17.6	*Charton*
σ_d	19.1	$>$	22.2	
ν_{ef}	0.0	$\approx$	1.6	
σ_I^*	18.8	$>$	17.1	*Charton*
σ_R^*	17.1	$<$	23.0	(modified by *Tomasik*)
ν_{ef}	0.1	$\approx$	0.2	
r	−0.78	$<$	0.38	*Yukawa-Tsuno*

Multiparametric correlation approaches have been used for analyzing the wave numbers of C=O stretching vibrations in order to study the separation of overall substituent effect into inductive, field, resonance, and steric components. The comparison of the slopes a^1, a^2, and a^3 corresponding to substituent constants x^1, x^2, and x^3 of *ortho*-substituted acetanilides with those for the *para*-substituted series is schematically illustrated in Table 3. It follows from the above table that both inductive and field effects are always more important in the case of *ortho*-substituted compounds (**1**), whereas the transmission of resonance effects is more significant in the *para*-substituted series (**2**). The correlations, including *Charton*'s sterical constants (ν_{ef}), indicate that the steric effects of substituents X on the C=O stretching vibration are rather negligible in both series.

Finally, it follows from Table 2 that the wave numbers of the NH stretching vibration of *ortho*-substituted acetanilides **1** which are free of intramolecular hydrogen bonds also correlate satisfactorily with *Hammett's* σ_p constants. From this correlation, however, compounds **1a–1d**, **1p** and **1s–1u** must be excluded. That means that not only vicinal interactions of type **11** and **12** occur, but that the NH group also slightly interacts (*via* intramolecular hydrogen bonding) with *ortho*-substituents containing a heteroatom with lone electron pairs in the α-position, *i.e.* N, S, and O.

The theoretical calculations were carried out by the AM1 quantum chemical method using full optimization and standard parametrization [16]. The input data were obtained by the molecular mechanistic MMX method [17]. For unsubstituted acetanilide (**1k**), the heats of formation (ΔH_f) were calculated for all theoretical possible conformations and tautomeric forms **3–8**. In the case of compound **1k**, the forms **3** and **5** and **4** and **6**, respectively, are mutually identical, and the difference between ΔH_f for two existing conformations **3** and **4** is only 1.2 $kJmol^{-1}$; conformation **4** is slightly more advantageous than the conformation **3**. The tautomeric forms **7** and **8** are by 67 $kJmol^{-1}$ and 35 $kJmol^{-1}$ less stable than the conformations **3** and **5**, respectively, form **8** being the more stabilized one. This is probably due to the formation of an intramolecular hydrogen bond between the OH group and the π-electrons of the benzene ring. To distinguish the differences between the heats of formation of conformations **3**–**6**, the data for substituted compounds of series **1** should be compared. For this purpose, the ΔH_f values were calculated for two selected *ortho*-substituted acetanilides (**1a** and **1p**) bearing substituents with extreme electron withdrawing and electron donating effects. The results show that the conformations **3** and **4** are by 6.7–21.3 kJmol^{-1} more stable than the conformations **5** and **6**, where the CH_3 or C=O groups are sterically hindered by the *ortho*-substituents *X*. For all *ortho* and *para*-substituted acetanilides investigated the electronic structure and optimal geometry has been calculated for conformations **3** and **4**. The C=O and NH bond orders are listed in Tables 4 and 5. It follows from the differences between the heats of formation and from the rotation angles that the most preferred conformation is **4**. The energy differences between two conformations are rather small (in most cases less than 15 kJmol^{-1}); therefore, conformations **3** and **4** probably exist in a thermodynamic equilibrium at room temperature which can be shifted towards **3** as a consequence of intramolecular hydrogen boding, *i.e.* 'dimerization' (**9**). In the case of compounds undergoing intramolecular hydrogen bonding interactions of types **10**–**12**, the differences between the heats of formations for conformations **3** and **4** are up to 14 kJmol^{-1} due to a better coplanarity of the whole system. This effect is accompanied by a diminution of the rotation angles of the acetyl group as well as of the

Table 4. Theoretical data for *ortho*-substituted acetanilides

	Conformation 2			Conformation 4		
	p(C=O)	*p*(NH)	ΔH_f (kJ·mol^{-1})	*p*(C=O)	p(NH)	ΔH_f (kJ·mol^{-1})
1a	1.7609	0.8821	−21.7	1.7631	0.8898	−23.8
1b	1.7693	0.8839	−215.1	1.7675	0.8936	−222.1
1c	1.7606	0.8817	83.2	1.7723	0.8909	81.3
1d	1.7692	0.8781	−60.2	1.7780	0.8793	−65.7
1e	1.7640	0.8867	−92.1	1.7761	0.8973	−93.2
1f	1.7626	0.8857	−112.5	1.7766	0.8972	−112.8
1g	1.7628	0.8853	−126.8	1.7765	0.8955	−126.8
1h	1.7606	0.8824	−117.1	1.7746	0.8915	−117.3
1i	1.7677	0.8837	49.8	1.7743	0.8919	44.6
1j	1.7788	0.8861	−248.5	1.7783	0.8948	−254.8
1k	1.7665	0.8882	−61.6	1.7710	0.8988	−62.8
1l	1.7766	0.8822	−89.2	1.7805	0.8903	−94.6
1m	1.7796	0.8796	13.0	1.7846	0.8879	6.8
1n	1.7787	0.8801	−37.1	1.7830	0.8878	−43.1
1o	1.7941	0.8785	−713.8	1.7924	0.8912	−723.4
1p	1.7890	0.8828	73.1	1.7900	0.8938	64.3
1q	1.7594	0.8655	−211.6	1.7666	0.8766	−217.3
1r	1.7938	0.8797	−218.7	1.7713	0.8747	−233.2
1s	1.7893	0.8667	−410.2	1.7788	0.8733	−420.6
1t	1.7905	0.8812	−65.6	1.7794	0.8796	−79.3
1u	1.7912	0.8773	−212.3	1.7800	0.8772	−226.1
1v	1.8052	0.8653	−43.1	1.7969	0.8735	−43.3

Table 5. Theoretical data for *para*-substituted acetanilides

	Conformation analogous to **3**		Conformation analogous to **4**	
	p(C=O)	ΔH_f (kJ·mol^{-1})	p(C=O)	ΔH_f (kJ·mol^{-1})
2a	1.7623	−218.2	1.7715	−219.7
2b	1.7649	−93.6	1.7752	−96.0
2c	1.7717	−248.7	1.7788	−252.6
2d	1.7733	−90.3	1.7816	−94.4
2e	1.7767	6.2	1.7855	1.6
2f	1.7762	−41.0	1.7847	−45.5
2g	1.7861	−714.9	1.7927	−721.0
2h	1.7830	70.6	1.7900	64.9
2i	1.7972	−46.9	1.8016	−54.7

interatomic distances between the hydrogen atom of the NH group and the oxygen atom in the C=O and N=O moieties of substituents X. The AM1 conformation results are in a good correspondence with those obtained previously by molecular mechanics [8].

The wave numbers of the C=O and NH stretching vibrations measured for series **1** and **2** correlate with theoretical values of corresponding bond orders (Table 6), whereby the statistically most significant results are obtained always with conformation **4** or an analogous conformation in the case of *para*-substituted acetanilides. Since the influence of intramolecular hydrogen bonding interactions is considered in AM1 calculations, it was also possible to include all twenty-two *ortho*-substituted acetanilides (**1a**–**1v**) into the ν(C=O) *vs.* p(C=O) correlation (for data in $CHCl_3$) at a significance level of $r = 0.926$.

Table 6. Correlations of the wave numbers of the C=O and NH stretching vibrations with C=O and NH bond orders for *ortho*- and *para*-substituted acetanilides $y = ax + b$

Series	y	Solvent	x	Conformation	n	r	s	F	a	b
1	ν(C=O)	CCl_4	p(C=O)	**3**	16[a]	0.881	3.2	49	557.3±79.8	720.2
1	ν(C=O)	CCl_4	p(C=O)	**4**	16[a]	0.937	2.4	102	810.3±80.4	267.4
1	ν(C=O)	$CHCl_3$	p(C=O)	**3**	22	0.747	5.9	25	465.6±92.6	862.9
1	ν(C=O)	$CHCl_3$	p(C=O)	**4**	22	0.926	3.4	120	976.1±89.3	−45.5
2	ν(C=O)	CCl_4	p(C=O)	[b]	9	0.908	3.6	33	676.6±117.7	506.7
2	ν(C=O)	CCl_4	p(C=O)	[c]	9	0.924	3.3	41	801.3±125.0	278.8
1	ν(C=O)	$CHCl_3$	p(C=O)	**3**	6[d]	0.867	6.5	12	665.6±190.9	499.6
1	ν(C=O)	$CHCl_3$	p(C=O)	**4**	6[d]	0.972	3.1	69	1103.0±132.9	−272.2
1	ν(N-H)	CCl_4	p(N-H)	**3**	17[e]	0.755	35.3	20	7848.6±1759.2	−3509.9
1	ν(N-H)	CCl_4	p(N-H)	**4**	17[e]	0.940	18.4	113	6392.6±601.7	2275.6

[a] For compounds **1a**–**1p**; [b] conformation analogous to **3**; [c] conformation analogous to **4**; [d] compounds with vicinal hydrogen bonding interactions (**1q**–**1v**); [e] compounds **1a**, **1h**, **1q**, **1r**, and **1v** omitted

It can be finally concluded that the analysis of both the infrared spectroscopic and theoretical data confirms that *ortho*-substituted acetanilides preferably exist in a thermodynamic equilibrium of conformations **3** and **4**. According to the results of AM1 calculations, conformation **4** is probably more stable than conformation **3**. In the case of intramolecular hydrogen bonding between two molecules, however, the equilibrium is shifted towards conformation **3**. The participation of the NH group of the acetylamino moiety in the intramolecular hydrogen bonds strongly supports the preference of conformation **3**. On the other hand, the absence of steric effects on the C=O group as well as the importance of the inductive mechanism in the transmission of substituent effects denies the existence of structures **5** and **6**.

Experimental

The preparation, purification, and some properties of compounds **1** have been described previously [8, 15].

The infrared spectra were measured in the regions of 1730–1630 cm^{-1} and 3470–3290 cm^{-1} at room temperature using a Zeiss Specord M 80 spectrometer. The measurements were carried out in solutions in $CHCl_3$ and CCl_4 employing NaCl cells of 0.1 and 1.0 mm thickness. Both CCl_4 and $CHCl_3$ were of spectral purity (Uvasol, Merck). The concentrations of the solutions were chosen to reach a maximal absorption of 75–80%. For the investigation of intermolecular hydrogen bonding in unsubstituted acetanilide (**1k**), diluted solutions of concentrations of 10^{-2}–10^{-5} $mol{\cdot}dm^{-3}$ in CCl_4 and NaCl cells of 1, 2.5, 5, and 10 mm path length were used. The maxima of the absorption bands were determined with an accuracy of ± 0.2 cm^{-1} for C=O stretching vibrations and ± 0.4 cm^{-1} for NH stretching vibrations.

Acknowledgements

This work was performed in the framework of the CEEPUS SK-20 project. The authors wish to thank Mrs. *Zora Šusteková* from the Institute of Chemistry, Comenius University in Bratislava, for assistance with the IR spectroscopic measurements and the preparation of the manuscript.

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Received December 27, 1996. Accepted (revised) February 24, 1997