Synthetic and ^{1}H and ^{13}C NMR Spectral Studies on *N*-(Mono-substituted-phenyl)-acetamides and Substituted Acetamides, 2/3/4-YC_6H_4NH-CO-$CH_{3-i}X_i$ (Y = CH_3, F, Cl, Br, NO_2; X = Cl, CH_3; *i* = 0, 1, 2, 3)

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Nineteen *N*-(2/3/4-methyl/halo/nitro-phenyl)-acetamides and substituted acetamides, 2/3/4-YC_6H_4NH-CO-$CH_{3-i}X_i$ (Y = CH_3, F, Cl, Br or NO_2; X = Cl or CH_3 and *i* = 0, 1, 2 or 3), have been prepared, characterized, and their ^{1}H and ^{13}C NMR spectra in solution measured and correlated. ^{1}H and ^{13}C NMR chemical shifts were assigned to the protons and carbon atoms, respectively, in line with those for similar compounds. Since the chemical shifts are dependent on the electron density around the nucleus or associated with the atom to which it is bound, the incremental shifts of the aromatic protons or carbon atoms due to -NH-CO-$CH_{3-i}X_i$ and –CO-$CH_{3-i}X_i$ (X = Cl or CH_3 and *i* = 0, 1, 2, 3) in all the *N*-phenyl-substituted acetamides, C_6H_5NH-CO-$CH_{3-i}X_i$, are calculated by comparing the proton or carbon chemical shifts of these compounds with those of benzene or aniline. The incremental shifts due to the groups in the parent compounds have also been computed by comparing the chemical shifts of the protons or carbon atoms in these compounds with those of benzene or aniline, respectively. The computed incremental shifts and other data were used to calculate the ^{1}H and ^{13}C NMR chemical shifts of the substituted compounds in three different ways. The calculated chemical shifts by the three methods compared well with each other and with the observed chemical shifts, testing the validity of the principle of additivity of the substituent effects in these compounds. The variation of ^{1}H NMR chemical shifts of either the aromatic or N-H protons, with the substituents in *N*-(phenyl)- and *N*-(2/3/4-chloro/methylphenyl)-acetamides and substituted acetamides did not follow the same trend, while the variation of the ^{13}C NMR chemical shifts of C-1 and C=O carbon atoms and those of alkyl carbon atoms of these compounds followed more or less the same trend.

Key words: ^{1}H and ^{13}C NMR Spectra; *N*-Aryl-acetamides; *N*-Aryl-substituted Acetamides.

1. Introduction

The amide moiety is an important constituent of many biologically significant compounds [1]. Thus an understanding of the formation, properties and reactions of amides is central to future development in such areas as polypeptide and protein chemistry. Many imides, hydroxamic acids and hydrazides exhibit pharmacological activity, which has further stimulated recent interest in their chemistry. Further, many acetanilides exhibit fungicidal, herbicidal and pharmacological activities. We have recently reported the infrared, Raman [2], NMR [3] and NQR [4] spectra and crystal structures [5] of several *N*-(aryl)-acetamides and substituted acetamides. As part of these efforts of correlating spectroscopic parameters with the chemical bond parameters, amides of the formulae 2/3/4-YC_6H_4NH-CO-$CH_{3-i}X_i$ (Y = CH_3, F, Cl, Br or NO_2; X = Cl or CH_3 and *i* = 0, 1, 2 or 3) have been prepared, characterized, their NMR spectra measured in solution and correlated.

2. Experimental

2.1. Materials and Methods

N-Phenyl- and *N*-(2/3/4-methyl/halo/nitro-phenyl)-acetamides/substituted acetamides of the general formulae C_6H_5NH-CO-$CH_{3-i}X_i$ and 2/3/4-YC_6H_4NH-CO-$CH_{3-i}X_i$ (where Y = CH_3, F, Cl, Br or NO_2; X = Cl or CH_3 and *i* = 0, 1, 2 or 3) (Table 1) were prepared from substituted anilines, substituted acetic acids (Aldrich, Germany) and thionyl chloride [2 – 7].

Table 1. Melting points (M. p.) and N-H and C=O infrared absorption frequencies of *N*-(substituted-phenyl)-substituted acetamides, j-YC_6H_4NH-CO-$CH_{3-i}X_i$.

j-Y, $CH_{3-i}X_i$	Compound	M. p. (°C)	γ_{N-H} (str) (cm^{-1})	$\gamma_{C=O}$ (str) (cm^{-1})
2-NO_2, CH_3	*N*-(2-Nitrophenyl)-acetamide	94	3348.2s	1701.0s
3-NO_2, CH_3	*N*-(3-Nitrophenyl)-acetamide	155	3305.8s	1708.8s
4-NO_2, CH_3	*N*-(4-Nitrophenyl)-acetamide	215 – 217	3224.8s	1678.0s
4-F, CH_3	*N*-(4-Fluorophenyl)-acetamide	153 – 155	3290.3s	1670.2s
4-Br, CH_3	*N*-(4-Bromophenyl)-acetamide	167 – 169	3228.6s	1685.7s
3-Cl, CH_3	*N*-(3-Chlorophenyl)-acetamide	79 – 81	3301.9s	1708.8s
3-Cl, CH_2Cl	*N*-(3-Chlorophenyl)-2-chloroacetamide	80 – 82	3274.9s	1681.8s
3-Cl, $CHCl_2$	*N*-(3-Chlorolphenyl)-2,2-dichloroacetamide	87	3271.0s	1674.1s
3-Cl, CCl_3	*N*-(3-Chlorolphenyl)-2,2,2-trichloroacetamide	119 – 121	3267.2s	1654.8s
3-Cl, CH_2CH_3	*N*-(3-Chlorophenyl)-2-methylacetamide	91 – 92	3255.6s	1666.4s
3-Cl, $CH(CH_3)_2$	*N*-(3-Chlorophenyl)-2,2-dimethylacetamide	110	3251.8s	1666.4s
3-Cl, $C(CH_3)_3$	*N*-(3-Chlorophenyl)-2,2,2-trimethylacetamide	128	3298.0s	1658.7s
3-CH_3, CH_3	*N*-(3-Methylphenyl)-acetamide	65 – 67	3282.6s	1658.7s
3-CH_3, CH_2Cl	*N*-(3-Methylphenyl)-2-chloroacetamide	84	3292.3s	1674.1s
3-CH_3, $CHCl_2$	*N*-(3-Methylphenyl)-2,2-dichloroacetamide	87	3271.0s	1678.0s
3-CH_3, CCl_3	*N*-(3-Methylphenyl)-2,2,2-trichloroacetamide	98	3278.8s	1693.4s
3-CH_3, CH_2CH_3	*N*-(3-Methylphenyl)-2-methylacetamide	72	3305.8s	1662.5s
3-CH_3, $CH(CH_3)_2$	*N*-(3-Methylphenyl)-2,2-dimethylacetamide	92 – 94	3274.9s	1673.4s
3-CH_3, $C(CH_3)_3$	*N*-(3-Methylphenyl)-2,2,2-trimethylacetamide	118	3301.9s	1658.7s

s, Strong.

Table 2. ^1H NMR chemical shifts (δ, ppm) of various aromatic and other protons in *N*-(3-chloro-/3-methyl-phenyl)-substituted acetamides, 3-Cl/3-$CH_3C_6H_4NH$-CO-$CH_{3-i}X_i$.

CO-$CH_{3-i}X_i$	Chemical shifts (δ, ppm)					
	H-2	H-4	H-5	H-6	N-H	Alkyl H
	3-ClC_6H_4NH-CO-$CH_{3-i}X_i$					
CO-CH_3	7.33d	7.04d	7.17t	7.66s	8.73	2.16
CO-CH_2Cl	7.59s	7.23d	7.27d	7.62d	10.1	4.14
CO-$CHCl_2$	7.39m	7.14m	7.25t	7.64t	8.77	6.16
CO-CCl_3	7.67s	7.29s	7.31s	7.70s	10.4	–
CO-CH_2CH_3	7.33d	7.03d	7.17t	7.65s	8.19	2.38, 1.20
CO-$CH(CH_3)_2$	7.36d	7.03d	7.16t	7.68s	8.26	2.55, 1.20
CO-$C(CH_3)_3$	7.32d	7.00d	7.13t	7.65s	7.85	1.27
H	6.41	6.65	6.95	6.41	–	–
	3-$CH_3C_6H_4NH$-CO-$CH_{3-i}X_i$					
CO-CH_3	7.27t	6.89d	7.15t	7.34s	8.00	2.30, 2.09
CO-CH_2Cl	7.21s	6.95d	7.17d	7.32t	8.37	2.31, 4.11
CO-$CHCl_2$	7.18t	6.95s	6.98s	7.35d	9.06	2.26, 6.27
CO-CCl_3	7.34s	7.03d	7.26m	7.39d	8.32	2.36
CO-CH_2CH_3	7.29s	6.87d	7.14t	7.34d	8.02	2.34, 2.22, 1.18
CO-$CH(CH_3)_2$	7.29t	6.89d	7.16t	7.41s	7.64	2.50, 2.21, 1.21
CO-$C(CH_3)_3$	7.28d	6.87d	7.14t	7.41s	7.55	2.28, 1.27
H	6.33	6.51	6.96	6.33	–	–

Table 3. ^1H NMR chemical shifts (δ, ppm) of various aromatic and other protons in *N*-(substituted-phenyl)-acetamides, j-YC_6H_4NH-CO-CH_3.

j-Y	Chemical shifts (δ, ppm)						
	H-2	H-3	H-4	H-5	H-6	N-H	Alkyl H
2-Cl [3]	–	7.30d	7.16t	7.17d	8.10d	7.76	2.20
3-Cl	7.33d	–	7.04d	7.17t	7.66s	8.73	2.16
4-Cl [3]	7.58d	7.22d	–	7.22d	7.58d	9.61	2.06
2-CH_3 [3]	–	7.22d	7.10t	7.00t	7.54d	7.62	2.16, 1.90
3-CH_3	7.27t	–	6.89d	7.15t	7.34s	8.00	2.30, 2.09
4-CH_3 [3]	7.39d	7.06d	–	7.06d	7.39d	8.18	2.10, 2.26
2-NO_2	–	8.73d	7.15t	7.61t	8.16d	10.2	2.24
3-NO_2	8.73d	–	8.17m	7.16m	7.63m	10.3	2.29
4-NO_2	7.82m	8.13m	–	8.13m	7.82m	10.2	2.18
4-F	7.45m	6.97m	–	6.97m	7.45m	8.05	2.11
4-Br	7.42d	7.26s	–	7.26s	7.42d	7.66	2.14

Table 4. ^1H NMR chemical shifts (δ, ppm) of various aromatic and other protons in *N*-(phenyl)-substituted acetamides, C_6H_5NH-CO-$CH_{3-i}X_i$ (X = Cl, CH_3; $i = 0, 1, 2, 3$).

CO-$CH_{3-i}X_i$	Chemical shifts (δ, ppm)				
	H-2,6	H-3,5	H-4	N-H	Alkyl H
CO-CH_3	7.50d	7.20t	7.02t	8.94	2.05
CO-CH_2Cl	7.47d	7.27t	7.10t	8.33	4.00
CO-$CHCl_2$	7.52d	7.32t	7.17t	8.53	6.11
CO-CCl_3	7.53d	7.33t	7.18t	8.48	–
CO-CH_2CH_3	7.60d	7.22t	6.97	9.57	2.35, 1.15
CO-$CH(CH_3)_2$	7.57d	7.26t	7.06t	7.97	2.52, 1.20
CO-$C(CH_3)_3$	7.49d	7.22t	7.01t	7.76	1.25
H	6.48	7.05	6.67	3.39	–

The commercial anilines (Sisco Research Laboratories, India) were purified by either double distillation or zone refining. All other reagents employed in the preparations and purification of reagents were of analytical grade. Pure samples of the respective anilines (aniline, 2-methylaniline, 2-chloroaniline, 2-nitroaniline, 3-methylaniline, 3-chloroaniline, 3-nitroaniline, 4-methylaniline, 4-fluoroaniline, 4-chloroaniline, 4-bromoaniline or 4-nitroaniline) were treated with mixtures of respective acetic acids (acetic acid, 2-chloroacetic acid, 2,2-dichloroacetic acid, 2,2,2-tri-

NH-CO-$CH_{3-i}X_i$	H-2,6	H-3,5	H-4	$COCH_{3-i}X_i$	H-2,6	H-3,5	H-4
NH-CO-CH_3	0.23	−0.07	−0.25	CO-CH_3	1.02	0.15	0.35
NH-CO-CH_2Cl	0.20	0.0	−0.17	CO-CH_2Cl	0.99	0.22	0.43
NH-CO-$CHCl_2$	0.25	0.05	−0.10	CO-$CHCl_2$	1.04	0.27	0.50
NH-CO-CCl_3	0.26	0.06	−0.09	CO-CCl_3	1.05	0.28	0.51
NH-CO-CH_2CH_3	0.33	−0.05	−0.30	CO-CH_2CH_3	1.12	0.17	0.30
NH-CO-$CH(CH_3)_2$	0.27	−0.01	−0.21	CO-$CH(CH_3)_2$	1.09	0.21	0.39
NH-CO-$C(CH_3)_3$	0.22	−0.05	−0.26	CO-$C(CH_3)_3$	1.01	0.17	0.34

Table 5. The incremental chemical shifts (δ, ppm) of aromatic protons due to the groups –NH-CO-$CH_{3-i}X_i$ and -CO-$CH_{3-i}X_i$ in C_6H_5NH-CO-$CH_{3-i}X_i$ (X = Cl, CH_3; i = 0, 1, 2, 3).

chloroacetic acid, 2-methylacetic acid, 2,2-dimethylacetic acid or 2,2,2-trimethylacetic acid) and thionyl chloride with constant stirring. The resulting mixtures were slowly warmed to expel HCl. Excess thionyl chloride was hydrolyzed by adding cold water dropwise under ice cold conditions. The solids separated were filtered under suction, washed thoroughly with water and dried. *N*-Phenyl- and *N*-(2/3/4-methyl/halo/nitro-phenyl)-acetamides/substituted acetamides could also be prepared by treating the respective anilines with the corresponding chloroacetyl chlorides in acetone or benzene. HCl produced was removed by treating with 2 M NaOH. The *N*-aryl-substituted acetamides thus prepared were recrystallized from ethanol several times to constant melting points. The compounds have been characterized by determining their melting points and by recording their infrared spectra and comparing with the literature values (Table 1).

2.2. Spectral Measurements

The ^{1}H and ^{13}C NMR spectra of all the *N*-(2/3/4-methyl/halo/nitro-phenyl)-acetamides and substituted acetamides were measured on a BRUKER Ac 300F, 300 MHz FT-NMR spectrometer. The spectra were recorded in $CDCl_3$ and DMSO with tetramethylsilane [$(CH_3)_4Si$] as internal standard.

3. Results and Discussion

3.1. ^{1}H NMR Spectra

^{1}H NMR chemical shifts of aromatic and alkyl protons of all the *N*-(2/3/4-methyl/halo/nitro-phenyl)-acetamides and substituted acetamides are shown in Tables 2 – 4. The various chemical shifts were assigned to the protons in line with those for similar compounds [3]. Since the chemical shift depends on the electron density around the nucleus or associated with the atom to which it is bound, the incremental shifts of the aromatic protons (ppm) due to -NH-CO-$CH_{3-i}X_i$ (where X = Cl or CH_3 and i = 0, 1, 2, 3) in all the *N*-phenyl-substituted acetamides, C_6H_5NH-CO-$CH_{3-i}X_i$, were computed by comparing the proton chemical shifts of these compounds (Table 4) [3] with those of the benzene proton value of 7.27 ppm (Table 5). Similarly, the incremental shifts of the aromatic protons (ppm) due to –CO-$CH_{3-i}X_i$ (where X = Cl or CH_3 and i = 0, 1, 2 or 3) of these compounds were also computed by comparing their proton chemical shifts with those of the aniline proton values of H-2,6 = 6.48 ppm, H-3,5 = 7.05 ppm, H-4 = 6.67 ppm (Table 5).

The chemical shifts of all the aromatic protons in all the *N*-(2/3/4-methyl/halo/nitro-phenyl)-acetamides and substituted acetamides, 2/3/4-YC_6H_4NH-CO-$CH_{3-i}X_i$ (where Y = CH_3, F, Cl, Br or NO_2; X = Cl or CH_3 and i = 0, 1, 2 or 3) were then calculated in three ways by adding either the substituent contributions [8] to the corresponding ^{1}H NMR chemical shifts of *N*-phenyl-substituted acetamides (Table 4) [3] or by adding the incremental shifts due to –NH-CO-$CH_{3-i}X_i$ or –CO-$CH_{3-i}X_i$ groups (Table 5) to the ^{1}H NMR chemical shifts of protons of the corresponding substituted benzenes or anilines, respectively. The calculated chemical shifts by the three procedures of calculation (values not shown) led to almost the same values and were in good agreement with the experimental chemical shifts, indicating that the validity of the principle of additivity of the substituent effects is quite good with these compounds.

3.2. ^{13}C NMR Spectra

The measured ^{13}C NMR chemical shifts of the aromatic and alkyl carbon atoms of all the *N*-(2/3/4-methyl/halo/nitro-phenyl)-acetamides and substituted acetamides are shown in Tables 6 – 8. The various chemical shifts are assigned to the different carbon atoms in the benzene rings in conformity with the literature for similar compounds [2, 3]. The ^{13}C NMR

Table 6. ^{13}C NMR chemical shifts (δ, ppm) of *N*-(3-chloro-phenyl)-substituted acetamides.

CO-CH$_{3-i}$X$_i$	3-ClC$_6$H$_4$NH-CO-CH$_{3-i}$X$_i$ (X = Cl, CH$_3$; i = 0, 1, 2, 3)							
	C-1	C-2	C-3	C-4	C-5	C-6	C=O	Alkyl C
CO-CH$_3$	139.2	120.3	134.4	124.2	129.8	118.2	169.5	24.3
CO-CH$_2$Cl	138.5	120.7	136.6	124.8	128.1	118.4	164.4	42.9
CO-CHCl$_2$	137.3	120.8	134.8	125.9	130.1	118.7	162.6	66.7
CO-CCl$_3$	135.7	120.5	129.6	122.4	128.3	118.8	159.5	92.9
CO-CH$_2$CH$_3$	139.2	120.2	134.4	124.1	129.8	118.1	173.0	30.6, 9.6
CO-CH(CH$_3$)$_2$	139.3	120.4	134.4	124.1	129.8	118.3	176.3	36.4, 19.5
CO-C(CH$_3$)$_3$	139.2	120.6	134.2	124.0	129.6	118.5	177.1	39.5, 27.3
H	147.6	114.5	134.2	117.8	130.1	113.0	–	–
	3-CH$_3$C$_6$H$_4$NH-CO-CH$_{3-i}$X$_i$ (X = Cl, CH$_3$; i = 0, 1, 2, 3)							
CO-CH$_3$	138.8	120.8	137.9	125.0	128.7	117.2	168.8	24.4, 21.4
CO-CH$_2$Cl	136.6	120.8	138.9	125.9	128.8	117.3	164.0	42.9, 21.3
CO-CHCl$_2$	136.1	121.5	139.9	126.6	128.9	118.0	162.8	67.0, 21.3
CO-CCl$_3$	135.8	121.0	139.4	126.9	129.1	117.5	159.2	95.1, 21.4
CO-CH$_2$CH$_3$	138.7	120.7	138.0	124.8	128.6	117.1	172.7	30.5, 21.3, 9.7
CO-CH(CH$_3$)$_2$	138.8	120.7	138.1	124.9	128.7	117.0	175.6	36.6, 21.4, 19.6
CO-C(CH$_3$)$_3$	138.5	120.8	137.9	124.8	128.5	117.2	176.6	39.4, 27.4, 21.3
H	146.4	115.6	138.6	119.0	128.8	112.0	–	–

Table 7. ^{13}C NMR chemical shifts (δ, ppm) of *N*-(substituted-phenyl)-acetamides, *j*-YC$_6$H$_4$NH-CO-CH$_3$.

j-Y	Chemical shifts (δ, ppm)							
	C-1	C-2	C-3	C-4	C-5	C-6	C=O	Alkyl C
2-Cl [3]	133.5	127.7	129.2	123.6	128.6	122.9	162.2	24.4
3-Cl	139.2	120.3	134.4	124.2	129.8	118.2	169.5	24.3
4-Cl [3]	137.6	120.4	127.0	128.0	127.0	120.4	168.3	23.68
2-CH$_3$ [3]	135.5	126.3	130.4	124.2	125.5	124.2	168.9	23.8, 17.7
3-CH$_3$	138.8	120.8	137.9	125.0	128.7	117.2	168.8	24.4, 21.4
4-CH$_3$ [3]	135.5	120.3	129.3	133.8	129.3	120.3	169.0	24.3, 20.8
2-NO$_2$	134.9	136.6	123.1	125.6	135.8	122.3	168.6	25.4
3-NO$_2$	135.8	122.0	136.2	123.1	134.7	125.6	168.9	25.4
4-NO$_2$	144.9	118.3	124.1	142.0	124.1	118.3	169.1	23.9
4-Br	137.0	121.5	132.0	117.0	132.0	121.5	168.4	24.6
4-F	134.1	122.0	115.5	157.8	115.5	122.0	168.9	24.2

Table 8. ^{13}C NMR chemical shifts (δ, ppm) of *N*-(phenyl)-substituted acetamides, C$_6$H$_5$NH-CO-CH$_{3-i}$X$_i$ (X = Cl, CH$_3$; i = 0, 1, 2, 3).

CO-CH$_{3-i}$X$_i$	Chemical shifts (δ, ppm)					
	C-1	C-2,6	C-3,5	C-4	C=O	Alkyl C
CO-CH$_3$	138.1	120.4	128.5	124.0	169.3	23.8
CO-CH$_2$Cl	136.8	120.4	128.9	125.1	164.2	42.9
CO-CHCl$_2$	136.2	120.6	129.2	125.8	162.3	66.9
CO-CCl$_3$	135.9	120.6	129.1	126.0	159.3	92.9
CO-CH$_2$CH$_3$	139.0	119.3	128.7	122.8	172.2	29.7, 9.5
CO-CH(CH$_3$)$_2$	138.2	120.0	128.8	124.0	175.9	36.4, 19.6
CO-C(CH$_3$)$_3$	138.1	120.4	128.3	123.7	176.6	39.2, 27.2
H	146.2	114.6	128.8	117.8	–	–

chemical shifts of benzene, substituted benzenes, aniline and substituted anilines were also measured under identical conditions and data used for computation of incremental shifts.

The incremental shifts of the aromatic carbon atoms (ppm) due to –NH-CO-CH$_{3-i}$X$_i$ (where X = Cl or CH$_3$ and i = 0, 1, 2 or 3) groups were computed by comparing the ^{13}C NMR chemical shifts of *N*-(phenyl)-substituted acetamides, C$_6$H$_5$NH-CO-CH$_{3-i}$X$_i$ (where X = Cl or CH$_3$ and i = 0, 1, 2 or 3) [3], with the benzene carbon value of 128.5 ppm (Table 9). Similarly, the incremental ^{13}C NMR shifts of the aromatic carbon atoms due to –CO-CH$_{3-i}$X$_i$ (where X = Cl or CH$_3$ and i = 0, 1, 2, 3) groups in these compounds were computed by comparing their chemical shifts with those of the aniline carbon values of C-1 = 146.2 ppm, C-2,6 = 114.6 ppm, C-3,5 = 128.8 ppm, C-4 = 117.8 ppm (Table 9). Then the ^{13}C NMR chemical shifts of all the aromatic carbon atoms in all the *N*-(2/3/4-methyl/halo/nitro-phenyl)-acetamides and substituted acetamides were calculated in three ways by adding either the substituent contributions [2, 3] to the ^{13}C NMR chemical shifts of *N*-(phenyl)-substituted acetamides (Table 8) or the incremental shifts due to –NH-CO-CH$_{3-i}$X$_i$ or –CO-CH$_{3-i}$X$_i$ groups (Table 9) to the ^{13}C NMR chemical shifts of the corresponding substituted benzenes or anilines, respectively. The calculated ^{13}C NMR chemical shifts by the three procedures of calculation led to almost the same values and were in good agreement with the experimental chemical shifts, indicating the validity of the principle of additivity of the substituent effects with these compounds.

4. Comparisons and Conclusions

The variation of ^{1}H NMR chemical shifts of either the aromatic or N-H protons with the substituents in *N*-(phenyl)-, *N*-(2-chlorophenyl)-, *N*-(3-chlorophen-

Table 9. The incremental shifts in chemical shifts of aromatic carbon atoms due to -NH-CO-$CH_{3-i}X_i$ and -CO-$CH_{3-i}X_i$ groups in *N*-(phenyl)-substituted acetamides, C_6H_5NH-CO-$CH_{3-i}X_i$ (X = Cl, CH_3; i = 0, 1, 2, 3).

NH-CO-$CH_{3-i}X_i$	C-1	C-2,6	C-3,5	C-4	CO-$CH_{3-i}X_i$	C-1	C-2,6	C-3,5	C-4
NH-CO-CH_3	9.6	−8.1	0.0	−4.5	CO-CH_3	−8.1	5.8	−0.3	6.2
NH-CO-CH_2Cl	8.3	−8.1	0.4	−3.4	CO-CH_2Cl	−9.4	5.8	−0.1	7.3
NH-CO-$CHCl_2$	7.7	−7.9	0.7	−2.7	CO-$CHCl_2$	−10.0	6.0	0.4	8.0
NH-CO-CCl_3	7.4	−7.9	0.6	−2.5	CO-CCl_3	−10.3	6.0	0.3	8.2
NH-CO-CH_2CH_3	10.5	−9.2	0.2	−5.7	CO-CH_2CH_3	−7.2	4.7	−0.1	5.0
NH-CO-$CH(CH_3)_2$	9.7	−8.4	0.3	−4.5	CO-$CH(CH_3)_2$	−8.0	5.4	0.0	6.2
NH-CO-$C(CH_3)_3$	9.6	−8.0	-0.2	−4.8	CO-$C(CH_3)_3$	−8.1	5.8	−0.5	5.9

yl)- and *N*-(4-chlorophenyl)-, *N*-(2-methylphenyl)-, *N*-(3-methylphenyl)- and *N*-(4-methylphenyl)-acetamides and substituted acetamides did not follow the same trend, while the variation of ^{13}C NMR chemical shifts of C-1 carbon atoms of these compounds followed more or less the same trend. The variations of ^{13}C NMR chemical shifts of C=O carbon atoms and those of alkyl carbon atoms of the above compounds also followed similar trends.

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