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NMR studies of benzoannulation in lithium, sodium and potassium *ortho*-formylphenolates

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ABSTRACT

Lithium, sodium and potassium derivatives of (benzo)salicylaldehydes have been prepared and characterized by ^{1}H and ^{13}C NMR in order to see how the metal cation and benzoannulation affect spectral parameters. There is no qualitative effect of the alkali metal atom in the compounds studied (from this point of view salicylaldehydes remind β-diketones). On the other hand, ^{1}H chemical shifts of the hydroxyl and formyl protons and ^{13}C chemical shifts of C2 (bearing OX, X = H, Li, Na or K) and of that the formyl carbon show the most significant variations being the best indicators of aromatic character of the six-membered quasi-ring of salicylaldehyde. In contrast, C1 (bearing formyl moiety) is almost inert to the alkali cations but reflects nicely the position of benzoannulation.

1. Introduction

According to the concept of resonance, π-electron delocalization is a very important phenomenon in the suitably substituted, *e.g.* benzoannulated molecules [1]. It is also a very significant factor affecting physical and chemical properties of the compounds, such as stability of the tautomeric species [2]. Studies on the Schiff bases derived from *o*-hydroxy-benzaldehydes show that composition of the tautomeric mixture depends on stability of the keto/enol forms, which in turn is related to the π-electron delocalization in the molecule and to the strength of the intramolecular hydrogen bond [3].

2*p* orbitals of the sp^2 hybridized atoms may overlap if the distance between them is sufficiently short. This enables, *e.g.* formation of the hydrogen bond between the acidic hydrogen and electronegative atoms. For the same reason the sp^2 hybridized lithium atom in the respective enolates of β-dicarbonyl compounds interacts with the carbonyl oxygen atom [4–7]. Since the size of *p* orbital of the sp^2 hybridized Na and K atoms precludes its effective overlapping with the *p* orbital of the carbonyl oxygen atom, formation of the six-membered quasi-rings in the molecules of the sodium and potassium enolates of β-diketones seems impossible. Systems that contain such quasi-rings including the lithium atom bound and coordinated to two other atoms that show some aromatic character are especially interesting. Such a situation requires the unoccupied 2*p* orbital of the Li atom to be parallel to the same type orbital of the proximate atom [8–10]. Aromaticity of the quasi-rings **Q** in the lithium salts of the enol form of malonaldehyde (Scheme 1a, X = Li) and in the enolimine form of *ortho*-hydroxy Schiff bases (Scheme 1b, X = Li) was found to be rather low [11,12].

The geometry- [13,14] and magnetism-based calculations [15] give no unequivocal answer to the question which of the six-membered quasi-rings involving the hydrogen and lithium atoms is more aromatic. This conclusion refers also to aromaticity of the quasi-ring formed in *ortho*-acylphenols and in the respective lithium phenolates [16] as well as in alkali metal *ortho*-methoxybenzoates [17,18]. Recent magnetism-based calculations indicate the current of π-electrons in the six-membered quasi-rings such as discussed above to be absent [19]. The observed equalization of the bond lengths in the quasi-ring present in lithium *ortho*-acylphenolates and *ortho*-acylphenols themselves is attributed instead to the electrostatic effect of $Li^{\oplus}$ on C=O bonds of the quasi-ring [20].

The more or less substantial π-electron delocalization in the quasi-rings of lithium derivatives of the enaminone tautomer of *ortho*-hydroxy Schiff bases (Scheme 1b, X = Li) [12] may be explained by a possibility of participation of the low-lying unoccupied *p* orbitals of $Li^{\oplus}$ in delocalization of π-electrons in the quasi-ring [14]. This conclusion is in line with energies of 2*p* orbitals of the hydrogen (14.48 eV) and lithium (0.53 eV) atoms calculated at the UHF/cc-pVQZ level [14]. Undoubtedly, the *p*-type orbitals of Li involved in bonding in the quasi-ring have dramatically lower

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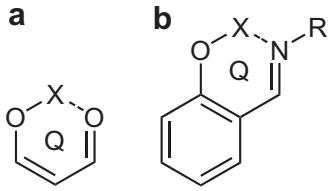
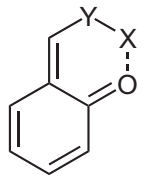
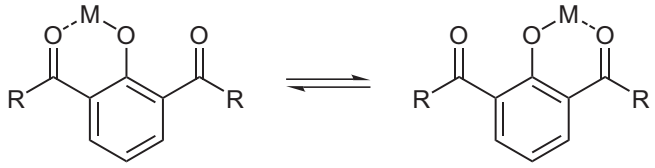


Scheme 1. Noncovalent interactions in malonaldehyde, *ortho*-hydroxy Schiff bases and some their *O*-substituted derivatives.

energy than that of the H atom. So far no π-electron delocalization in the quasi-ring of salicylaldehyde and its *O*-alkali metal derivatives (Scheme 2, Y = O, X = Li, Na, K) have been studied. There is no qualitative difference in chelation of the sodium and potassium cations in the respective derivatives of β-diketones [5–7]. This effect was found to be the most and less strong in the lithium and potassium enolates, respectively [5]. The NMR spectra of lithium, sodium, and potassium derivatives are believed to be affected by the size of the cation and degree of the salt dissociation [4]. The observed carbon chemical shifts represent the averaged values of the chemical shifts of associated salt and free anion, dependent on the populations of these two species. The degree of dissociation is low in solution of the lithium derivatives. This process is probably complete for the potassium salts [4].



Scheme 2. General formula of hydroxy- and aminomethylenecyclohexa-2,4-dienone and their *O*-alkali metal derivatives.



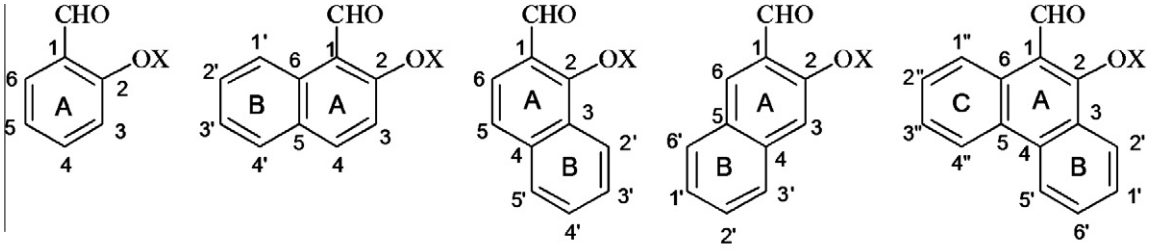
Scheme 3. Noncovalent interactions in 2,6-diacylphenols and their *O*-alkali metal derivatives.

There is no doubt about intramolecular hydrogen bond to appear in *ortho*-acylphenols [21]. Variable temperature ^{1}H NMR spectral measurements show that in solution there is a competition between two equivalent hydrogen bonded forms of 2,6-diacylphenols (Scheme 3, M = H) [21]. Similar observations for the respective lithium derivatives (Scheme 3, M = Li) would confirm presence of the intramolecular "lithium" bond [10,22]. Unfortunately, intramolecular interactions in such compounds are of quite different character: two isomeric tetramers were found to compete [21]. Formation of the polymers by organolithium compounds [23–25] as well as by lithium phenolates [26] is a very common phenomenon. Different character of the sigma bonds formed between base and proton (polar covalent) and alkali metal cations (largely ionic) [27–34] are believed to be responsible for the differences observed in chelation of these species. As this can be seen (*vide infera*), the hitherto efforts were ineffective to show unequivocally the character of metal–oxygen interactions in lithium, sodium and potassium *ortho*-formyl(benzo)phenolates. In the present paper we compared the ^{1}H, ^{7}Li, and ^{13}C chemical shifts for salicylaldehyde and its *O*-lithium, sodium and potassium derivatives just to discover if the metal–oxygen interactions are independent of the metal atom present in the molecule. Since benzoannulation is known to affect properties of the compounds significantly [1] and no such effect on structure of *ortho*-acylpenols and alkali metal *ortho*-acylphenolates nor the nature of metal–oxygen interactions in the later compounds has been studied earlier, their 3,4-, 4,5- and 5,6-benzoannulated derivatives are also included. Formulas of the compounds studied are presented in Scheme 4. It shows also the numbering of positions and rings in their molecules.

2. Result and discussion

Experimental chemical shifts of the hydroxyl proton for **1H**–**5H** presented in Table 1 are in agreement with the previous findings [16,35]. Intramolecular hydrogen bond in *ortho*-hydroxybenzaldehydes lengthens the O–H bond [36]. Increased acidity of the protons is reflected by their deshielded signals. The data shown in Table 1 prove that in 5,6- (**2H**) and 3,4-benzoannulated (**3H**) and in 3,4,5,6-dibenzoannulated (**5H**) derivatives the hydroxyl proton is more acidic than in salicylaldehyde (**1H**) and in its 4,5-benzoannulated derivative (**4H**) [16,35].

Chemical shifts of the hydroxyl proton in the compounds studied can be used to monitor the effect of benzoannulation in these molecules. Lengthening of the O–H bond should result in shortening of the C1–C2 bond. Due to increased contribution of the quin-



No	X	No	X	No	X	No	X	No	X
1H	H	**2H**	H	**3H**	H	**4H**	H	**5H**	H
1Li	Li	**2Li**	Li	**3Li**	Li	**4Li**	Li	**5Li**	Li
1Na	Na	**2Na**	Na	**3Na**	Na	**4Na**	Na	**5Na**	Na
1K	K	**2K**	K	**3K**	K	**4K**	K	**5K**	K

Scheme 4. Formulas of the compounds studied.

Table 1
^{1}H and ^{7}Li NMR chemical shifts (δ) of *ortho*-formylphenols and of the respective Li, Na, and K phenolates for 0.5 M solutions in DMSO-d_6 at 30 °C (data for the protons in the rings **B**, *e.g.* H1′, and **C**, *e.g.* H1″, are always given in the second and third row, respectively).

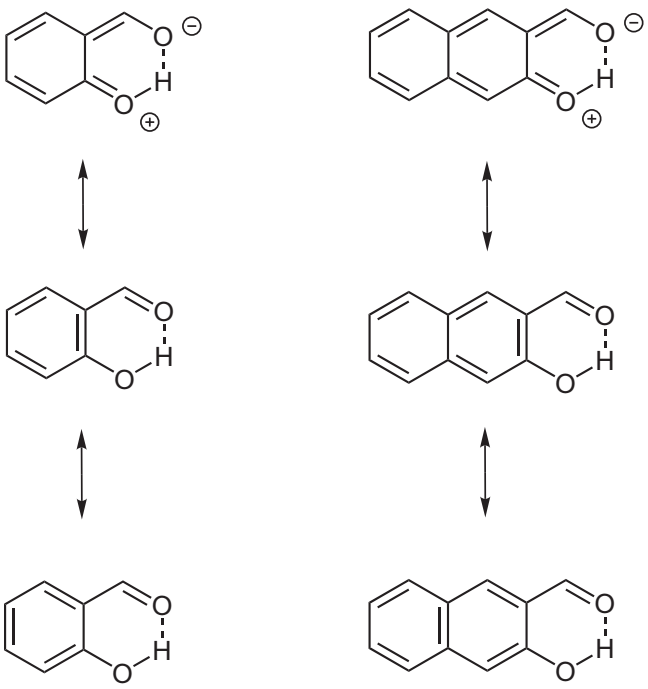
	HI	H2	H3	H4	H5	H6	CHO	X
1H	–	–	6.98	7.45	6.90	7.65	10.21	10.71[a]
ILi	–	–	6.38	7.09	6.18	7.21	9.41	0.74[b]
			6.29[c]	6.90[c]	5.80[c]	7.30[c]	10.30[c]	
INa	–	–	6.74	7.23	6.45	7.42	10.24	–
IK	–	–	6.17	7.87	5.81	7.15	10.00	–
2H	–	–	7.25	8.10	–	–	10.82	12.06[a]
	8.91	7.60	7.41	7.86	–	–		
2Li	–	–	6.99	7.85	–	–	10.64	−0.43[b]
	8.97	7.44	7.21	7.67	–	–		
2Na	–	–	6.48	7.41	–	–	10.28	–
	9.05	7.17	6.88	7.35	–	–		
2K	–	–	7.40	7.35	–	–	10.22	–
	9.07	7.14	6.84	7.30	–	–		
3H	–	–	–	–	7.48	7.71	10.20	12.30[a]
	7.61	8.36	–	–	7.93	7.72		
3Li	–	–	–	–	6.58	7.25	9.53	[d]
	7.26	8.30	–	–	7.54	7.45		
3Na	–	–	–	–	6.29	7.26	9.95	–
	7.14	8.22	–	–	7.40	7.33		
3K	–	–	–	–	7.39	7.68	10.19	–
	7.57	8.36	–	–	7.88	7.69		
4H	–	–	7.30	–	–	8.35	10.41	10.57[a]
	7.35	7.53	7.76	–	–	7.97		
4Li	–	–	6.83	–	–	8.03	10.26	0.00[b,e]
	6.96	7.23	7.37		7.68	7.68		
4Na	–	–	7.30	–	–	8.33	10.42	–
	7.34	7.53	7.74	–	–	7.97		
4K	–	–	6.31	–	–	7.69	10.40	–
	6.58	6.93	7.05	–	–	7.37		
5H	–	–	–	–	–	–	10.86	14.56[a]
	7.76	8.47	–	–	8.82	7.92		
	8.63	7.67	7.59	8.75	–	–		
5Li	–	–	–	–	–	–	10.84	−0.62[b]
	7.74	8.47	–	–	8.80	7.90		
	8.67	7.65	7.56	8.73	–	–		
5Na	–	–	–	–	–	–	10.80	–
	7.71	7.51	–	–	8.75	7.87		
	8.70	7.61	7.51	8.68	–	–		

[a] ^{1}H.
[b] ^{7}Li.
[c] In DMF-d_7 [33].
[d] Very broad signal slightly shielded from the standard.
[e] Overlapping with signal of the standard.

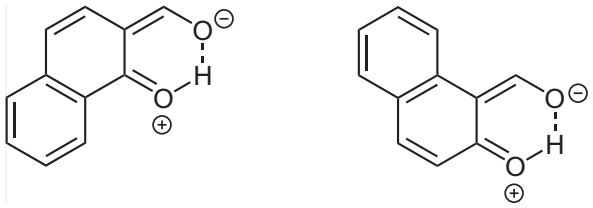
oid resonance structures (Scheme 5), aromatic character of compounds **1H** and **4H** is partly annihilated. On the other hand, such resonance structures for two other *ortho*-hydroxy-naphthaldehydes are still partly aromatic (Scheme 6). Thus, these compounds are much less susceptible to benzoannulation than their 4,5-benzoannulated isomer (**4H**).

The NMR chemical shifts of the formyl proton for the compounds studied (Table 1) are, in general, moderately dependent on the OX substituent (X = H, Li, Na and K). The values of δC^{1}**HO** change in the following order: **5** > **2** > **4** > **1** ≈ **3**. Although range of the ^{7}Li NMR chemical shifts is quite narrow (12 ppm) [38], analysis of the δ (^{7}Li) values (Table 1) show that in general benzoannulation of *o*-OHC–C_6H_4–OLi deshields the lithium atom (δ^{7}Li: **1Li** > **4Li** > **2Li** > **5Li**).

^{13}C NMR chemical shifts of C1 and C2 for hydroxybenzaldehydes studied (Table 2) can also be divided into two different categories. C1 atom in **1H** (122.18 ppm) and **4H** (124.12 ppm) is



Scheme 5. Contributing resonance forms of salicylaldehyde and its 4,5-benzo derivative.



Scheme 6. Quinoid resonance forms of 3,4- and 5,6-benzosalicylaldehydes.

deshielded with respect to this in **2H** (112.37 ppm) and **3H** (115.34 ppm). The most shielded shifts are found for **5H** (108.39 ppm), **5Li** (108.38 ppm), and **5Na** (108.36 ppm). Bond equalization in the molecules of **1H** and **4H** completely annihilates aromatic character of the molecule (Scheme 5). On the other hand, two other *ortho*-hydroxynaphthaldehydes are still partly aromatic (Scheme 6). Shielding of C2 was found to be the most effective in **4H**. On the other hand, the most deshielded C2 is that in **3H**. ^{13}C NMR chemical shifts for the formyl group do not show any special trend that reflects the type of annulation.

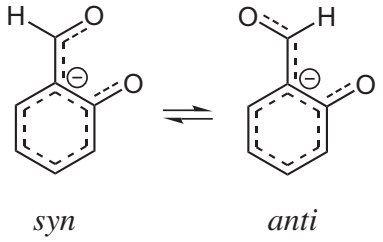
Comparison of the *ab initio* calculated and experimental carbon chemical shifts of potassium *ortho*-formylphenolate, *o*-OHC–C_6H_4–OK, revealed that the *anti* form (Scheme 7) prevails in DMF-d_7 solution (aprotic solvents of relatively high dielectric constant that can solvate cation efficiently promotes dissociation of the salts) [37]. On the other hand, the *syn* conformer dominates for the respective lithium derivative, *o*-OHC–C_6H_4–OLi (there is a weak repulsion between the C=O group and $O^{\ominus}$ in the *syn* form of the anion) [37]. A careful analysis of the experimental and calculated J(^{1}H, ^{13}C) and J(^{1}H, ^{1}H) values supported the above conclusion, but just from the ^{1}H and ^{13}C chemical shifts differences its is impossible to conclude what is the conformation of the lithium derivative [37].

Analysis of the NMR spectra shows that *ortho*-hydroxybenzaldehydes remind β-diketones [5–7]: there is no qualitative difference in chelation of the lithium, sodium and potassium cations in their *O*-alkali metal derivatives.

Table 2
^{13}C NMR chemical shifts (δ) of *ortho*-formylphenols and of the respective Li, Na, and K phenolates for 0.5 M solutions in DMSO-d_6 at 30 °C (data for the carbon atoms in the rings **B**, *e.g.* C1′, and **C**, *e.g.* C1′, are always given in the second and third row, respectively).

	Cl	C2	C3	C4	C5	C6	CHO
1H	122.18	160.92	117.31	136.39	119.54	130.31	192.93
ILi	123.85	174.32	124.38	135.70	109.54	135.70	192.17
	124.77[a]	175.28[a]	124.95[a]	136.11[a]	110.08[a]	136.87[a]	192.83[a]
INa	123.47	169.11	120.88	135.63	113.60	128.19	190.81
IK	123.83	174.85	124.21	135.05	108.99	127.50	190.21
	125.17[a]	179.16[a]	127.06[a]	135.21[a]	106.63[a]	127.82[a]	190.73[a]
2H	112.37	163.89	118.68	138.27	128.73	131.69	192.81
	122.01	129.15	124.12	128.73	127.51	131.69	
2Li	112.50	170.19	122.81	37.40	126.00	133.12	191.37
	121.91	128.42	122.29	128.28	126.00	133.12	
2Na	112.38	180.39	129.92	136.01	123.65	135.58	189.60
	121.71	127.19	119.31	127.50	123.65	135.58	
2K	112.09	180.45	130.23	135.67	123.34	135.67	189.18
	121.61	126.92	118.80	127.24	123.34	135.67	
3H	115.34	160.06	124.26	137.09	119.24	125.90	195.63
	126.21	123.41	124.26	137.09	127.79	130.28	
3Li	116.14	173.05	131.73	138.27	109.49	123.12	189.34
	123.12	125.34	131.73	138.27	126.60	128.87	
3Na	116.41	175.27	133.41	138.59	107.55	127.01	187.68
	122.38	125.27	133.41	138.59	126.44	128.13	
3K	115.52	161.35	125.07	137.22	118.29	125.73	194.85
	125.87	123.59	125.07	137.22	127.67	130.06	
4H	124.12	155.64	110.62	137.42	126.82	131.94	192.19
	123.90	129.23	125.98	137.42			
4Li	127.30	165.77	112.72	139.43	123.49	133.16	193.85
	120.14	127.98	124.75	139.43	123.49	129.60	
4Na	124.29	156.06	110.68	137.52	126.72	131.64	192.13
	123.81	129.19	125.96	137.52	126.72	129.72	
4K	129.12	173.16	113.90	140.76	120.69	128.11	194.12
	116.85	126.31	123.60	140.76	120.69	129.85	
5H	108.39	162.89	123.98	134.30	124.70	129.37	195.53
	127.46	124.45	123.98	134.30	123.30	131.80	
	120.59	128.27	125.18	123.53	124.70	129.37	
5Li	108.38	163.68	124.51	134.34	124.49	129.70	195.11
	127.34	124.51	124.51	134.34	123.24	131.65	
	120.67	128.20	124.88	123.44	124.49	129.70	
5Na	108.36	164.50	124.25	134.37	125.07	130.02	194.66
	127.19	124.56	124.25	134.37	123.14	131.46	
	120.76	128.11	124.56	123.33	125.07	130.02	

[a] In DMF-d_7 [33].



Scheme 7. *Syn* and *anti* conformers of *ortho*-formylphenolate anion.

3. Conclusions

There does not exist any clear effect on the ^{1}H and ^{13}C NMR chemical shifts of salicylaldehyde caused via its *O*-substitution by alkali metal cations. Although this is known, in benzoannulated salicyladehydes the situation is different owing to π-electron delocalization, which is further reflected in their NMR parameters. Among them ^{1}H chemical shifts of hydroxyl proton and ^{13}C chemical shifts of hydroxyl and formyl bearing carbons are the most useful ones showing most directly the changes in the aromatic character in the intra-molecularly hydrogen bonded six-membered quasi-ring of salicylaldehyde.

4. Experimental

4.1. Compounds

Compounds **1H** and **2H** are commercial products. Aldehydes **3H**, **4H**, and **5H** are these used by us recently [3].

4.2. Lithium and sodium ortho-formylphenolates

Pieces of lithium or sodium (5 mmol) were added to the aldehyde (5 mmol) dissolved in dry diethyl ether (15 mL). Reaction mixture was refluxed and stirred even for few days until all metal is consumed (the apparatus was protected from the moisture with a trap filled with granulated anhydrous calcium chloride). The solvent was distilled off and product recrystallized from 95% ethanol. It was then dried in the vacuum desiccator over the sodium hydroxide pellets.

4.3. Potassium ortho-formylphenolates

Solutions of aldehyde (5 mmol) in hot 95% ethanol (15 mL) and potassium hydroxide (5 mmol) in the same solvent (15 mL) were combined and refluxed for 1 h. Part of the solvent (10 mL) was distilled off. The solid material precipitated after cooling of the residue was washed with dry diethyl ether and dried in the vacuum desiccator over the sodium hydroxide pellets. Unfortunately, this procedure was not efficient to obtain **5K**.

4.4. NMR spectroscopy

All NMR spectra were run for 0.5 M solutions in $CDCl_3$ with Bruker Avance DRX 500 NMR spectrometer operating at 500.13 MHz for ^{1}H and 126.77 MHz for ^{13}C, and 194.37 MHz for ^{7}Li, respectively. The ^{1}H and ^{13}C chemical shifts are referenced to the trace signal of $CHCl_3$, 7.26 ppm from internal TMS, and to the centre peak of $CDCl_3$ heptet, 77.00 ppm from internal TMS, respectively. The ^{7}Li chemical shifts are referenced to the signal of an external 1 M aqueous LiCl in a 1 mm diameter capillary inserted coaxially inside the 55 mm diameter NMR-tube. The PFG ^{1}H, ^{13}C HMQC and HMBC spectra were run using standard pulse sequences, hmqcgpqf and hmbcgplpndqf, from Bruker pulse library.

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